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What mesoscopic structures really "remember": insufficiency of the open boundary approximation

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Abstract

We analyze the influence of contact electrons on quantum transport in a resonant-tunneling diode (RTD), using a many-body density matrix formalism for open systems. We explicitly relate the net current in the RTD to the memory-containing effective interaction between the RTD active region and the contacts. This effect can only be captured if the RTD active region is treated fully as a dynamically open system.

Keywords: Quantum transport; Resonant-tunneling diode; Open system

Mesoscopic physics is one of the most active areas of today's solid-state research. Dimensions of mesoscopic structures range from a few nanometers to a few microns, and the structures are expected to operate within a wide range of temperatures: from milli-kelvin quantum dots to room-temperature semiconductor devices. But all mesoscopic structures have at least one thing in common: they challenge our understanding of electronic transport, as they firmly refuse to be described by semiclassical approaches.

Treatment of the contact–active-region interaction has long been a sore spot of semiconductor device simulation [1]. In this paper, we present an analysis of transient transport in a resonant-tunneling diode (RTD), including the interaction with the contacts (electron–electron and hopping; see below). This analysis implements our theoretical work on the many-body density matrix formalism for transport in open quantum systems [2–4]. An open system S (with Hamiltonian h_S) is allowed to interact with the environment E

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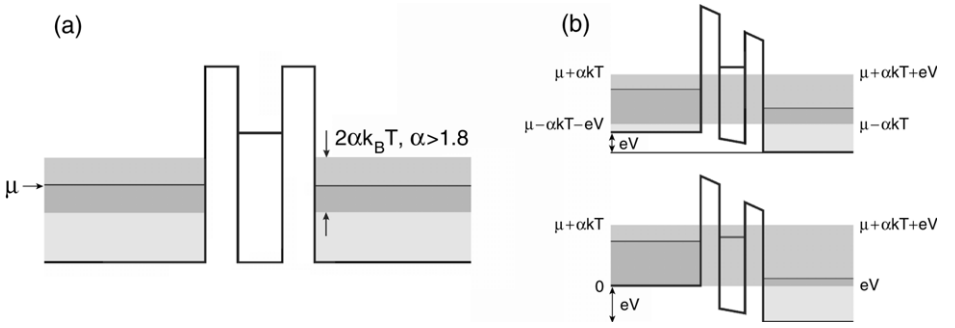

Fig. 1. (a) The RTD in equilibrium. (b) The RTD under bias, for $eV < \mu - kT$ (top panel) and $eV > \mu - kT$ (bottom panel). The dark area correspond to the energy interval in which transport occurs, and the single-particle states within this interval are allowed to have variable occupation number.

(Hamiltonian h_E) via an interaction described by the Hamiltonian h_{int}. The evolution of the total $S + E$ density matrix is tracked within the total $S + E$ Liouville space, and the Hamiltonians defined above determine the corresponding Liouville operators. The total $S + E$ Liouville operator L governs the density matrix evolution, but, in many-body cases, the dimension of the environmental Liouville space is large, and it is therefore not advisable to solve the Liouville equation directly. We have devised a way to compute certain submatrices instead, but we will not go into details of this formalism [2–4].

In the case of an RTD, the active region (quantum well) represents the system, while the left and the right reservoir constitute the environment (Fig. 1(a)). No scattering is at present taken into account. In the tight-binding picture, and including the intra-well electron–electron interaction, the active-region Hamiltonian is given by

$$h_S = \frac{\hbar^2}{ma^2}\sum_{i=1}^{N_S} c_i^+ c_i - \frac{\hbar^2}{2ma^2}\sum_{i=1}^{N_S-1}(c_i^+ c_{i+1} + c_{i+1}^+ c_i) + \frac{e^2}{8\pi\varepsilon_0\varepsilon}\sum_{\substack{i,j=1\\ i\neq j}}^{N_S}\frac{c_i^+ c_i\, c_j^+ c_j}{|x_i - x_j|}, \quad (1)$$

where $c_i^+(c_i)$ is the creation (annihilation) operator at the ith site, and a is the mesh size. On the other hand, the interaction Hamiltonian consists of two parts: the electron–electron interaction with contact electrons, and the hopping terms that connect the boundary points of the reservoirs and the well. The Hamiltonian of the interaction between the left contact and the well is

$$h_{L-S} = \frac{e^2}{4\pi\varepsilon_0\varepsilon}\sum_{\substack{i\in L\\ \alpha\in S}}\frac{c_i^+ c_i\, c_\alpha^+ c_\alpha}{|x_\alpha - x_i|} - \frac{\hbar^2}{2ma_L^2}(c_{1,L}^+ c_{1,S} + c_{1,S}^+ c_{1,L}). \quad (2)$$

We will assume that the reservoirs contain a free electron gas (no electron–electron interaction in the reservoirs), with the tight-binding single-particle spectrum given by $E(k) = t_L[1 - \cos(ka_L)]$, where $t_L = \hbar^2/ma_L^2$ is the hopping energy for the left reservoir, and $k = 2\pi n/N_L$ is a wavevector in the Brillouin zone of the lattice induced by discretization. This dispersion relation is approximately parabolic near the bottom of the band, giving a good approximation for the free-particle spectrum. Resorting to the

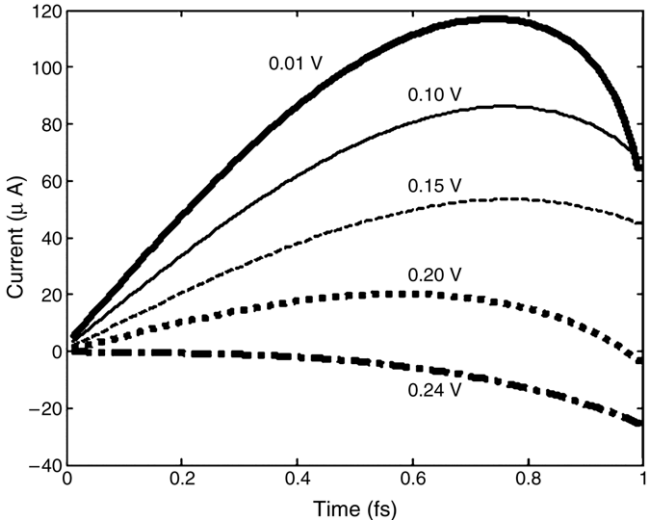

Fig. 2. The net current in the RTD well during the first femtosecond after the bias was applied, for several different values of the applied bias.

free-particle approximation for the contacts simplifies the construction of their Fock space. That is, at a given chemical potential μ, applied bias V, and $\alpha > 1.8$, in the left reservoir we consider only those states that are between the energies $\max\{0, \mu - \alpha k_B T - eV\}$ and $\mu + \alpha k_B T$, while in the right reservoir we consider those between $\max\{eV, \mu - \alpha k_B T\}$ and $\mu + \alpha k_B T + eV$ (Fig. 1(b)). These states are dominant in transport, so they should be allowed to have filling of either 0 or 1 (no spin at present taken into account), and we use them to construct the many-body environmental states.

The Hamiltonians given above allow us to perform certain approximations [5] in the equations of motion for the active-region reduced density matrix ρ_S, and finally arrive at the following equations:

$$\begin{aligned} \frac{\mathrm{d}\rho_S(t)}{\mathrm{d}t} &= -i[L_{11} - X(t)]\rho_S(t), \\ \frac{\mathrm{d}X(t)}{\mathrm{d}t} &= -iX(t)^2 + iX(t)L_{11} + iL_{12}L_{21}, \qquad X(t_0) = 0. \end{aligned} \tag{3}$$

Here, L_{11} is generated by an effective active-region Hamiltonian $h_{S,\mathrm{eff}}$, containing h_S from Eq. (1) and a correction due to the electron–electron interaction; X is the memory-containing effective interaction with the contacts, and L_{12} and L_{21} are the off-diagonal terms of the Liouvillian, due mainly to the hopping term in Eq. (2).

It is important to note that the electron–electron interaction does not yield current flow through the RTD well, because the electron–electron part of the Hamiltonian in Eq. (2) commutes with the occupation number at every site. However, as mentioned above, the effective Hamiltonian $h_{S,\mathrm{eff}}$ does contain a correction due to the electron–electron

interaction between the well and the contacts, so the electron–electron interaction indirectly influences the magnitude of the current [5].

Since $[h_{S,\mathrm{eff}}, n] = 0$, where $n = \sum_i c_i^+ c_i$ is the number operator for the active region, it can be shown that the net current through the well is given by

$$e\frac{\mathrm{d}\langle n(t)\rangle}{\mathrm{d}t} = ie\,\mathrm{Tr}[nX(t)\rho_S(t)], \tag{4}$$

which unequivocally shows that the well gets charged/discharged depending on X, the memory-containing effective interaction [4] with the contacts, predominantly due to the hopping term in Eq. (2). In Fig. 2, the net current flowing through the well is depicted as a function of time during the first femtosecond after the bias was applied. We observe initial charging of the well for low voltages, and discharging for higher. Zero net current in the first few tenths of a femtosecond corresponds to applying the resonant voltage [5].

In conclusion, we have analyzed transient transport in an RTD using the many-body density matrix formalism of [2–4]. We find that the net current in the well is due to the memory-containing effective interaction with the contacts, which is a feature that can be captured only if the RTD active region is treated fully as a dynamically open system. The open boundary approximation is, in general, insufficient to capture this effect.

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