A quantum many-body density matrix model for sub-femtosecond transport in mesoscopic structures*

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In conventional semiconductor devices, the theoretical description of transient transport is achieved by solving the semiclassical Boltzmann equation using ensemble Monte Carlo. 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. However, it is well established that the transient-regime transport in nanostructures is governed by the exchange of particles and information between the current-limiting active region and the contacts. We present a theoretical model for transient transport in mesoscopic structures, and illustrate the approach with numerical simulation of a resonant-tunneling diode (RTD). We introduce a *second-order master equation* for the evolution of the many-body reduced density matrix of the active region. This contains *full quantum-mechanical information* about the processes in the current-limiting active region. The master equation is derived directly form the Liouville equation for the active region+contacts, by using the partial-trace-free approach, and it incorporates the memory terms that describe the information exchange between the contacts and the active region. In this way, the state of the contacts is accounted for, but does not explicitly enter the calculation, allowing us to compute the full many-body reduced density matrix for the active region. The model accounts for the presence of the bias by assuming a special form of the forcing term in the master equation. The numerical simulation shows that incorporation of the memory terms is crucial for description of charging/discharging in the well, and obtaining the proper transient behavior. Electron-electron interaction between the active region and the contacts, as well as phonon scattering (within the relaxation-time approximation), have been taken into account. In the top panel of Fig.1, the time evolution of the net current, and the current through the left contact, are presented for a 20mV voltage drop across the active region (2.5 nm well+2 nm barriers). The current through the left contact saturates at a positive value of about $50\mu A$ (since the calculation is one-dimensional, we are not dealing with current density, but the actual current). The period of oscillation is 12.5 fs, corresponding to a frequency of 80 THz, which is in general agreement with experimental findings. In the bottom panel of Fig. 1, the probability of finding an electron is plotted as a function of position in the well, for 4 different characteristic points from the top panel. At the beginning, (a) injection from the left contact, where the bias is applied, is obviously dominant. Plots corresponding to points (b) and (d) specify the saddle points on the "total probability vs. time" curve, and indicate what the steady-state distribution will be. The curve corresponding to point (c) represents maximum occupation of the well, after which the well discharges, due to the feedback from the contacts, which is inherent to the model.

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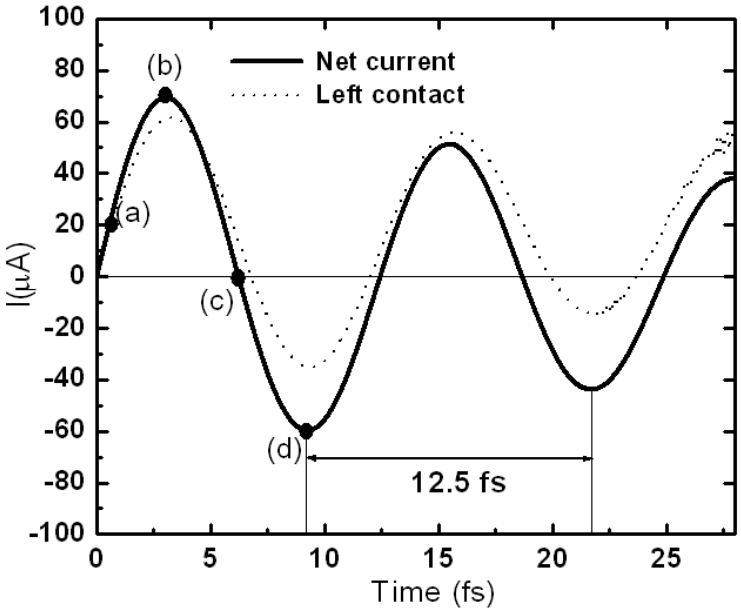

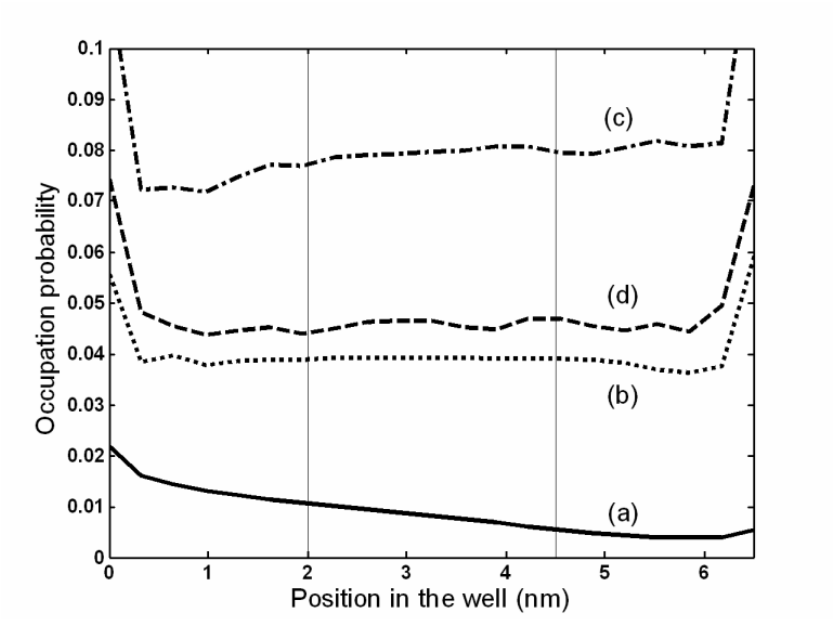

Fig. 1. Top panel: Evolution of net current in the well (solid line) and current through the left contact (dotted line), in the first 25 fs after application of 20 mV across the active region.

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 probability density, but unitless probability, because we work with discrete mesh). Vertical lines indicate where the barriers end and the well begins.

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