Time-dependent aspects of quantum transport.

E.K.U. Gross

Max Planck Insitute of Microstructure Physics, 06120 Halle (Saale), Germany

Electronic transport through single molecules or atomic wires, sandwiched between semi-infinite leads, is studied within the Anderson impurity model with one or more interacting sites at various levels of approximation
The system is driven out of equilibrium by an external bias and the non-equilibrium properties are determined by real-time propagation using both time-dependent density functional theory (TDDFT) and many-body perturbation theory (MBPT). In the MBPT calculations, the self-energy is approximated at the Hartree-Fock (HF), second-Born (2B) and GW level. In the TDDFT calculations, the exchange-correlation functional is approximated by an adiabatic LDA-type functional derived from the exact Bethe-ansatz solution of the 1D Hubbard model (ABALDA).
In the Coulomb blockade regime, we find that no steady state exists. The time-propagation leads, after some transient regime, to undamped oscillations of the density and current which correspond to a periodic charging and discharging of the device [1]. Outside the regime of Coulomb blockade, assuming the existence of a steady state and solving directly the steady-state equations, we find multistability in the density and current within the HF approximation and the ABALDA. In these cases we investigate if and how these solutions can be reached through time evolution and how to reversibly switch between them.
Finally, by comparison with MBPT results, we investigate whether and to which extent the bistability results are real or a consequence of the approximations made. It turns out that the inclusion of dynamical correlation effects in the form of frequency dependent MBPT-self-energies tends to suppress the phenomenon of bistability [2,3].

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[3] A.-M. Uimonen, E. Khosravi, A. Stan, G. Stefanucci, S. Kurth, R. van Leeuwen, E. K. U. Gross, Phys. Rev. B **84**, 115103 (2011).