Transient-regime transport in nanostructures

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In structures consisting of a quasiballistic, nanometer-size active region attached to much larger reservoirs, electronic transport cannot be described by using the semiclassical Boltzmann transport formalism. Rather, the active region is an open quantum-mechanical system whose dynamics is governed by coupling to the contacts and by the rapid dephasing inside the contacts. To correctly describe transport in this regime, one must resort to a quantum-mechanical scattering formalism that properly accounts for the open system nature of the current-limiting active region and adequately eliminates the large number of degrees of freedom that exist in the leads [1].

Here, we present a computational method for calculating the transient dynamics of 2-terminal nanostructures by using several convenient approximations to reduce the complexity of the described problem [2]. We work within the open systems formalism [3], where the active region/environment system is represented as a composite system Hamiltonian with an environment, active region, and interaction terms and the initial statistical operator is assumed to be of a tensor-product form that guarantees the existence of a non-Markovian subdynamics.

In particular, we calculate the transient response of a quantum point contact (QPC) formed by the split-gate technique on a two-dimensional electron gas. The QPC, an open system coupled to reservoirs, is modeled by a solution to the coupled, two-dimensional Schrödinger and Poisson equations using a discrete subset of the normal-mode basis. The normal modes are projected onto the traveling-wave solutions that match the incoming reservoir plane waves. The occupation of the open system states carries the information about the time evolution and is calculated by solving a coarse-grained quantum master equation with suitably defined open system/contact interaction Hamiltonians. The final electronic transient response is obtained by enforcing the current continuity across the open system/contacts boundaries through a time-dependent reservoir drift wavevector. We investigate the transient current response to a voltage step and its dependence on the split-gate bias and relaxation time in the contacts [4].

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