VMC: a code for Monte Carlo simulation of quantum transport

Physical model, case examples, user's guide

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The Wigner-Boltzmann equation for electrons in semiconductor devices is solved numerically by means of a novel Monte Carlo method. The equation describes both quantum interference and dissipation effects due to carrier scattering. The methodology for deriving the method is summarized in the following. The integral form of the Wigner-Boltzmann equation is used as a starting point for deriving the method. The kernel of the adjoint equation has been decomposed into a linear combination of conditional probability densities. These densities represent the transition density used for the construction of numerical trajectories. The properties of the transition density employed allow a particle picture to be introduced. In this picture dissipation and interference phenomena are taken into account by two alternative processes involving quasi-particles. Dissipation caused by interaction with phonons and other scattering sources is accounted for by drift and scattering processes corresponding to the semi-classical Boltzmann transport picture.

Interference effects due to the Winger potential are associated with generation of pairs of particles having statistical weight +1 and -1. The classical force term is separated from the Wigner potential and included in the Liouville operator. With this modification, the developed model corresponds to a Boltzmann equation augmented by a generation term. The challenge of employing such method is to handle the avalanche of numerical particles properly. The problem has been solved for stationary conditions: Particles of opposite weight and a sufficiently small distance in phase space are continuously removed in the course of a simulation. The cancellation is due to the fact that such particles have a common probabilistic future but opposite contribution to the statistics.

Experience about the properties of the MC method has been collected by simulation of different types of resonant tunneling diodes. The novel MC method has been validated by comparison with NEMO-1D and comparison with measurements. In some cases phonon scattering is found to play an important role, as predicted by both simulators.