Novel Monte Carlo algorithms for ultrafast transport phenomena in semiconductors

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In this work novel Monte Carlo algorithms are studied for investigation the ultrafast evolution of electron-phonon interaction in the presence of an applied electric field. The research efforts are directed to solve the Levinson equation which is a particular case of the Barker-Ferry equation with infinite electron life-time. In contrast to the Boltzmann equation which has a non-negative kernel, the kernel of the quantum transport equation is oscillatory and can take negative values. In a stochastic approach to the equation this property of the kernel gives rise to statistical weights with inverse signs. The numerical aspects of the approach are characterized by a large variance of the simulation results - the so called negative sign problem in quantum-mechanical simulations.

Various variance reduction algorithms are proposed for solving this problem. The properties of these algorithms, such as computational complexity and accuracy, are investigated by Monte Carlo simulations. The algorithms have been applied for solving the quantum kinetic equation for a diversity of evolution times. The long time behavior of the solutions are studied. A physical model with GaAs material parameters has been adopted in the simulations.