Operator-Split Method for Variance Reduction in Stochastic Solutions of the Wigner Equation

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The stochastic approach to Wigner transport in nanoscale semiconductor devices utilizes trajectories built up according to the rules of the numerical Monte Carlo theory. Under stationary conditions these trajectories begin at a device boundary and are simulated until they exit the device again of a boundary. A physical quantity of interest is associated with a random variable. During the evolution a trajectory accumulates statistical weight W, which is a sample of the possible values taken by that variable. The sample mean estimates the expectation value of the physical quantity. A peculiarity of the task is that W can alter its sign, while $|W|$ grows exponentially with the dwelling time in the device and the L_1 norm of the Wigner potential. Accordingly, also the variance of the sample mean and thus the numerical requirements of the task are growing, preventing the application of the approach to realistic devices.

We propose a method for variance reduction by means of storing part of the weight on a grid in the phase space. It is based on the notion that two trajectories which reach a given phase space point but carry opposite weights have the same probabilistic future but opposite contributions to the sample mean. These trajectories cancel each other which saves the time for the remainder of their simulation. In the formal derivation of the method the Wigner potential operator V_w is split into two operators $A = mV_w$ and $B = (1-m)V_w$, $0 < m < 1$. A is associated with the weight of the particle that continues with the trajectory, while B gives the weight stored at each step of the trajectory construction. V_w, A and B obey the following operator equality (I is the identity operator):

$$(I - V_w)^{-1} = (I - A)^{-1} + (I - V_w)^{-1} B (I - A)^{-1}.$$

An iterative algorithm has been derived, where the simulated trajectories begin consecutively from the boundary and from the grid. The algorithm has been applied to a resonant-tunneling diode. Simulation results are presented and discussed.