A Stable Backward Monte Carlo Method for the Solution of the Boltzmann Equation

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For the numerical study of non-equilibrium charge transport in semiconductors the Monte Carlo (MC) method found wide spread application. In particular the physically transparent forward MC method is used, which evaluates functionals of the distribution function. The more abstract backward MC method, however, remained virtually unimplemented. This method follows the particle history back in time and allows the distribution function to be evaluated in given points. It has significant advantages in cases where the solution is sought in sparsely populated regions of the phase space only. The value $f(k_0, t)$ of the distribution function f at momentum k_0 and time t is evaluated using the estimator

$$\nu_i = \frac{\lambda^*(k_0, t_0)}{\lambda(k_0, t_0)} \dots \frac{\lambda^*(k_{i-1}, t_{i-1})}{\lambda(k_{i-1}, t_{i-1})} f_0(k_i)\,,$$

where f_0 denotes the initial distribution, $\lambda = \int S(k, k')dk'$ the total scattering rate, and $\lambda^* = \int S(k', k)dk'$ the backward scattering rate. Although the MC algorithm based on this estimator is consistently derived from the integral form of the Boltzmann equation, computer experiments reveal a stability problem in that the particle energy becomes very large when the trajectory is followed backward in time. This fact can be understood from a property of the transition rate $S(k, k')$ known as the principle of detailed balance, which ensures that in any system particles scatter preferably to lower energies. Because for trajectory construction the backward transition rate $S^*(k, k') = S(k', k)$ is employed, the principle of detailed balance is inverted in the simulation and scattering to higher energies is preferred.

The stability problem can be solved by using the forward transition rate $S(k, k')$ also for the construction of the backward trajectory changing the estimator accordingly:

$$\nu_i = e^{\beta\Delta_0} \dots e^{\beta\Delta_i} f_0(k_i)$$

The Δ_i denote the difference in particle energy introduced by the i-th scattering event, and $\beta = 1/(k_B T)$. Bulk simulations using this estimator are presented, demonstrating the stability of the method.