Solution of the Space-dependent Wigner Equation Using a Particle Model

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The Wigner equation is well suited for numerical modeling of quantum electronic devices. A stationary, space-dependent Wigner equation is considered that takes into account scattering on a semi-classical level through the Boltzmann collision operator. The development of Monte Carlo algorithms is complicated by the fact that, as opposed to the semiclassical case, the integral kernel is no longer a strictly positive function. We present a particle model which interprets the nonlocal potential operator as a generation term of numerical particles of positive and negative statistical weight. The problem arising from the avalanche of numerical particles is thereby solved for the steady state. Sequential algorithms are proposed that follow only one sample particle whereas other numerical particles are stored on a state space grid at the same rate as particles are generated. Due to the opposite sign, particle weights annihilate to a large extent on the grid. The total residual weight on the grid must be kept as small as possible as it represents a measure for the numerical error of the method.

While particle states after scattering and after generation are determined stochastically, the particle state maintained for trajectory construction and the state stored on the grid are selected deterministically in a way to minimize the local residual weight. When constructing the algorithms particular emphasis has been put on the conservation laws implied by the Wigner equation. The first Monte Carlo algorithm to be presented generates particles pairwise with opposite sign which ensures exact mass conservation, whereas the second algorithm uses a reduced free-flight time and generates only one particle each time. The sign of the particle weight is selected randomly and mass is conserved only on average. Applications of the two algorithms to the simulation of realistic resonant tunneling diodes are shown.