A Weight Decomposition Approach to the Sign Problem in Wigner Transport Simulations

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A Monte Carlo (MC) method for simulation of quantum transport in one dimensional nano-scale devices is proposed. The coherent stationary Wigner equation is considered, where the solution $f_w(k,x)$ depends on the momentum $\hbar k$ and the position x. The method aims at evaluation of the mean value $\langle A\rangle = (A,f)$ of a generic physical quantity $A(x,k)$ such as carrier density or velocity. A forward formulation of the task is obtained from the conjugate integral form of the equation. The conjugate kernel is factorized into conditional probabilities enclosed in curly brackets, and a weight w

$$\left\{\nu(t)e^{-\int_0^t \nu(y)dy}\right\}_1\left(\left\{\frac{\nu(t)}{\mu(t)}\right\}_2\{\delta(k-k')\}_3+\left\{\frac{\gamma(t)}{\mu(t)}\right\}_{2'}\left\{\frac{|V_w(x(t),k-k')|}{\gamma(t)}\right\}_{3'}\right)w$$

Here V_w is the Wigner potential, $\gamma(x)=\int|V_w(x,k)|dk$, $\nu(x)$ is a positive function, $\mu=\nu+\gamma$, and $x=x(t)$ depends linearly on the time t. The subscripts denote the order of application of the probabilities used for trajectory construction. $\{.\}_1$ generates the time t, $\{.\}_{2,2'}$ selects the kernel component which generates the after-scattering state k'. $w=s\mu/\nu$, where $s=1$ or $s=sign(V_w)$ multiplies the total weight W accumulated by the trajectory. The method gives rise to huge values $\pm|W|$ leading to large variance of the simulation results - the so called sign problem in MC simulations. This restricts the application of the method to real quantum devices.

We propose an approach where the weight is split in the phase space instead of being accumulated over a single trajectory. The kernel is decomposed in a different way and a special choice of the function ν is used. The tree components of the kernel simultaneously create three after-scattering states at each iteration. These states, having a weight ±1 populate the phase space. Positive and negative states have opposite contribution to the statistics. They have the same probabilistic future if located close together and thus can be canceled. The active cancellation reduces the time for simulation of these states leading to a variance reduction. Simulation results of resonant tunneling diodes have been succesfully and efficiently carried out with this approach.