Efficient Monte Carlo-based algorithms for the Wigner transport equation

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Efficient Monte Carlo-based algorithms for the Wigner transport equation

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Abstract. The Wigner transport equation is solved by Direct Simulation Monte Carlo, based on the generation and annihilation of signed particles. In this framework, stochastic algorithms are derived using the theory of pure jump processes with a general state space. Numerical experiments on benchmark test cases are shown.

1. Introduction

The continuous scaling down of semiconductor devices is nowadays at a point, where active lengths are of the order of only a few tens of nanometers. Effects such as particle tunneling through source-to-drain potential profiles are now highly relevant and cannot be ignored. From this perspective, only full quantum models are capable of describing the appropriate physics. A well-known model is the Wigner equation which can be augmented by a Boltzmann-like collision operator accounting for the process of decoherence. The Wigner equation writes [1]:

$$\frac{\partial f_W}{\partial t} + \frac{\hbar}{m^*} k \cdot \nabla_x f_W = \mathcal{Q}(f_W) \quad , \quad \mathcal{Q}(f_W) = \int V_W(x, k-k') f_W(x, k')\, dk' \tag{1}$$

$$V_W(x,k) = \frac{1}{i\hbar(2\pi)^d} \int dx'\, e^{-ik\cdot x'} \left[V\left(x + \frac{x'}{2}\right) - V\left(x - \frac{x'}{2}\right) \right] \tag{2}$$

where V_W is the Wigner potential, and $V(x)$ is the potential energy. The Wigner potential is a non-local potential operator which is responsible of the quantum transport, it is real-valued, and anti-symmetric with respect to k.

The numerical solution of the Wigner equation can be obtained using high-order finite difference solvers [2–5]. To avoid discretization problems, particle Monte Carlo (MC) methods can be used (see [6] for a review), despite the large computational times.

In the realm of the MC methods, the *Signed particle Monte Carlo approach* [7, 8] seems to be the most promising, because it can be understood in a probabilistic framework. In fact, the quantum evolution term $(1)_2$ is interpreted as a *Gain* term of a collisional operator in which the *Loss* term is missing. But the Wigner potential (2) is not always positive and cannot be considered a scattering term. For this reason, it can be separated into a positive and negative parts $V_W^+, V_W^- \geq 0$ such that $V_W = V_W^+ - V_W^-$. Therefore the quantum evolution term can be

written as

$$\mathcal{Q}(f_W) = \int dk' w(k',k) f_W(x,k') - \gamma(x) f_W(x,k) \quad , \quad \gamma(x) = \int dk'\, V_W^+(x,k-k') \tag{3}$$

$$w(k',k) = V_W^+(x,k-k') - V_W^-(x,k-k') + \gamma(x)\delta(k-k') \tag{4}$$

where now $\mathcal{Q}(f_W)$ is written as the difference of *Gain* and *Loss* terms. The corresponding scattering mechanism is dictated by (4), where the first term represents the creation of a new positive particle, the second the creation of a negative one and the last term means that the initial particle is maintained. Hence a real-valued weight (or affinity) must be introduced, to describe this pair production. The intensity of the pair creation is ruled by γ, and the momentum of the new particles generated according to the probability V_W^+. The main drawbacks of this procedure reside in the exponential grow of the particle number, and in the evaluation of the γ and V_W^+ functions because they are rapidly oscillating.

This creation process has been recently understood in terms of the "piecewise deterministic Markov processes" theory (PDMP) [9, 10]. Each particle is characterized by a real-valued weight A, a position x and a wave-vector k. The particle position changes continuously, according to the velocity determined by the wave-vector. New particles (called offspring) are created randomly and added to the system. The main result is that appropriate functionals of this stochastic process satisfy a weak form of the Wigner equation. Moreover, this approach has certain advantages compared to other derivations. In particular, it suggests a variety of new algorithms as well as some of the algorithms previously considered in the literature.

2. New generation algorithms

According to PDMP, we shall introduce a new algorithm, which based on a majorant of the Wigner potential

$$|V_W(x,k)| \leq \hat{V}_W(x,k) \quad \forall x,k \quad , \quad \hat{\gamma}(x,c) = \frac{1}{2}\int_{\mathbb{B}} \hat{V}_W(x,k)\, dk \tag{5}$$

where $\mathbb{B} = \left\{k \in \mathbb{R}^d : \|k\| \leq c\right\}$ and c is a cutoff. A splitting time step $\Delta t \leq 1/\hat{\gamma}$ is used in order to separate the transport and the creation processes. The new algorithm performs the evolution of the system on the time interval $[0, \Delta t]$ according to the following steps:

1. Transport step : the particle positions change according to

$$x_j := x_j + \frac{\hbar}{m^*} k_j \, \Delta t \quad , \quad j = 1, ..., N$$

2. Creation step : for $j = 1, .., N$ new particles are created according to the following rules:
   (a) with probability $1 - \hat{\gamma}(x_j, c)\Delta t$ do not create anything.
   (b) Otherwise generate randomly a new $\tilde{k}$ according to the probability

$$\frac{1}{2\hat{\gamma}(x_j,c)} \hat{V}_W(x_j,k), \quad k \in \mathbb{B}$$

   (c) with probability

$$1 - \frac{|V_W(x_j,\tilde{k})|}{\hat{V}_W(x_j,\tilde{k})}$$

   do not create anything.

(d) Otherwise create the particle couple

$$[\tilde{A}(A_j, x_j, \tilde{k}_j), x_j, k_j + \tilde{k}] \quad , \quad [-\tilde{A}(A_j, x_j, \tilde{k}_j), x_j, k_j - \tilde{k}]$$

with $\tilde{A}(A, x, k) = A \operatorname{sign} V_W(x, k)$. Put $N := N + 2$.

3. Cancellation step: if $N \geq N_{canc}$ pairs of particles with opposite affinity, which belong to the same element of the phase-space are removed.

The particle creation rate, in this new algorithm, is dictated by the function $\hat{\gamma}$ $(5)_2$ obtaining a gain factor 2 with respect to standard creation procedure employing the function γ $(3)_2$; moreover, the new algorithm has the advantage that the calculation of the rate function γ, which is highly oscillating, is avoided. Recently we have developed another MC algorithm (which we shall call no-splitting), performing the particle evolution on a finite time interval $[0, T]$ without any time discretization error, i.e. avoiding the time step splitting error [11].

3. Benchmark studies

As benchmark, we have considered a potential barrier with the shape of a gaussian function, centered at x=0 with dispersion $\sigma = 1$ nm and height $a = 0.3$ eV. The Wigner potential (2), in the 1D case, writes

$$V_W(x, k) = \frac{2a\sigma\sqrt{2\pi}}{\pi\hbar} \exp\left[-2(\sigma k)^2\right] \sin(2kx) \quad . \tag{6}$$

The creation algorithm is based on the following majorant of $V_W(x, k)$

$$\hat{V}_W(x, k) = \frac{2a\sigma\sqrt{2\pi}}{\pi\hbar} \quad , \quad \hat{\gamma}(x, c) = \frac{2a\sigma\sqrt{2\pi}}{\pi\hbar}\, c \tag{7}$$

The initial condition for the Wigner equation is

$$f_W(x, k, 0) = \frac{1}{\pi} \exp\left[-\frac{(x - x_0)^2}{2\sigma_0^2}\right] \exp\left[-2\sigma_0^2(k - k_0)^2\right] \tag{8}$$

where x_0 = -15 nm, k_0= 0.7 nm^{-1}, σ_0 = 2.852 nm, and we have chosen absorption boundary conditions. In the x-space we have considered an uniform mesh [-30, 30](nm) with $N_x = 200$ grid-points; also in the k-space we have an uniform mesh [-10, 10](nm^{-1}) with N_k=400. The cutoff has been fixed $c = 8$ nm^{-1}, the initial particle number is $N_{ini} = 160000$, the cancellation parameter $N_{canc} = 480000$. Since for pure states the Wigner and Schrödinger equations are completely equivalent, we have compared the MC mean density with that obtained using a high-order deterministic Schrödinger equation solver [12]. The mean density, obtained at 20 fsec. with the two solvers, is shown in figure 1, for various time steps. We can observe that the MC solution converge to the Schrödinger one, showing clearly the error introduced by the time step. In figure 2 we plot the mean density obtained using the no-splitting algo (without any time step) and the Schrödinger one: the agreement between the two mean densities is very good. Figure 3 shows the CPU times versus the time step as well as the CPU obtained with the no-splitting algo, and, in figure 4, the max absolute error between the MC and the Schrödinger solutions. From these figures it is clear the advantage to use the no-splitting algorithm instead of standard ones.

4. Conclusions

The Wigner equation has been solved by using the Signed particle Monte Carlo method where, new pair of particles characterized by a sign, are created randomly and added to the system. This creation mechanism has been understood in terms of the Markov jump process. Numerical experiments have been performed successfully on a benchmark test case. Future researches will include simulation of silicon nanowires according to the guidelines in [13–15].

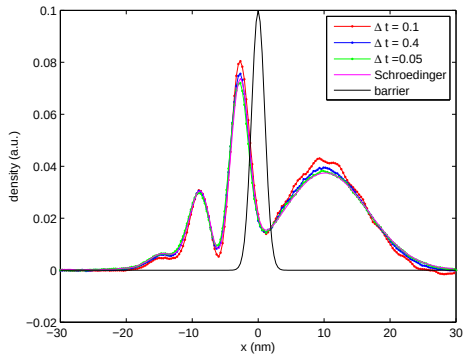

Figure 1. The mean density versus position at simulation time 20 fsec., obtained with some time steps Δt.

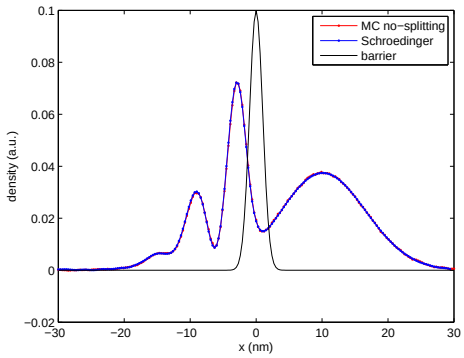

Figure 2. The mean density versus position at simulation time 20 fsec., obtained with the no-splitting algorithm.

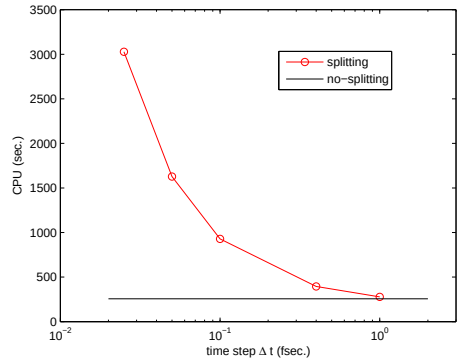

Figure 3. CPU time versus the time step Δt.

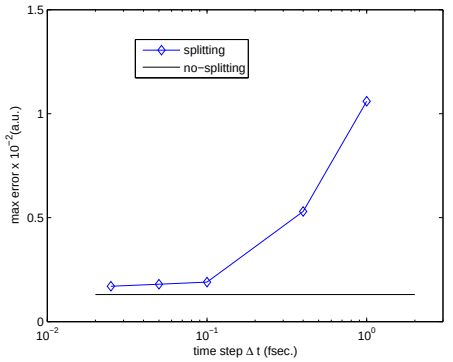

Figure 4. Max error versus the time step Δt.

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