The Role of Annihilation in a Wigner Monte Carlo Approach

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Abstract. The Wigner equation provides an interesting mathematical limit, which recovers the constant field, ballistic Boltzmann equation. The peculiarities of a recently proposed Monte Carlo approach for solving the transient Wigner problem, based on generation and annihilation of particles are summarized. The annihilation process can be implemented at consecutive time steps to improve the Monte Carlo resolution. We analyze theoretically and numerically this process applied to the simulation of important quantum phenomena, such as time-dependent tunneling of a wave packet through potential barriers.

1 Introduction

In the theory of carrier transport involving the concept of phase-space, there are strong similarities between classical and quantum regimes. From this perspective, the Wigner theory is a promising approach for the simulation of fully quantum transport phenomena in semiconductor devices. Investigations of this approach have been carried out in the recent past. Efforts have been performed to reuse successful ideas of the semi-classical transport regime.

Eventually, two particle models were derived. The first model, an ensemble Monte Carlo (MC) technique based on particles endowed with an affinity, has proved to be a reliable method. Unfortunately it needs heavy computational resources [1]. The second model is a single particle MC approach, based on the ergodicity of the system and thus restricted to stationary regimes determined by the boundary conditions [2]. As compared to the previous one, it has very different attributes, related to the generation of particles endowed with a sign. Particles are created in the phase space and are consecutively evolved to the boundary.

A generalization of the second approach has been recently developed. This new method exploits the concepts of momentum quantization and indistinguishable particles. These concepts treat properly quantum mechanics, entangled with the notions of classical trajectories, particle ensemble, and particle-with-sign

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generation giving rise to a time-dependent, fully quantum transport model which naturally includes both open and closed boundary conditions along with general initial conditions.

Focusing on this model we introduce a recently developed technique, a time-dependent renormalization by means of particles annihilation, which allows the simulation of time-dependent quantum phenomena. We apply this novel technique to the tunneling of a wave packet through a barrier.

2 Stochastic Aspects

The developed Monte Carlo algorithm aims to evaluate the expectation value $\langle A\rangle(t)$ of a generic physical quantity A at given evolution time t.

2.1 Monte Carlo Algorithm

By reformulating the semi-discrete Wigner equation as a Fredholm integral equation of the second kind one can derive a proper adjoint equation, which allows to express $\langle A\rangle$ as a series of terms:

$$\langle A\rangle(t) = \int_0^\infty dt' \int \mathrm{d}x_i \sum_{m'=-\infty}^{\infty} f_i(x_i, m') e^{-\int_0^{t'} \gamma(x_i(y))dy} g(x_i(t'), m', t') \tag{1}$$

where $x'(y) = x_i(y)$ is the Newtonian trajectory of a field-less particle, $g(x, m, t)$ is solution of the adjoint equation, represented by its resolvent series [2]:

$$g(x', m', t') = A_\tau(x', m', t') + \int_{t'}^\infty \mathrm{d}t \sum_{m=-\infty}^{\infty} g(x'(t), m, t) \Gamma(x', m, m') e^{-\int_{t'}^{t} \gamma(x'(y))dy} \tag{2}$$

with

$$A_\tau(x, m, t) = A(x, m)\delta(t - \tau)$$

$$\gamma(r) = \sum_{m=-\infty}^{\infty} V_w^+(r, m)$$

$$\Gamma(r, m, m') = V_w^+(r, m - m') - V_w^+(r, m' - m) + \gamma(r)\delta_{m,m'}$$

$$V_w^+ = \begin{cases} V_w & \text{if } V_w > 0 \\ 0 & \text{otherwise.} \end{cases}$$

The approach is a generalization of the stationary counterpart [2] for general transient transport problems. The terms in the resolvent expansion of (1) are ordered by consecutive applications of the kernel in (2), which is used to construct the transition probability for the numerical Monte Carlo trajectories. The latter consist of pieces of Newton trajectories linked by a change of the momentum number from m to m' according to Γ. Thus a numerical trajectory may be associated with a moving particle which undergoes scattering events. The exponent gives the probability that the particle remains on its Newton trajectory provided that the scattering rate is γ. If not scattered until time τ, the particle contributes to $< A >_0 (\tau)$ with the value $f_i(x_i, m')g(x_i(\tau), m')$. If scattered, the particle contributes to a next term in the expansion. It may be shown that a single particle contributes to one and only one term in the expansion and thus is an independent realization of the random variable sampling the whole sum: $< A > (t)$ is then estimated by averaging over N particles.

It is possible to give another interpretation to the equations due to the special appearance of Γ: after any free flight the trajectory forks into three contributive terms, the initial trajectory and two new trajectories with wave-vector offset equal to $l = m - m'$ and $-l$ around the initial wave number. Thus, a particle picture of a Monte Carlo branching process can be associated.

The process of creation of new couples is exponential [2]. The upper part of Fig. 1 shows what happens for one particle which moves in a constant field. The field magnitude is chosen to be 10339.2 V/m, so that the particle goes to the next k-space cell after 1 ps, and the total length of the domain is $1\,\mu m$. The following interpretation can be given: one initial particle evolves until, at some given random time, it generates a couple of positive and negative particles (recorded at 200 fs). Those particles evolve along with their parent particle, until they also generate couples. In turn, couples generate other couples until the final time is reached. This process triggers an avalanche of particle creations. From one particle, one ends up with 111 new particles at a recording time of 650 fs. We chose this final time since it is of the same order of typical final times to reach stationary regimes of practical nanodevices. Now, realistic simulations also involve several milions of initial particles. They rapidly generate a number of particles, which is of the order of several billions, a daunting numerical task.

2.2 The Annihilation Technique

The renormalization technique by annihilation described below represents a way to avoid this situation.

The renormalization technique is based on the fact that, in the Wigner formalism, particles are now mathematical objects deprived of any physical meaning. They are independent realizations of certain probability distributions related to the time-dependent solution of the Wigner equation. The unknown (and main object) of our problem is the Wigner quasi-distribution function. Furthermore, particles having the same wave number and position (i.e. being in the same cell of the phase-space), with opposite signs, do not contribute in the calculation of the average value for a macroscopic variable. They simply cancel the contribution of each other reciprocally or, in other words, annihilate.

These observations highlight the possibility of removing, periodically, the particles which do not contribute to the calculation of the Wigner function, i.e. one can apply a renormalization of the numerical average of the Wigner quasi-distribution by means of a particles annihilation process. This is in accordance to the Markovian character of the evolution to progress at consecutive time steps so that the final solution at a given time step becomes the initial condition for the next step. This method can be implemented as follows: one fixes a recording time at which the annihilating particles are checked. Particles found to annihilate are immediately removed from the simulation. This considerably reduces the number of particles at every recording time, as shown in the bottom of Fig. 1. In this case, the simulation ends up with 35 particles instead of 111 particles. This technique is advantageous since the reduction of the number of particles by means of the renormalization process allows the simulation of time-dependent technologically relevant cases with the Wigner formalism. Indeed, it is known

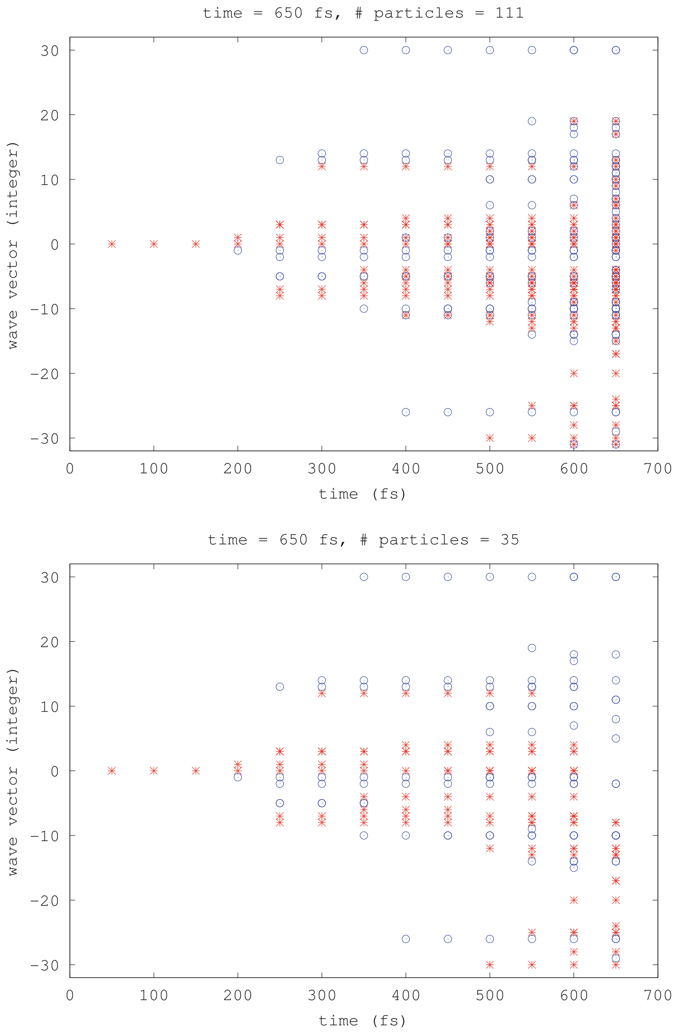

Fig. 1. Particle creation avalanche process with (bottom) and without (top) the annihilation technique. * = positive sign particles, o = negative sign particles.

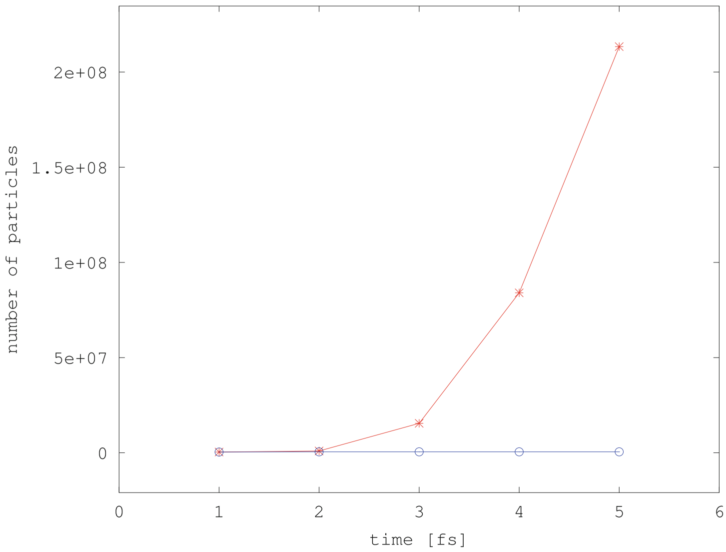

Fig. 2. Total number of particles with (dots) and without (stars) applying the annihilation technique.

that the particle's number grows exponentially in time, which destroys the simulation feasibility after a few time steps (see Fig. 2 and [2]).

3 Computational Aspects

The numerical experiment presented here consists of the simulation of a Gaussian wave packet tunneling through a barrier. The results have been obtained using the HPC cluster deployed at the institute of information and communication technologies of the Bulgarian academy of sciences. This cluster consists of two racks which contain HP Cluster Platform Express 7000 enclosures with 36 blades BL 280 C with dual Intel Xeon X5560 @ 2.8 Ghz (total 576 cores), 24 GB RAM per blade. There are 8 storage and management controlling nodes 8 HP DL 380 G6 with dual Intel X5560 @ 2.8 Ghz and 32 GB RAM. All these servers are interconnected via non-blocking DDR Infiniband interconnect at 20 Gbps line speed. The theoretical peak performance is 3.23 Tflops.

The software run on this machine is a modified version of Archimedes, the GNU package for the simulation of carrier transport in semiconductor devices [3]. This code was first released in 2005, and, since then, users have been able to download the source code under the GNU Public License (GPL). Many features have been introduced in this package. In this particular project, our aim is to include the quantum effects without recurring to quantum approximations such as effective potentials which are not satisfying when applied to nanodevices. The code is entirely developed in C and optimized to get the best performance from

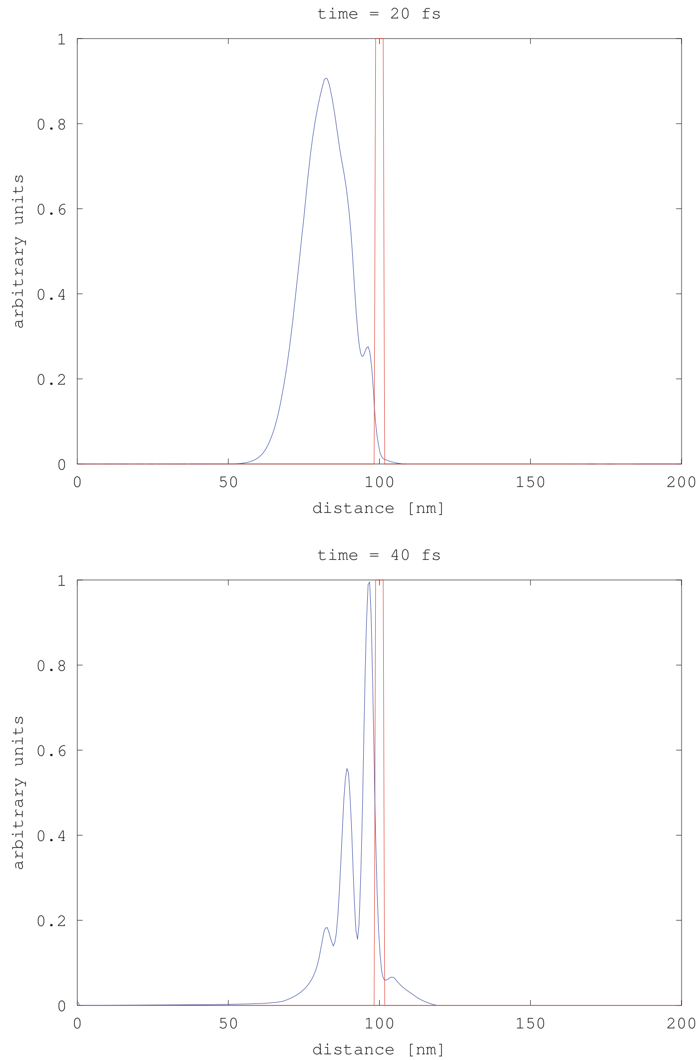

Fig. 3. Evolution at different times of a wave packet in proximity of a potential barrier.

the hardware [4]. The results of the new version will be, eventually, deployed on nano-archimedes website, dedicated to the simulation of nanodevices (see [5]).

The wave packet moves in a domain that has a potential barrier in the center. The domain is 200 nm long, and the barrier is 3 nm thick with an energy equal to 0.2 eV. The corresponding initial Wigner function reads:

$$f_W^0(r,n) = Ne^{-\frac{(r-r_0)^2}{\sigma^2}} e^{-(n\Delta k - k_0)^2\sigma^2} \tag{3}$$

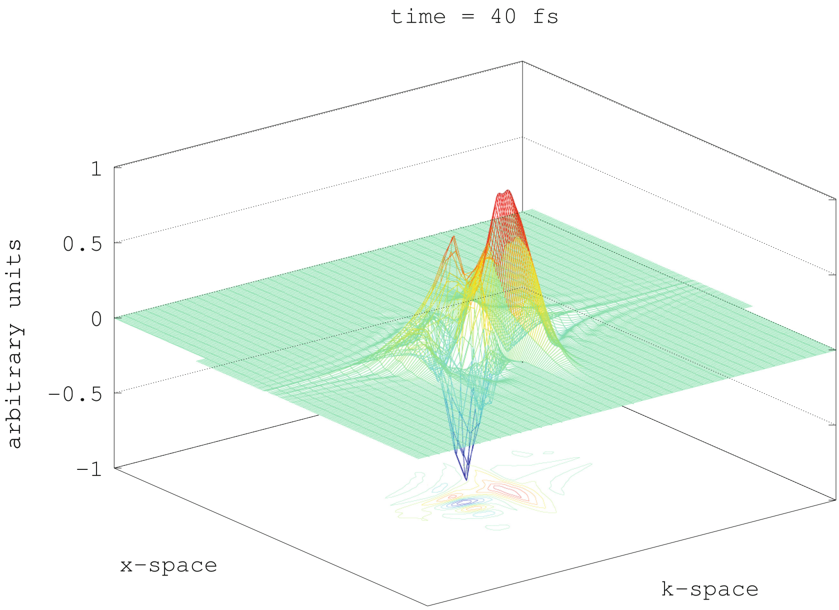

Fig. 4. Wigner distribution of a wave packet after 40 fs evolution.

N, k_0, r_0 and σ are, respectively, a constant of normalization, the initial wave vector, the initial position, and the width of the wave packet. The parameters defining the packet are chosen to make it collide with the potential barrier. The initial wave vector is equal to $4 \cdot 10^8\, m^{-1}$, the initial position of the center wave packet is at 68.5 nm, and the value for σ is 10 nm.

The rate of creation of particles depends on the shape of the function $\gamma(x)$. For the simulation of this particular transport problem, one needs at least 40 fs to observe relevant quantum effects. This is achievable only by applying a renormalization technique. Thus, we renormalize the Wigner quasi-distribution function by annihilation of particles every 1 fs. In this way one can reach long final times even equal to 80 fs.

Figures 3 and 4 show the wave packet at different evolution times, and the Wigner distribution function, respectively. The density obtained from the Wigner equation ressembles the time-dependent Schroedinger counterpart. A thorough comparison between Wigner and Schroedinger models will be presented somewhere else. Furthermore, the smoothness of the solution indicates the low stochastic noise of the method. Finally, Fig. 4 shows negative values in the calculated solution in the proximity of the barrier. This is a manifest of the quantum nature of the Wigner function as compared to the non-negative semi-classical distribution function.

4 Conclusions

We presented a renormalization technique for the Wigner quasi-distribution function, which involves the annihilation of particles at chosen recording times. We applied the method to the simulation of the tunneling process, where a Gaussian wave packet interacts with an energetic barrier. We have shown that, due to this renormalization technique, it is possible to calculate the time-dependent solution of the Wigner equation in realistic transport problems governed by quantum effects.

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