Two-dimensional Transient Wigner Particle Model

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***Abstract*—The Wigner equation represents a convenient approach when it comes to simulate the transient behavior of a wave packet at a nanoscale regime. It is a full quantum model that can include phonon scattering terms. A two-dimensional Monte Carlo technique has been recently implemented which is based on particles sign. In this paper we show that this is an efficient approach which works in realistic time-dependent and multi-dimensional situations.**

I. Introduction

The quantum phenomena inherent for nanometer systems are as a rule complemented with decoherence processes of phase breaking and energy dissipation caused by the environment. Such mixed transport regimes are conveniently described by the Wigner-Boltzmann (WB) formalism, which seamlessly approaches the classical limit, if decoherence processes begin to dominate. Indeed, as shown in [1], scattering strives to destroy the effect of the high order potential derivatives retaining only the electric field. The main challenges encountered in the implementation of the Wigner-Boltzmann formalism consist in the quantum component of the equation. Several approaches such as Wigner trajectories [2] and paths [3], the affinity method [4], [5], and the particle sign method [6] have been proposed. All of them reuse basic classical transport notions, but yet present limitations in one aspect or another and can not reach the viability and efficiency of the classical Monte Carlo models in particular: In the particle affinity method a real number assigned to the particles of an ensemble carries the quantum information of the system. This method has shown to be succesful for general time-dependent transport problems in realistic devices. However numerical issues related to the number of individual particles in the ensemble restricts the application to one-dimensional (1D) geometries. The particle sign model is a single particle approach, based on the ergodicity of the system. Signed particles generated by the Wigner potential reside on phase space points of generation, waiting to be consecutively evolved to the boundary. If an evolving particle meets a resident counterpart with opposite sign, both particles can annihilate each other. This method associates to the electron-potential interaction a clear heuristic picture, but is restricted to stationary transport determined by the boundary conditions.

In order to develop a general purpose approach, one may, eventually, combine some compatible ideas from this variety of concepts. In this paper we present a two-dimensional (2D) implementation of a new Wigner Monte Carlo approach, which is based on the concept of particle signs. This new method exploits the concepts of momentum quantization and indistinguishable particles. These concepts, proper to quantum mechanics, entangled with the classical notions of trajectories, particle ensemble, and particle-with-sign generation give rise to a time-dependent, multi-dimensional, full quantum transport model which includes both open and closed boundary conditions along with general initial conditions. The method, quantitatively validated in 1D benchmark problems including a comparison with the Schrödinger solution is now examined for 2D transport problems. We focus on qualitatively transparent physical phenomena allowing to analyze the numerical behavior. The main conclusion is that the method does not require special computational resources, thus making the implementation of quantum particle TCAD tools a reachable goal.

II. Model

According to one seminal consequence of quantum mechanics, the energy of particles is discretized and comes in *quanta*. The k-space is then naturally expressed in terms of a finite quantity $\Delta\mathbf{k} = \frac{\pi}{\mathbf{L}_C}$ (which imposes cellular automata rules [7]), where $\mathbf{L}_C = (L_C^x, L_C^y)$ is known as the coherence length. Thus, the Wigner equation can be expressed in terms of semi-discrete quantities and reads:

$$\frac{\partial f_W(\mathbf{x},\mathbf{M},t)}{\partial t} + \frac{\hbar\mathbf{M}\Delta\mathbf{k}}{m^*}\cdot\nabla_{\mathbf{x}} f_W(\mathbf{x},\mathbf{M},t) = \sum_{\mathbf{m}=-\infty}^{+\infty} V_W(\mathbf{x},\mathbf{M}-\mathbf{m},t) f_W(\mathbf{x},\mathbf{m},t) \quad (1)$$

In this case the Wigner potential also becomes semi-discrete:

$$V_W(\mathbf{x},\mathbf{M}\Delta\mathbf{k}) = \quad (2)$$
$$\frac{1}{i\hbar}\frac{1}{\mathbf{L}_C}\int_{-\frac{\mathbf{L}_C}{2}}^{+\frac{\mathbf{L}_C}{2}} d\mathbf{x}' e^{-i2\mathbf{M}\Delta\mathbf{k}\cdot\mathbf{x}'}\big(V(\mathbf{x}+\mathbf{x}') - V(\mathbf{x}-\mathbf{x}')\big)$$

In contrast to the semi-classical picture where particles are described in terms of continuous quantities, particles momenta are now described in terms of integer multiples $\mathbf{n}$ of a quantity $\Delta\mathbf{k}$. The problem is reformulated as a Fredholm integral equation of second kind, where the free term naturally includes general (open and closed) boundary conditions and initial conditions. The kernel of the equation Γ

$$\Gamma = V^+(t,\mathbf{r},\mathbf{n}-\mathbf{n}') - V^-(t,\mathbf{r},\mathbf{n}'-\mathbf{n}) + \gamma(t,\mathbf{r})\delta_{\mathbf{n},\mathbf{n}'} \quad (3)$$

$$V^+ = max\big(V_w, 0\big); \quad V^-(\mathbf{n}) = V^+(-\mathbf{n}); \quad \gamma = \sum_{\mathbf{n}} V^+ \quad (4)$$

$$V_w(t,\mathbf{r},\mathbf{n}) = \frac{1}{\hbar\mathbf{L}}\int_{-\mathbf{L}/2}^{\mathbf{L}/2} sin(2\mathbf{n}\Delta\mathbf{k}\mathbf{s})\left(\Delta V(t,\mathbf{r}\pm\mathbf{s})\right) d\mathbf{s} \quad (5)$$

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offers the following stochastic picture of the interaction with the Wigner potential: An initial particle with sign a at $\mathbf{n}$

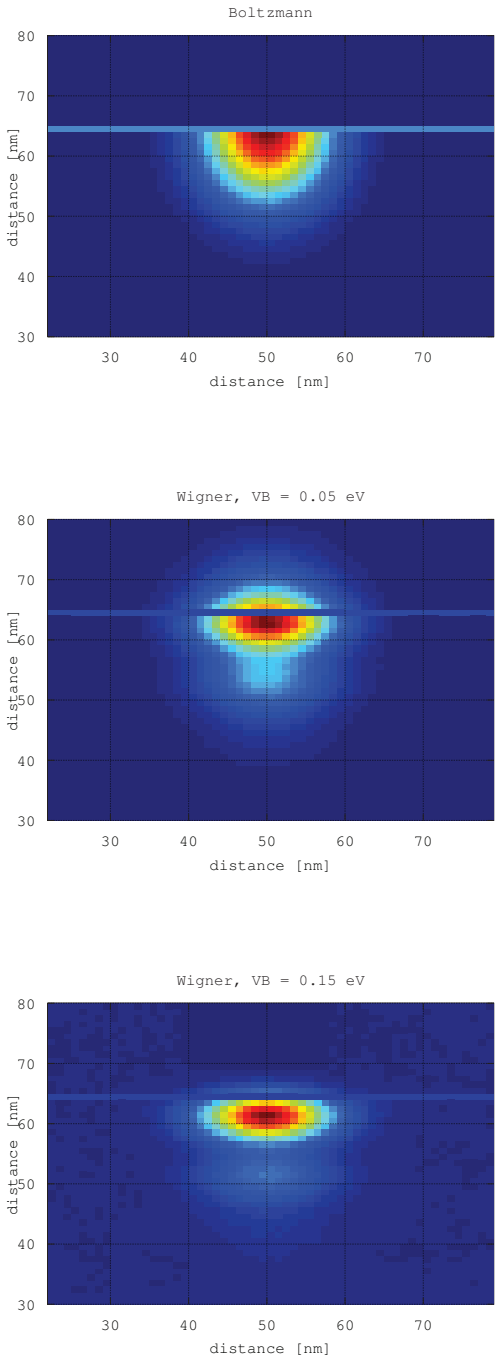

Fig. 1. Gaussian wave packet interacting with a perpendicular potential barrier at 30fs. Top: Boltzmann evolution. Middle and Bottom: Wigner evolutions with a potential barrier equal to 0.05eV and 0.15eV respectively.

generates, with a rate $V^+(\mathbf{l}) = V^-(-\mathbf{l})$, two primary particles with signs a, $-a$ and momenta

$$\mathbf{n}' = \mathbf{n} + \mathbf{l}; \qquad \mathbf{n}' = \mathbf{n} - \mathbf{l} \tag{6}$$

The initial particle does not feel the interaction and continues its evolution until time T. The created pair, in turn, generates new pairs, etc., and the number of particles increases exponentially. In order to keep the particle generation under control, we use the following strategy: At time T all K particles provide information about the mean value

$$\langle A \rangle = \sum_k A(\mathbf{r}_k(T), \mathbf{n}_k) sign(k), \tag{7}$$

where A is a generic physical quantity and $\mathbf{r}_k(T)$ is the position of the k-th particle over the Newton trajectory initialized by the phase space point, sign and time of birth. Two particles k and k' with opposite $sign$ and equal $\mathbf{n}$ do not have a net contribution in the limit $\mathbf{r}_k(T) \to \mathbf{r}_{k'}(T)$, thus, they annihilate. The Markovian dynamics allows to evolve at consecutive time steps ΔT, when a renormalization by annihilation is performed by recording on a phase space grid. This procedure keeps the particle avalanche under control. We note the fieldless character of the evolution: The electric field is incorporated into the Wigner potential. In this way the dynamics of the system is entirely expressed in terms of creation and annihilation of particles.

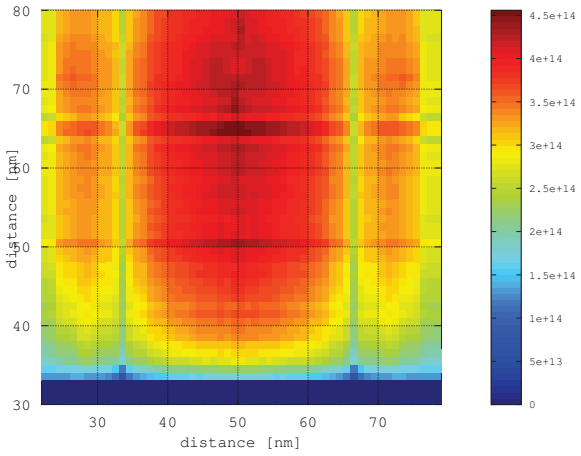

Fig. 2. Two-dimensional representation of the Gamma function in 1/sec.

III. Numerical Experiments

The simulator used to obtain the results presented in this section is a modified version of Archimedes, the GNU package for the simulation of carrier transport in semiconductor devices [8]. The code, known as nano-archimedes, implements two different parallelized algorithms. On one hand, the calculation of the Wigner potential, which consists of a set of nested loops, is spread among the available CPUs and the parallelization performance is almost ideal. This is obtained by using the parallel library OpenMP which represents a standard in the parallel coding community. On the other hand, the ensemble Monte Carlo particles are divided into subsets that are distributed among the available CPUs. The code is written in such a way that it can run both on a common personal computer (PC)

and on available clusters. For example, a typical simulation ran on our cluster [9], using 4 CPUs and less than 8 Gbytes takes about 2 hours. On a common PC with an Intel Core i5 processor a typical simulation will take about 10 hours.

We simulate three different instances of a 2D Gaussian wave packet moving against a potential barrier. The barrier is formed between the interface of a potential step and the absorbing boundary of the simulation domain. The interface is indicated in the figures by a line or a surface, in order to visualize the effects of tunneling and absorption by the boundaries. In the first case, the initial wave vector is perpendicular to the barrier, the evolution time is fixed, and we compare the process of tunneling with different barrier heights with the reference frame given by a hardwall reflection from the interface. In the second case, the initial wave vector is again perpendicular with respect to the barrier and the time evolution of the reflection and tunneling processes are followed. The third case is like the second one, but a parallel component of the initial wave vector is added. These three experiments can be reduced to a set of one-dimensional problems giving rise to a physically clear picture of the simulated processes. On the other side the numerical experiments represent genuine multi-dimensional arangements, so that any deviation of the physically expected behaviour will indicate numerical problems. We focus on the numerical feasibility of the 2D approach. For all experiments, the initial conditions consist of a Gaussian wave packet and read

$$f_W^0(\mathbf{x}, \mathbf{M}) = Ne^{-\frac{(\mathbf{x}-\mathbf{x}_0)^2}{\sigma^2}} e^{-(\mathbf{M}\Delta\mathbf{k}-\mathbf{k}_0)^2\sigma^2} \tag{8}$$

where N, $\mathbf{k}_0$, $\mathbf{x}_0$ and σ are, respectively, a constant of normalization, the initial wave vector, the initial position, and the width of the wave packet. which is fixed to 10nm. The initial energy of the wave packet of about 0.025eV is always smaller than the interface energy. Fig.1 shows the evolution of an initial Gaussian wave packet that goes perpendicular to the barrier at 30fs. The top plot represents a Gaussian wave packet which, following a Boltzmann evolution, bounces back from the interface by a specular reflection. The time is chosen in such a way that half of the initial particles have been already scattered by the interface. We note the spherical symmetry of the task in the lower half of the plot. The plots below correspond to a Wigner evolution so that the tunneling under the 0.05eV and 0.15eV high barriers is well pronounced. According to the physical picture the lateral components should not be affected by the independent process in normal direction and thus spread as in the Boltzmann case. The penetration under the barrier causes a deformation of the wave packet, which should reduce the spherical symmetry to a symmetry with respect to the vertical line in the center of the plot. This is exactly what happens with the behaviour of the Wigner density in the bottom two plots, which show that the numerical aspects of the 2D implementation are in accordance with the phenomenological picture. Two other peculiarities follow the same line: The increase of the potential reduces the tunneling so that the 0.15eV case is closer to the Boltzmann counterpart. This, however, holds for the upper

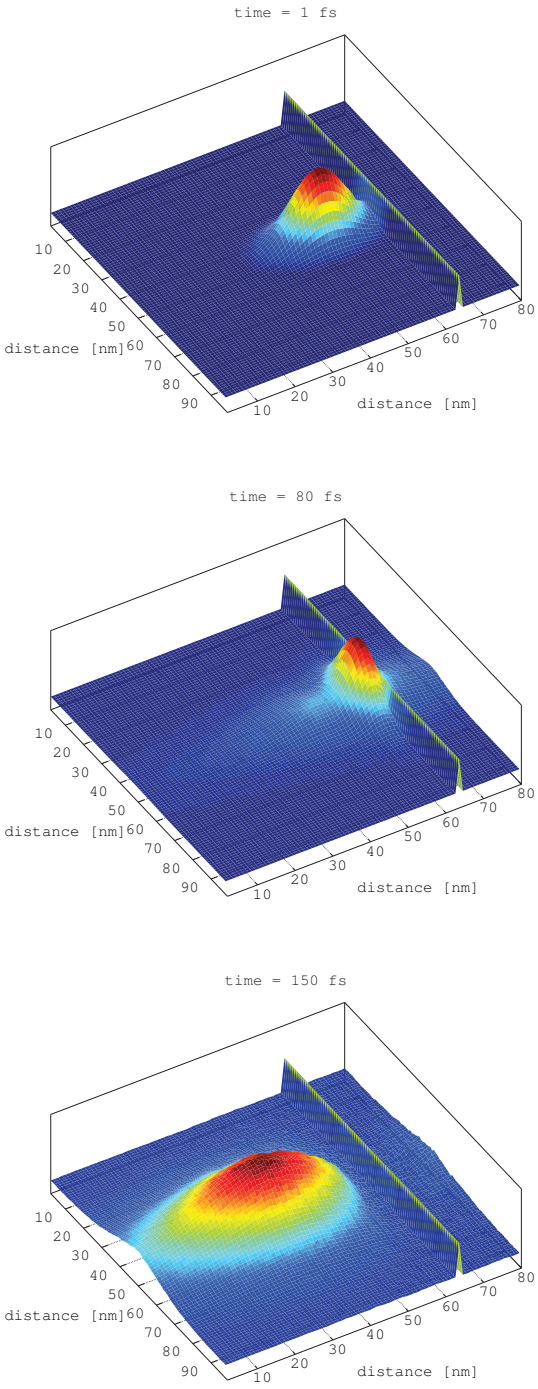

Fig. 3. Initial wave vector perpendicular to the potential barrier: Evolution of a 2D Gaussian wave packet at time 1fs, 80fs and 150fs respectively.

parts of the plots: At the bottom we observe a larger spread of the reflected waves with the increase of the barrier height. This is related to the fact that the quantum interaction is non-local and begins earlier in the sense that its magnitude spreads further away from the interface with the increase of the height. One can observe in the plots the magnitude of the electron-

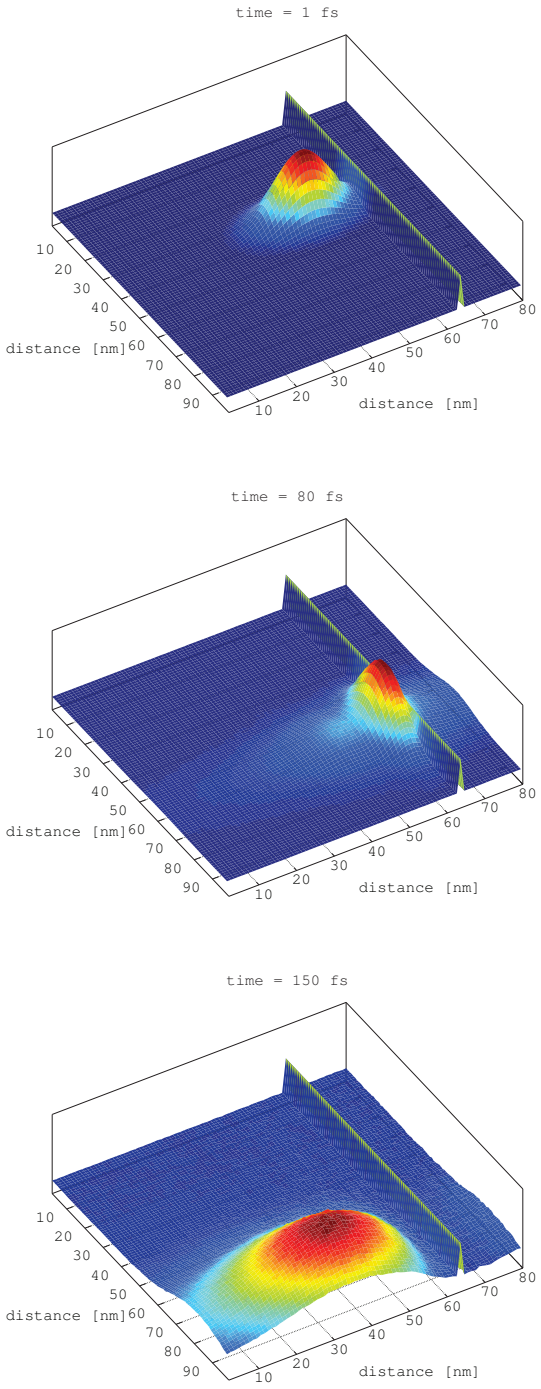

Fig. 4. Initial wave vector oblique to the potential barrier: Evolution of a 2D Gaussian wave packet at time 1fs, 80fs and 150fs respectively.

potential interaction quantity γ (see Fig. 2), which furthermore manifests the 2D character of the particle generation process.

Fig. 3 shows three different times of the evolution process corresponding to an interaction with a 0.05eV barrier and the right boundary. The initial wave packet (top plot) approaches the barrier. It is partially transmitted and partially absorbed by the barrier at 80fs (middle plot). Finally at 150fs (bottom plot) the tunneling part of the wave packet reaches the absorbing boundaries. This is indicated by the light-blue hump, whose smoothness and magnitude well demonstrates the precision of the stochastic approach. The same is true on the left boundary, reached by the bounced packet after 150fs, as can be seen in the bottom plot. This experiment is used as a reference for the next one, where we add a lateral component to the initial condition, cf. Fig. 4. From a phenomenological point of view this is equivalent of looking at Fig. 3 from a moving coordinate frame, so that the corresponding plots should be translationally equivalent. From a numerical point of view this is a very different 2D experiment due to the entirely different sequence of generation of particles in the four-dimensional phase space. Nevertheless the numerical picture is in accordance with the phenomenological one. Finally the bottom plot shows that the two absorbing boundaries do not influence the smoothness of the solution.

From all reported results, we can conclude that the method is not only effective but also efficient and can be applied to realistic and technologically relevant situations as it will be shown elsewhere.

IV. Acknowledgement

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[8] J.M. Sellier, *www.gnu.org/software/archimedes* This code was first released in 2005 under the GNU Public License (GPL). The code is entirely developed in C and optimized to get the best performance from the hardware. The results of the new version will be posted on the nano-archimedes website, dedicated to the simulation of nanodevices, see *www.nano-archimedes.com*.

[9] *http://www.grid.bas.bg/gate/index.php?option=com_content&view=article&id=61&Itemid=34* The machine used to obtain the simulations is 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 280c with dual Intel Xeon X5560 @ 2.8Ghz (total 576 cores), 24 GB RAM per blade. The theoretical peak performance is 3.23 Tflops.