Research Article

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A benchmark study of the Wigner Monte Carlo method

Abstract: The Wigner equation is a promising full quantum model for the simulation of nanodevices. It is also a challenging numerical problem. Two basic Monte Carlo approaches to this model exist exploiting, in the time-dependent case, the so-called particle affinity and, in the stationary case, integer particle signs. In this paper we extend the second approach for time-dependent simulations and present a validation against a well-known benchmark model, the Schrödinger equation. Excellent quantitative agreement is demonstrated by the compared results despite the very different numerical properties of the utilized stochastic and deterministic approaches.

Keywords: Wigner equation, Monte Carlo methods, quantum mechanics, Schrödinger equation

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1 Introduction

The Wigner equation represents a promising model for the simulation of nanodevices. It is a full quantum model able to capture the relevant physics in next generation semiconductor devices. It is well known that the pure state Wigner equation is an equivalent phase-space reformulation of the Schrödinger equation. At the same time the Wigner equation can be augmented by a Boltzmann-like collision operator accounting for the process of decoherence. Despite the initial enthusiasm around the Wigner model, the equation has represented a numerically daunting task and it has raised more problems than solutions. Several decades ago, some efforts have been put in the aim to numerically solve this equation for technologically relevant situations. The first works which appeared were all based on finite differences discretization [8], which raises problems in the treatment of the diffusion term $\frac{\hbar \mathbf{k}}{m^*} \cdot \nabla_{\mathbf{x}} f_W$ in the Liouville operator representing the differential part of the equation. Indeed the Wigner function $f_W(\mathbf{x}, \mathbf{k}, t)$ oscillates very rapidly in the phase-space, which makes the numerical calculation of its finite difference derivative a severe problem. This is thoroughly documented, for example, in [2].

More recently, two new approaches have been developed based on particle Monte Carlo methods. These approaches rely on the integral characteristics of the Liouville operator and thus avoid the problem of evaluating the diffusion term. The first model [7], an ensemble Monte Carlo (MC) technique, has proved to be effective and applicable to realistic technological situations such as one-dimensional resonant tunneling diodes. It is based on the concept of particles endowed with an affinity, a real number, having the meaning of a stochastic weight, employed in Monte Carlo methods for statistical enhancement of Boltzmann transport simulations [3, 6]. This method involves the use of heavy computational resources due to the increase of the number of particle states in the ensemble corresponding to the increasing quantum complexity of the problem [7]. The second model, relevant for stationary conditions, relies on the ergodicity of the problem determined by the boundary conditions, and, as such, has been developed within a single particle MC approach [4]. As compared to the affinity approach, it is very different and related to the generation of particles endowed with a sign. Based on these concepts we develop a new model for general transport conditions. It exploits the concepts of momentum quantization and indistinguishable particles. These concepts, intrinsic to quantum mechanics and entangled with the notions of classical trajectories, particle ensemble, and

particle-with-sign generation, give rise to a time-dependent, full quantum transport model which naturally includes both open and closed boundary conditions along with general initial conditions. In particular, this new method does not have an analog among the Boltzmann equation approaches.

In this paper we focus on the stochastic aspects of the particle sign model and present a thorough validation by comparing the Wigner MC results with the Schrödinger equation solution, an already traditional benchmark experiment [7, 11]. An excellent quantitative agreement is demonstrated despite the very different numerical aspects of the two approaches.

The paper is organized in the following way. We first introduce the particle sign Wigner MC algorithm from a mathematical perspective and describe some details needed to make the method able to deal with the process of particles creation and annihilation. The numerical procedure used to derive the model is described in detail in the next section. In the last section we describe the benchmark test for the comparisons between the Schrödinger and Wigner equations. We finally report the results of our simulations and discuss them.

2 Quantum dynamics in phase-space

The Wigner formulation of quantum mechanics [12] offers a description of the electron state in terms of a phase-space function $f_w(x, k, t)$, where x is the position and k is the wave number ($\hbar k$ momentum) variable. The pure state Wigner function is related to the solution of the Schrödinger equation $\Psi(x, t)$ via the Wigner–Weyl transform:

$$f_w(x, k, t) = \frac{1}{i\hbar 2\pi} \int dx' e^{-ikx'} \Psi\left(x + \frac{x'}{2}, t\right) \Psi^*\left(x - \frac{x'}{2}, t\right). \tag{2.1}$$

The Wigner equation is obtained from the Schrödinger equation and its adjoint [5] as follows:

$$\frac{\partial f_W}{\partial t} + \frac{1}{\hbar} \nabla_k \epsilon(k) \nabla_x f_W = Q[f_W], \tag{2.2}$$

where the functional $Q[f]$ acts over a pseudo-distribution function (in the Wigner formalism distribution functions can have negative values):

$$Q[f_W](x, k, t) = \int dk' V_W(x, k - k', t) f_W(x, k', t)$$

and the function $V_W = V_W(x, k, t)$, defined over the phase-space and known as the Wigner potential, reads

$$V_W(x, k, t) = \frac{1}{i\hbar 2\pi} \int dx' e^{-ikx'} \left(V\left(x + \frac{x'}{2}, t\right) - V\left(x - \frac{x'}{2}, t\right) \right).$$

The function $V = V(x, t)$ is the potential over the spatial domain, which in this general case may vary in time. Physically, it can represent, e.g., a force applied over a particle, a potential barrier, etc. The transport problem consists, at this point, of (2.2) along with a defined simulation domain containing the initial and boundary conditions.

The fact that particle energy in this regime is a discrete quantity suggests that the corresponding phase-space should be discretized to be in accordance with the principles of quantum mechanics. Thus, one can reformulate the Wigner equation in a semi-discrete phase-space with a continuous spatial variable x and a discretized wave-vector k described in terms of a step

$$\Delta k = \frac{\pi}{L_C}$$

(L_C is the so-called coherence length). By discretizing the phase-space, the Wigner equation now reads

$$\frac{\partial f_W}{\partial t} + \frac{\hbar}{m^*} m \Delta k \nabla_x f_W = \sum_{m'=-\infty}^{+\infty} V_W(x, m') f_W(x, m - m'). \tag{2.3}$$

3 Wigner Monte Carlo method

The purpose of this section is to present the main ideas behind the Wigner MC method based on particles sign. The aim of this method is the evaluation of the expectation value $\langle A \rangle(t)$ of some generic physical quantity, given in the Wigner picture by a phase-space function $A = A(x, k)$ at a given evolution time t. The computational problem is to calculate the inner product (A, f_W) with the solution of (2.2). It can be shown that this task can be reformulated in a way which involves the solution of the adjoint equation. Doing this, we first obtain an integral form of (2.2), and then the adjoint equation.

3.1 Integral formulation

In this section, we rewrite equation (2.2) in an integral form. First, let us define a function γ as

$$\gamma(x) = \sum_{m=-\infty}^{\infty} V_w^+(x, m) = \sum_{m=-\infty}^{\infty} V_w^-(x, m), \tag{3.1}$$

where V_w^+ takes the values of V_w if $V_w > 0$ and 0 otherwise, and V_w^- takes the values of $-V_w$ if $V_w < 0$ and 0 otherwise. In the stationary case, the Wigner potential is antisymmetric. It is clear that if $V_w^+(x, -m) = 0$, then $V_w^-(x, -m) \neq 0$ and, moreover, $V_w^-(x, -m) = V_w^+(x, m)$. Thus, equation (2.2) can be rewritten by adding and subtracting the term $\gamma(x(t'))$.

Let us, now, denote by Γ the following expression:

$$\Gamma(x(t'), m, m') = \left(V_w^+(x(t'), m - m') - V_w^+(x(t'), -(m - m')) + \gamma(x(t'))\delta_{m,m'} \right). \tag{3.2}$$

For the sake of simplicity, we assume the evolution of an initial condition $f_i(x, m)$ starts at time 0. A common inclusion of both boundary and initial conditions, which formally resembles the free term of the Boltzmann integral equation, is performed and by integration over the interval $(0, t)$, one recovers the following equation:

$$f_w(x, m, t) - e^{-\int_0^t \gamma(x(y))dy} f_i(x(0), m) = \int_0^t dt' \sum_{m'=-\infty}^{\infty} f_w(x(t'), m', t')\Gamma(x(t'), m, m')e^{-\int_{t'}^t \gamma(x(y))dy}$$

$$= \int_0^\infty dt' \sum_{m'} \int dx' f_w(x', m', t')\Gamma(x', m, m')$$
$$\times e^{-\int_{t'}^t \gamma(x(y))dy} \theta(t - t')\delta(x' - x(t'))\theta_D(x'). \tag{3.3}$$

To ensure the explicit appearance of the variables $Q = (x, m, t)$ and $Q' = (x', m', t')$, the kernel has been augmented by the θ and δ functions which retain the value of the integral unchanged. In particular θ_D keeps the integration within the simulation domain (if any). In the same way, the expectation value of the physical quantity A at moment τ is augmented and reads

$$\langle A \rangle(\tau) = \int dt \int dx \sum_{m=-\infty}^{\infty} f(x, m, t)A(x, m)\delta(t - \tau) = \int dQ f(Q)A_\tau(Q). \tag{3.4}$$

3.2 Adjoint equation

The expectation value (3.4) can be rewritten by introducing an adjoint equation, having a solution g and a free term g_0 determined below. If we formally write (3.3) and its adjoint equation as

$$f(Q) = \int dQ' K(Q, Q')f(Q') + f_i(Q),$$

$$g(Q') = \int dQ K(Q, Q')g(Q) + g_0(Q')$$

and
(i) the first equation is multiplied by $g(Q)$,
(ii) integrated on Q,
(iii) the second one is multiplied by $f(Q')$, integrated on Q',
(iv) the two equations are subtracted,
one obtains

$$\int dQ f_i(Q) g(Q) = \int dQ' g_0(Q') f(Q') \quad \leftrightarrow \quad \int dQ' f_i(Q') g(Q') = \int dQ g_0(Q) f(Q),$$

where the dummy variables have been exchanged for a more convenient comparison with (3.4). This shows that

$$g_0(Q) = A_\tau(Q), \quad \langle A \rangle = \int_0^\infty dt' \int dx' \sum_{m'=-\infty}^\infty f_i(x', m') e^{-\int_0^{t'} \gamma(x'(y)) dy} g(x', m', t'), \tag{3.5}$$

where $x'(y)$ is the trajectory initialized by x', m', t', $x(0) = x'$. Thus, the adjoint equation is obtained by integration on the unprimed variables:

$$g(x', m', t') = A_\tau(x', m', t') + \int_0^\infty dt \sum_{m=-\infty}^\infty \int dx\, g(x, m, t) \Gamma(x', m, m') e^{-\int_{t'}^t \gamma(x(y)) dy} \theta(t - t') \delta(x' - x(t')) \theta_D(x'). \tag{3.6}$$

This equation will be reformulated by reverting the parametrization of the field-less trajectory. Now $x(t') = x''$, m and t' initialize the trajectory and x becomes the variable changing with time t. The position argument of g becomes $x'(t)$ and one obtains

$$g(x', m', t') = A_\tau(x', m', t') + \int_{t'}^\infty dt \sum_{m=-\infty}^\infty g(x'(t), m, t) \Gamma(x', m, m') e^{-\int_{t'}^t \gamma(x'(y)) dy} \theta_D(x'). \tag{3.7}$$

Equation (3.5) is reformulated in the same way, by reverting the parametrization of the field-less trajectory. In this particular case the initialization is changed from x', m', t' to $x_i = x'(0), m', 0$ so that

$$x'(y) = x_i(y) = x_i + \frac{\hbar m' \Delta k}{m^*} y, \quad x' = x'(t') = x_i(t'), \quad dx' = dx_i,$$

$$\langle A \rangle = \int_0^\infty dt' \int dx_i \sum_{m'=-\infty}^\infty f_i(x_i, m') e^{-\int_0^{t'} \gamma(x_i(y)) dy} g(x_i(t'), m', t'). \tag{3.8}$$

3.3 Quantum particle method

Now, a particle method can be devised by considering the consecutive iterations of (3.6) into (3.8). The zeroth order term

$$\langle A \rangle_0(\tau) = \int_0^\infty dt' \int dx_i \sum_{m'=-\infty}^\infty f_i(x_i, m') e^{-\int_0^{t'} \gamma(x_i(y)) dy} A(x_i(t'), m') \delta(t' - \tau)$$

has the following interpretation. According to the Monte Carlo theory for solving integrals, we consider a part of the integrand as a product of conditional probabilities. Assuming that f_i is normalized to unity, we generate random points x_i, m' at time 0. These initialize particle trajectories $x_i(y)$. The exponent gives the probability for the particle to remain over the trajectory provided that the scattering rate is γ. This probability filters out these particles, such that the randomly generated scattering time is less than τ. If not scattered until time τ, the particle contributes to $\langle A \rangle_0(\tau)$ with the value of the rest of the integrand: $f_i(x_i, m') A(x_i(\tau), m')$. Otherwise, scattered particles do not contribute. The term $\langle A \rangle_0(\tau)$ is estimated by the mean value obtained from N initialized particles.

The first iteration term is obtained by a replacement of $g(x_i(t'), m', t')$ in (3.8) by the kernel of (3.7) written for this term (i.e. in (3.7) we replace x' by $x_1 = x_i(t')$). Note that the trajectory in the exponent becomes

initialized by x_1, m, t'. We have

$$\langle A \rangle_1(\tau) = \int\limits_0^\infty dt' \int dx_i \sum_{m'=-\infty}^\infty f_i(x_i, m') e^{-\int_0^{t'} \gamma(x_i(y)) dy} \int\limits_{t'}^\infty dt \sum_{m=-\infty}^\infty g((x_1(t), m, t) \Gamma(x_1, m, m') e^{-\int_{t'}^t \gamma(x_1(y)) dy} \theta_D(x_1).$$

Then, $g((x_1(t), m, t)$ is replaced with the free term of (3.7) in the corresponding point: $A((x_1(t), m, t) \delta(t - \tau)$. Moreover, we augment the equation by completing some probabilities enclosed in curly brackets and reorder other terms:

$$\langle A \rangle_1(\tau) = \int\limits_0^\infty dt' \int dx_i \sum_{m'=-\infty}^\infty f_i(x_i, m') \left\{ \gamma(x_i(t')) e^{-\int_0^{t'} \gamma(x_i(y)) dy} \right\}$$

$$\times \theta_D(x_1) \int\limits_{t'}^\infty dt \sum_{m=-\infty}^\infty \left\{ \frac{\Gamma(x_1, m, m')}{\gamma(x_i(t'))} \right\} \left\{ e^{-\int_{t'}^t \gamma(x_1(y)) dy} \right\} A((x_1(t), m, t) \delta(t - \tau).$$

Now, a particle is initialized at $x_i, m', 0$. It follows the trajectory until time t' which is the time of scattering given by the probability density in the first curly brackets. Indeed, the enclosed term, if integrated over time between 0 and ∞, gives unity. Moreover, the exponent is the probability not to scatter until time t', while $\gamma(x_i(t'))dt'$ is the probability to scatter in the interval dt' after t'. The phase-space position now is $x_1 = x_i(t'), m' t'$ and the evolution continues if the particle is still in the simulation domain (otherwise the contribution is zero). The term in the next curly bracket is analyzed below for interpretation as a source of scattering from m' to m (locally in space at point x_1 and at the time of scattering t'). Thus, at moment t' the particle initializes the trajectory x_1, m and, with the probability given by the exponent in the last curly brackets, remains over the trajectory until time τ: t is set to τ by the δ function provided that $t' < \tau$, otherwise the contribution is zero. We note however that in this case the particle has a contribution to the zeroth iteration term. The first three iterations show how to continue with higher order terms:

$$\sum_{s=1}^3 \langle A \rangle_s(\tau) = \int\limits_0^\tau dt_i \int dx_i \sum_{m_i=-\infty}^\infty \underset{\Uparrow x_i, m_i, 0}{f_i(x_i, m_i)} e^{-\int_0^{t_i} \gamma(x_i(y)) dy}$$

$$\times \left[\underset{\Uparrow x_1 = x_i(t_i)}{A(x_1, m_i) \delta(t_i - \tau)} + \int\limits_{t_i}^\tau dt_1 \sum_{m_1=-\infty}^\infty \theta_D(x_1) \underset{\Uparrow x_1, m_1, t_i}{\Gamma(x_1, m_1, m_i)} e^{-\int_{t_i}^{t_1} \gamma(x_1(y)) dy} \right.$$

$$\left. \times \left[\underset{\Uparrow x_2 = x_1(t_1)}{A(x_2, m_1) \delta(t_1 - \tau)} + \int\limits_{t_1}^\tau dt_2 \sum_{m_2=-\infty}^\infty \theta_D(x_2) \underset{\Uparrow x_2, m_2, t_1}{\Gamma(x_2, m_2, m_1)} e^{-\int_{t_1}^{t_2} \gamma(x_2(y)) dy} \underset{\Uparrow x_3 = x_2(t_2)}{A(x_3, m_2) \delta(t_2 - \tau)} \right] \right].$$

The initialization coordinates of the novel trajectories are also given, beginning with the symbol $\Uparrow$.

One observes that the iteration expansion of $\langle A \rangle$ actually branches, and the total value is given by the sum of all branches. Thus instead of scattering, three trajectory pieces or, equivalently three particles, appear:

$$\frac{\Gamma(x_1, m, m')}{\gamma(x_1)} = \left\{ \frac{V_w^+(x_1, m - m')}{\gamma(x_1)} \right\} - \left\{ \frac{V_w^-(x_1, m - m')}{\gamma(x_1)} \right\} + \{ \delta_{m,m'} \}. \tag{3.9}$$

According to the last term, the genuine particle survives and two more particles are generated with the first two probabilities. In other words, we generate the first state $m - m' = l$ with probability

$$\frac{V_w^+(x_1, l)}{\gamma(x_1)}.$$

Then, with the same probability (using just another random number) we generate another value, say l', for the second state $m' - m = l'$. These values can be combined into a single choice of l by reordering the sum over m for the second term so that $V_w^-(x_1, m - m')$ to appear in the place of V_w^+. Indeed, we recall that if $V_w^+(l)$ is not zero, then $V_w^+(-l) = 0$, and that $V_w^-(-l) = V_w^+(l)$. In this way the two states

$$m - m' = l, \quad m - m' = -l, \quad \leftrightarrow \quad m = m' + l, \quad m = m' - l,$$

with the second one having a flipped sign, have the same probability to appear.

To summarize: by applying the kernel of (3.7) in the form (3.9), one can order the terms in the resolvent expansion of (3.8). This is used to construct the transition probability of the numerical Monte Carlo trajectories which consist of pieces of Newton trajectories linked by a change of the momentum number from m to m' according to Γ. These numerical trajectories are interpreted as moving particles under scattering events. The exponent gives the probability that a particle remains on its field-less Newton trajectory with a scattering rate equal to γ. If the particle does not scatter until time τ, then particles contribute to $\langle A \rangle_0(\tau)$ with the value $f_i(x_i, m')g(x_i(\tau), m')$, otherwise they contribute to a next term of the expansion. It can be proved that a particle contributes to one and only one term of this expansion. Thus, the macroscopic value $\langle A \rangle(t)$ is estimated by averaging over N particles.

By exploiting the special appearance of the term Γ, it is possible to depict a Monte Carlo algorithm for the integration of the ballistic semi-discrete Wigner equation (2.3). After any free flight the initial particle creates two new particles with opposite signs and wave-vector offset (around the initial wave-vector) equal to $+l$ and $-l$ where $l = m - m'$. The initial particle and the two created ones represent three contributive terms to the series. We, thus, have an MC algorithm for our model.
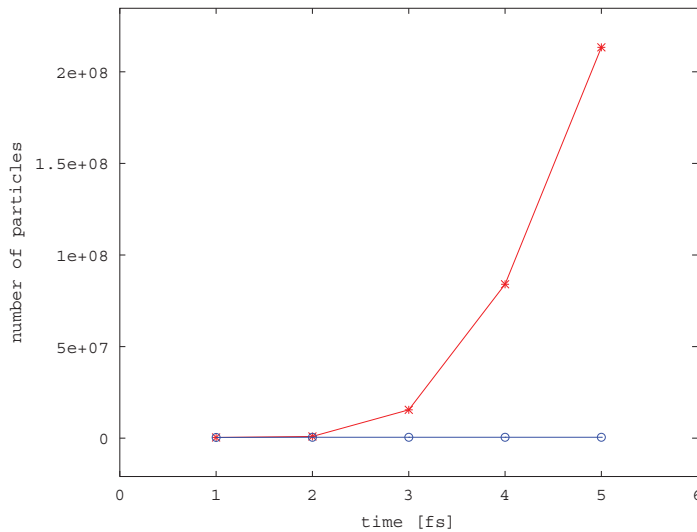

Figure 1. Total number of particles with (dots) and without (stars) applying the annihilation of particles. This technique keeps the total number of particles during the simulation under control.

It can be demonstrated that the process of creation of new couples is exponential by nature [4], as it is clearly shown in Figure 1 (stars). By exploiting the fact that particles are indistinguishable and annihilate, when they belong to the same phase-space cell with opposite signs, it is possible to remove a significant number of particles during the simulation. The technique works as follows: one fixes a recording time step at which one checks if particles are annihilating in some region of the phase-space. In the positive case, they are simply removed. All non-annihilating particles are kept in the simulation, since they contribute to the construction of the time-dependent solution. This technique is very efficient as one can see from Figure 1 (dots), especially for realistic simulations which typically involve several millions of initial particles. Without this technique, the time-dependent MC simulation of the ballistic Wigner equation would simply be a numerical daunting task.

4 Benchmark problem and results

The benchmark test we choose for the validation of our Wigner MC method consists of the interaction of a Gaussian wave packet with a potential barrier. We compare the results obtained with the solution of the

Schrödinger equation. This model is very well known and trusted by the nanodevice simulations community. It is clear that a good agreement between the presented Wigner MC technique and the Schrödinger equation represents a way to gain trust in this new method.

It is not the first time that a Wigner simulation is compared to the solution of the Schrödinger equation. During the early developments of the Wigner MC affinity method, some comparisons have been performed, but only a *qualitative* agreement has been reached between these two models, see, e.g., [7] and [11]. Here, we show that a satisfactory *quantitative* agreement can be reached with our Wigner MC method based on particle signs.

The length of the domain for our numerical experiment is 200 nm and a potential barrier of width 6 nm and energy 0.3 eV is placed in the center. We evolve this initial wave-packet until time 40 fs. This is a long enough time to see an actual interaction with the potential barrier. Thus, it is possible to observe in this numerical experiment both quantum reflection and quantum tunneling [1].

Concerning the initial conditions of our experiment, in the continuous case, they would be

$$f_W(x, k, t) = N' e^{-\frac{(x-x_0)^2}{\sigma^2}} e^{-(k-k_0)^2 \sigma^2}, \tag{4.1}$$

where N' is a normalization constant, x_0 the initial position of the peak and σ the width of the packet [7, 11] (obtained from the continuous Wigner–Weyl transform). In our case, these conditions are not valid. Indeed the semi-discrete Wigner-Weyl transform must be applied:

$$f_W(x, k, t) = \frac{1}{2L_C} \int\limits_{-L_C}^{+L_C} dx' e^{-ikx'} \rho\left(x + \frac{x'}{2}, x - \frac{x'}{2}, t\right), \tag{4.2}$$

where the function $\rho = \rho(x, y, t)$ is the density matrix (obtained from the wave-function $\Psi(x, t)$). The application of the semi-discrete transform gives the following initial conditions:

$$f_W^0(x, k) = A' e^{-\frac{(x-x_0)^2}{\sigma^2}} \int\limits_{-\frac{L_C}{2}}^{+\frac{L_C}{2}} dx' e^{-\frac{x'^2}{\sigma^2} - i2(k-k_0)x'} \tag{4.3}$$

with A' a normalization constant. Note that the semi-discrete initial conditions are in integral form. In this paper, we perform a numerical integration by means of a Gaussian quadrature technique.

Concerning the discretization scheme for the time-dependent Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m^*} \frac{\partial^2 \Psi}{\partial x^2} - qV(x)\Psi(x) \tag{4.4}$$

an explicit finite difference discretization technique would involve instabilities and create spurious oscillations [1]. Thus, we solve it by using an implicit discretization technique [1], i.e.

$$\Psi_j^{n+1} = \Psi_j^n + \frac{i\Delta t}{\Delta x^2}\left(\Psi_{j+1}^{n+1} - 2\Psi_j^{n+1} + \Psi_{j-1}^{n+1} + q\Delta x^2 V_j \Psi_j^{n+1}\right), \tag{4.5}$$

with $j = 1, \ldots, N_x$ (N_x is the number of cells in space) and n the time step index. This technique is proven to be numerically stable.

The numerical experiment is performed for the time-dependent Schrödinger equation (4.4), using the implicit discretization technique (4.5), and the Wigner equation, using the Monte Carlo technique based on particles sign. We then compare the square of the modulus of the wave functions obtained with the two different models. This corresponds to compare the probabilities of finding a particle inside the domain. The solutions of both methods are reported in Figures 2–4 at times, respectively, 0, 10, 20, 30 and 40 fs. The continuous (red) line shows the solution obtained from the time-dependent Schrödinger equation, while the dashed (blue) line shows the solution obtained from the Wigner MC method. One sees a very good agreement between the two models even for long times such as 40 fs, especially, if compared to previous MC techniques based on the particles affinity, where only qualitative agreement could be achieved [7, 11]. This represents a step ahead towards the simulation of time-dependent quantum systems which eventually also include the effects of phonon scattering. Furthermore, one should stress the fact that while models based on Schrödinger

equation have intrinsic difficulties in implementing general boundary conditions, our model can implement all kind of boundaries such as open, close or even imposed distribution functions at the contacts. This represents a big advantage in the simulation of realistic devices.
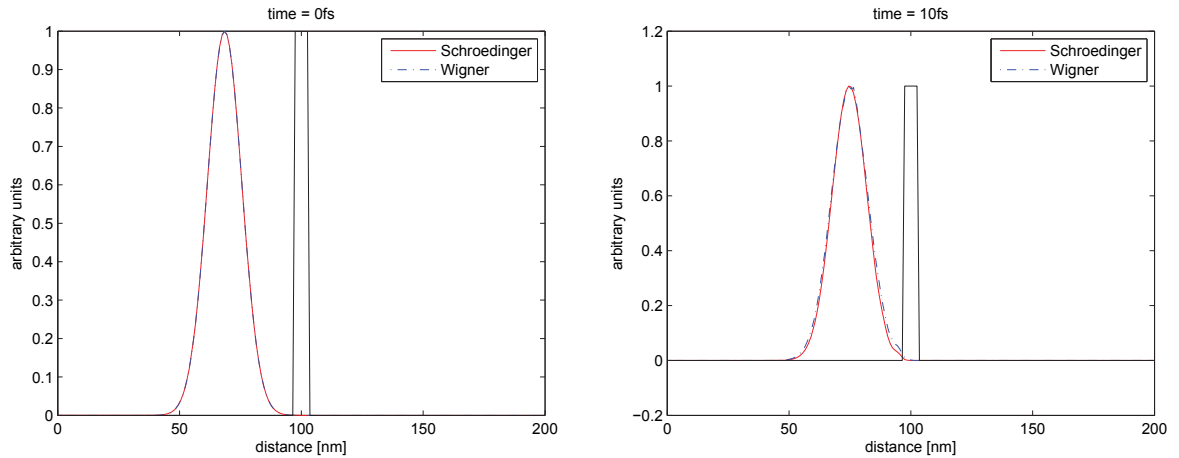

Figure 2. Evolution of a Gaussian wave packet at 0fs and 10fs respectively. continuous (red) line = Schrödinger, dashed (blue) line = Wigner.
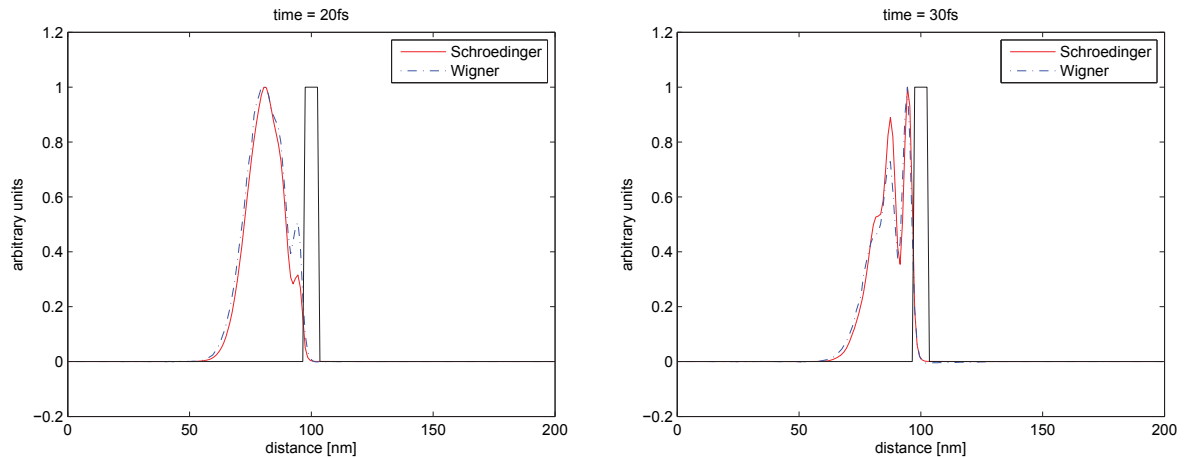

Figure 3. Evolution of a Gaussian wave packet at 20fs and 30fs respectively. continuous (red) line = Schrödinger, dashed (blue) line = Wigner.

The results presented have been obtained using the HPC cluster deployed at the Institute of Information and Communication Technologies (IICT) of the Bulgarian Academy of Sciences. This cluster consists of two racks with HP Cluster Platform Express 7000 enclosures with 36 blades BL 280c with dual Intel Xeon X5560 @ 2.8 Ghz (total 576 cores), 24 GB RAM per blade. There are eight 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 simulator used to obtain the results presented in this paper is a modified version of Archimedes, the GNU package for the simulation of carrier transport in semiconductor devices [10]. 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
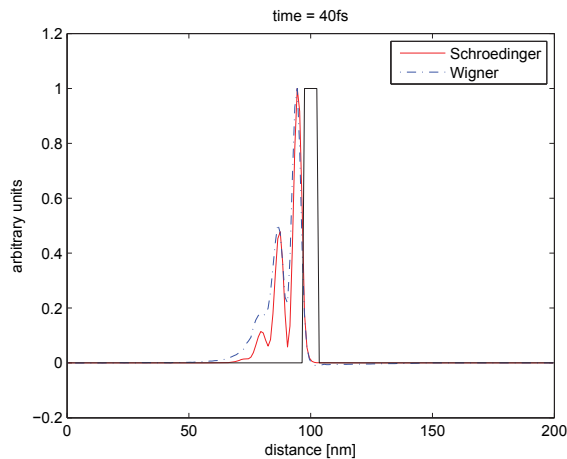
Figure 4. Evolution of a Gaussian wave packet at 40fs. continuous (red) line = Schrödinger, dashed (blue) line = Wigner.

to develop a full quantum, time-dependent and multi-dimensional simulator for nanotechnology devices. The code is entirely developed in C and optimized to get the best performance from the hardware. The results of the new version are periodically posted on the nano-archimedes website, dedicated to the simulation of nanodevices and chemical systems, see [9].

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