A Comparison of Approaches for the Solution of the Wigner Equation

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Abstract

As nowadays semiconductor devices are characterized by active lengths on the nanometer scale, it is important to use models including fully the quantum mechanical effects. In this paper we focus on the Wigner equation, a convenient reformulation of the Schrödinger equation in terms of a phase-space, and present a Monte Carlo technique to solve it, based on signed particles. Then we adapt the concept of potential decomposition, widely utilized to simplify the numerical treatment of the Wigner equation, to our method. Both approaches are compared to the direct solution of the Schrödinger equation. We show that excellent agreement is reached with our Monte Carlo technique which is also computationally efficient. The numerical experiment chosen for the comparisons consists of a Gaussian wave packet tunneling through a realistic source-to-drain potential profile. This is a technologically relevant situation for today's semiconductor devices for which quantum mechanical effects are prominent.

Keywords: Wigner equation, Monte Carlo, electrostatic potential decomposition, Schrödinger equation, full quantum transport

1. Introduction

The continuous scaling 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 higly relevant and cannot be ignored. They must be included in simulations to achieve reliable, predictive results. From this perspective, only full quantum models are capable of describing the appropriate physics. A well-known model is the Wigner equation, an equivalent phase-space reformulation of the Schrödinger equation [23].

Despite the numerical difficulties, there has been a high interest around the Wigner formalism. Efforts towards the simulation of this model started several decades ago and were based on finite difference discretization methods [13]. Serious problems were introduced by the treatment of the diffusion term $\frac{\hbar \mathbf{k}}{m^*} \cdot \nabla_{\mathbf{x}} f_W$. Indeed, the Wigner quasi-distribution function $f_W(\mathbf{x}, \mathbf{k}, t)$ oscillates very rapidly in the phase-space (with both positive and negative values). This

can eventually cause problems in the calculation of the derivatives by means of finite difference methods [6].

Recently, two new approaches to solve the Wigner equation, based on Monte Carlo (MC) techniques, have been developed. They both avoid the problem of evaluating the diffusion term, since they use the integral characteristics of the Liouville operator, which are Newtonian trajectories. The first model [20], [21], [22], [12] is an ensemble MC technique based on the concept of quantum affinity, a real number having the meaning of a stochastic weight (ranging in the set $[-\infty; 1]$) similar (but not equal) to what happens in MC methods for the statistical enhancement of Boltzmann transport simulations [7], [11], which is calculated according to the Wigner potential [12]. The method has proved to be reliable and applicable to several technologically relevant situations such as the simulation of one-dimensional (1D) resonant tunneling diodes. Despite its success, the method can hardly be applied to multi-dimensional simulations due to the demand of significant computational resources. In fact, the number of particle states in the ensemble increases during the simulation according to the complexity of the problem [12]. The second model [19], based on the concept of signed particles [8], is time-dependent, can take into account general initial and boundary conditions (BCs) and, to some phenomenological extent, can include the effects of lattice vibrations [17] (one should note that open BCs in the Wigner formalism still represent an open problem [14], in this paper we use absorbing BCs only which are in agreement with [3]). By exploiting some of the tenets of quantum mechanics, such as indistinguishabity of particles and energy quantization, along with the classical notions of trajectories, ensembles and signed particle generation, it is possible to depict a MC approach to the Wigner equation, which is time-dependent and multi-dimensional [10], [18], [17].

Finally, a concept shown to be very successful and useful for the simulation of nanometer scaled semiconductor devices is the decomposition of the potential profile [4]. This method consists in separating the full potential acting on the domain in two parts, a smooth (classical) component and a rapidly varying (quantum) component. This allows the inclusion of quantum corrections in precedently implemented Monte Carlo simulators. However this concept is challenged by recently developed multi-dimensional Wigner MC methods [18].

In this paper we utilize the signed particle Wigner MC method (full WMC) [19] and simulate the evolution of a Gaussian wave packet moving in a precalculated potential profile corresponding to a 1D $n^+ - n - n^+$ diode. Then, we adapt the potential decomposition [4] to our MC method and apply it to the same numerical experiment. Finally, these approaches are compared to the time-dependent Schrödinger equation. An excellent quantitative agreement is demonstrated between the full WMC and the solutions of the Schrödinger equation.

2. The Monte Carlo approach to solving the Wigner equation

The Wigner equation is an intuitive formulation of quantum mechanics in terms of a quasi distribution function $f_W = f_W(x, k, t)$ defined over a phase-

space. It reads [9]:

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

with

$$Q[f_W](x,k,t) = \int dk' V_W(x, k-k', t) f_W(x, k', t) \tag{2}$$

and

$$V_W(x,k,t) = \frac{1}{i\hbar 2\pi} \int dx' e^{-ik\cdot x'} \big(V(x + \frac{x'}{2}, t) - V(x - \frac{x'}{2}, t) \big) \tag{3}$$

(known as the Wigner potential). Here the function $V = V(x,t)$ is the (eventually time-dependent) electrostatic potential defined over the spatial domain.

Now, it is possible to reformulate the Wigner equation over a semi-discrete phase-space. Indeed, by introducing the quantity $\Delta k = \frac{\pi}{L_C}$ (where L_C is a cut-off length, sometimes know as the coherence length), the k-space can be expressed as a set of multiples $k = m\Delta k$ (with m an integer). The semi-discrete Wigner equation reads

$$\frac{\partial f_W}{\partial t} + \frac{\hbar}{m^*} m\Delta k \cdot \nabla_x f_W = \sum_{m'=-\infty}^{+\infty} V_W(x, m') f_W(x, m - m') \tag{4}$$

The transport problem is completed by specifying the initial and boundary conditions for (4). The unknown is the Wigner quasi-distribution function which is used to calculate the expectation value $\langle A \rangle(t)$ of a given macroscopic quantity $A = A(x,k)$, which can be expressed in terms of a series [8], [10]

$$\langle A \rangle = \int_0^\infty dt' \int \dot{\mathrm{x}}_i \sum_{m'=-\infty}^{\infty} f_i(x_i, m') e^{-\int_0^{t'} \gamma(x_i(y))dy} g(x_i(t'), m', t') \tag{5}$$

where

$$\gamma(x) = \sum_{m=-\infty}^{\infty} V_w^+(x, m) \tag{6}$$

with V_w^+ is the positive part of V_w. The function $f_i = f_i(x,m)$ is the initial condition and $g = g(x,m,t)$ is the solution of the adjoint equation [8], whose kernel $\Gamma = \Gamma(x, m, m')$ is defined as

$$\frac{\Gamma(x,m,m')}{\gamma(x)} = \left\{ \frac{V_w^+(x, m-m')}{\gamma(x)} \right\} - \left\{ \frac{V_w^+(x, -m+m')}{\gamma(x)} \right\} + \{\delta_{m,m'}\} \tag{7}$$

Following the reasoning of [8] and [10] the kernel can have a physical interpretation. In its formulation three particles appear, the initial one and two new ones. Indeed, by means of the probability

$$\frac{V_w^+(x,l)}{\gamma(x)} \tag{8}$$

we generate the first state $m - m' = l$ (with the same particle sign of the initial one) and, with the same probability, we generate the second state $m' - m$ (with the sign flipped with respect to the original one). A MC algorithm for the integration of the semi-discrete Wigner equation (4) is now depicted (full WMC). After any free flight, the initial particle creates two new particles with opposite signs. Their new wave-vectors are calculated from the offsets (around the initial wave-vector) $+l$ and $-l$ where $l = m - m'$. One should note that, being this approach of MC nature, it has the immediate advantage of being highly scalable on parallel machines [1].

The process of creating new couples is exponential [8] and a technique must be utilized to maintain the number of particles manageable. We exploit the fact that particles are indistinguishable and annihilate, when they are in the same phase-space cell with opposite signs. Thus, by fixing a recording time step at which we check if particles are annihilating, we can remove (annihilate) a significant number of redundant particles during the simulation. Only non-annihilating particles are kept, being the ones contributing to the construction of the solution. This method is known as *creation-annihilation technique* and has proved to be efficient, in particular, when millions of particles are involved [10].

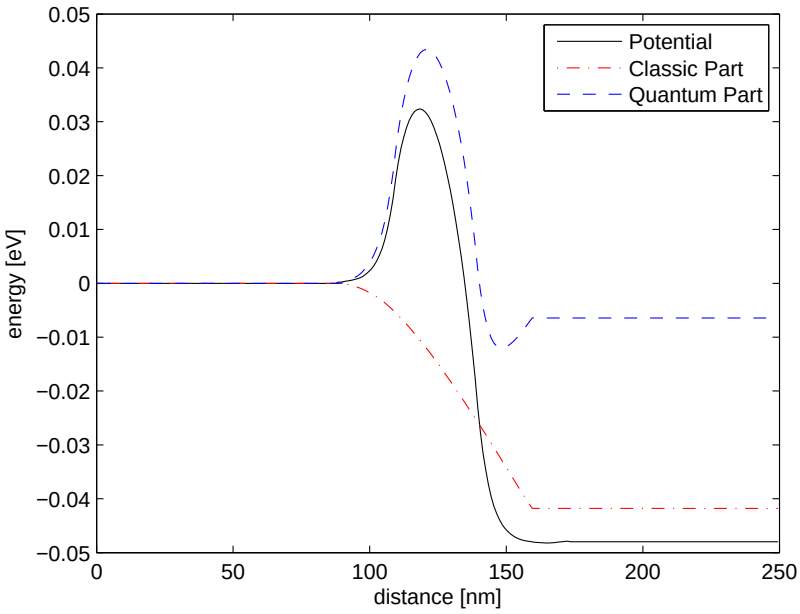

Figure 1: Decomposition of the electrostatic potential.

3. Decomposition of the electrostatic potential

The decomposition of the electrostatic potential is a well-known approach typically utilized to simplify the numerical complexity involved in the simulation of the Wigner equation [4]. It has been successfully applied to one-dimensional situations [12], [8], [2]. Our goal is to use this technique to make comparisons against the full WMC method described in the previous section. It consists of separating the electrostatic potential into a smooth classical component and a rapidly varying quantum component. This approach is originally defined for the case of a continuous phase-space. Since the full WMC method involves a semi-discrete phase-space, we modify the decomposition accordingly.

The original method is based on the Fourier analysis of the potential $V = V(x)$, which is known to diverge for $k = 0$ in the continuous case. In order to avoid this problem, a cut-off wave length λ_c and a cut-off wavenumber q_c are introduced $q_c = \frac{2\pi}{\lambda_c}$. Thus, the electrostatic potential can be decomposed over the device in two main contributions, a classical (slowly varying) and quantum (rapidly varying) contribution.

$$V(x) = V_{cl}(x) + V_{qu}(x) \tag{9}$$

In a continuous phase-space, the classical component $V_{cl} = V_{cl}(x)$ is defined as [4]:

$$V_{cl}(x) = \frac{1}{2\pi} \int_{-q_c}^{q_c} dq \hat{V}(q) e^{iqx} \tag{10}$$

$\hat{V}(q)$ is the Fourier transform of the potential (low-pass filter with cut-off q_c). In order to assure that we stay inside the device, the transform domain is truncated accordingly (otherwise it would span over the range $[-\infty, +\infty]$) and we assume that the electrostatic potential is constant outside the device (i.e. constant voltage in the leads).

Taking into account the semi-discrete nature of the phase-space and the truncated Fourier domain, it is possible to rewrite the classical contribution in a discrete form.

$$V_{cl}(x_j) = \frac{\sum_l w_{jl} V(x_j)}{\sum_l w_{jl}} \tag{11}$$

with

$$w_{jl} = \frac{sin\left[(j-l)q_c\Delta x\right]}{(j-l)q_c\Delta x} \tag{12}$$

In the continuous approach [4], the value for λ_c can be chosen in a rather arbitrary fashion and the index l varies in the range $-\frac{n_k}{2} \leq l \leq \frac{n_k}{2}$ (range of the Fourier transform), where n_k is also arbitrary. Since the transform (11) does not correspond to a numerical discretization any longer, but rather to the transform due to the discrete nature of the k-space, λ_c and n_k cannot be chosen arbitrarily anymore. In the semi-discrete case two theoretical constraints appear. First of all, to make the decomposition meaningful, the classical component has to be smooth. Second, we must stay in the same grid defined by the Wigner MC

method (described by the quantity Δk). Naturally, this still leaves some freedom in the choice of λ_c and n_k, but, from the performed numerical experiments, we observe that the best choice is $\lambda_c = 2L_C$ and $n_k = N_k$, where N_k is the maximum index allowed in the Wigner MC approach (positive direction of the k-space). In our case, other choices produces a non-smooth classical potential which invalidates the use of a potential decomposition.

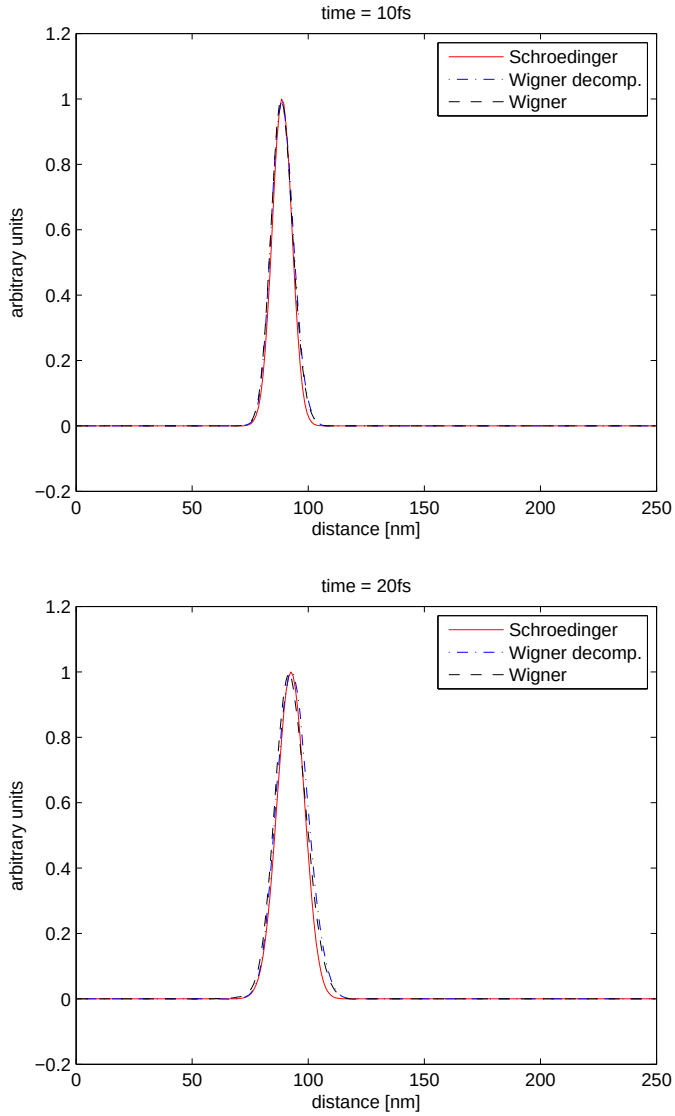

Figure 2: Evolution of a Gaussian wave packet inside a realistic potential at 10fs and 20fs. Comparison between Schrödinger, full WMC, and potential decomposition.

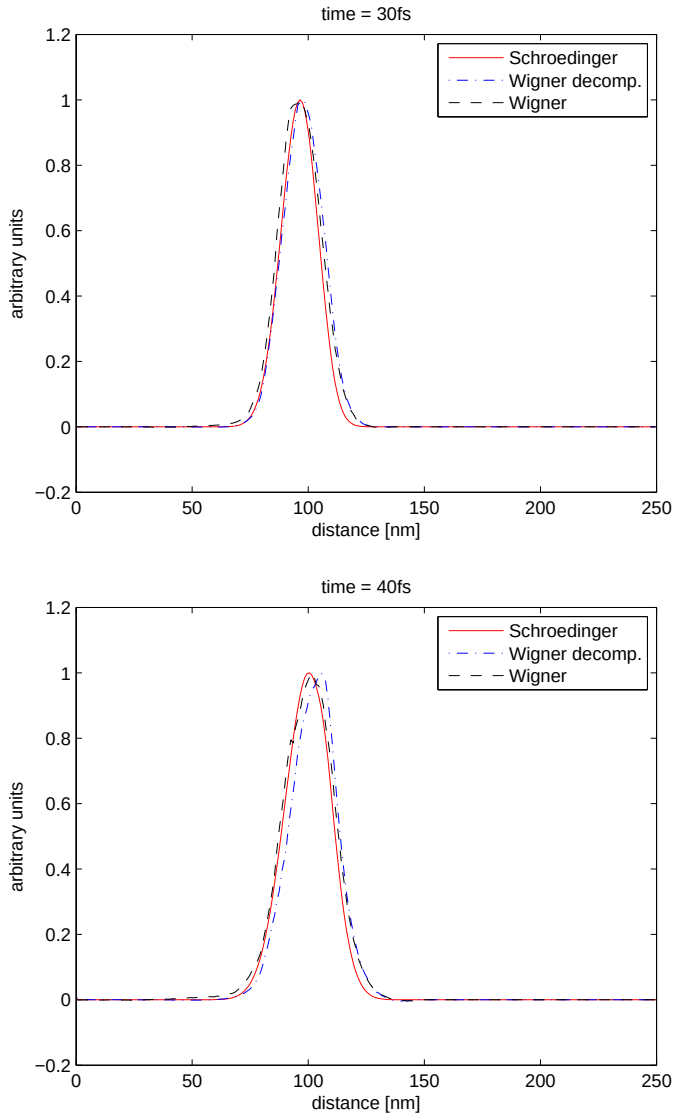

Figure 3: Evolution of a Gaussian wave packet inside a realistic potential at 30fs and 40fs.

4. A numerical experiment

We now present a numerical experiment consisting of a Gaussian wave packet moving in a realistic electrostatic potential which is obtained from a previous self-consistent semi-classical MC simulation [15]. The device is a $n^+ - n - n^+$ Silicon diode with lengths equal to 100nm, 50nm and 100nm respectively. The

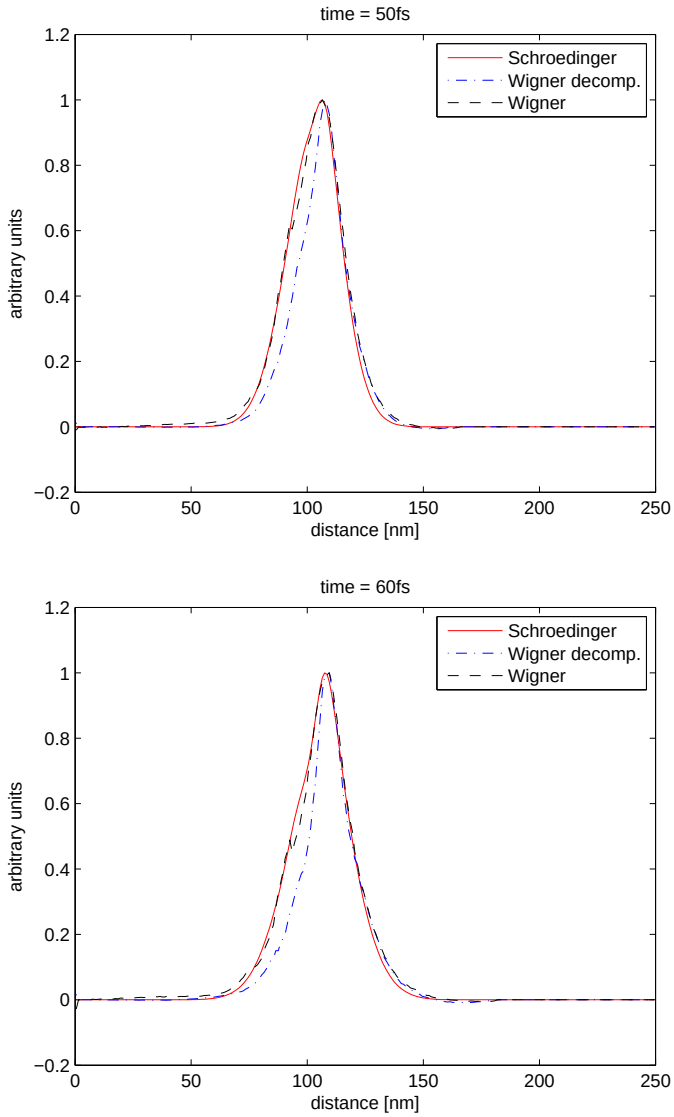

Figure 4: Evolution of a Gaussian wave packet inside a realistic potential at 50fs and 60fs.

n^+ doping concentration is $10^{24}m^{-3}$ while in the n region is $10^{22}m^{-3}$. The applied bias is equal to 0.05V (drain contact). The wave packet starts to move in the proximity of the drain contact (left side of the domain) towards the source contact (right side of the domain). The packet is expected to tunnel through the potential hump, in other words a barrier, visible in the channel (middle of the domain), see the (black) continuous curve in Fig.1. The evolution of the

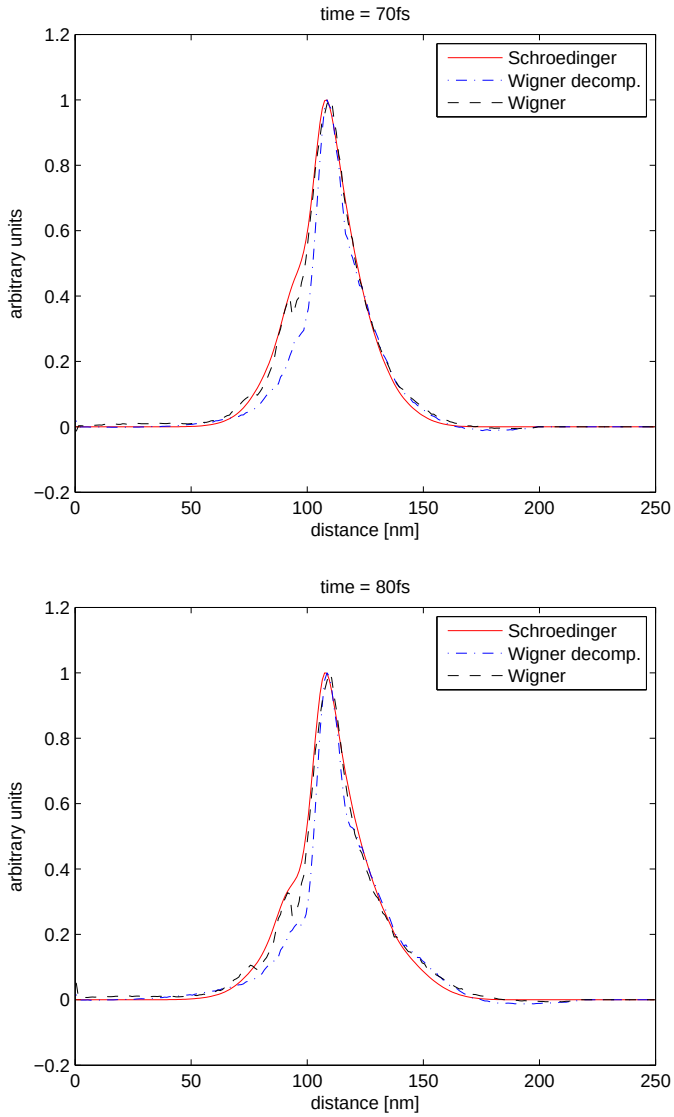

Figure 5: Evolution of a Gaussian wave packet inside a realistic potential at 70fs and 80fs.

packet is calculated in three different ways: the full WMC method, the potential decomposition technique, and a time-implicit finite differences discretization of the Schrödinger equation [5] (and all methods use the same spatial discretization). We consider the solution of the discretized Schrödinger equation as the benchmark and compare it to the other two methods. We show that the full WMC technique is applicable to realistic situations, such as source-to-drain tun-

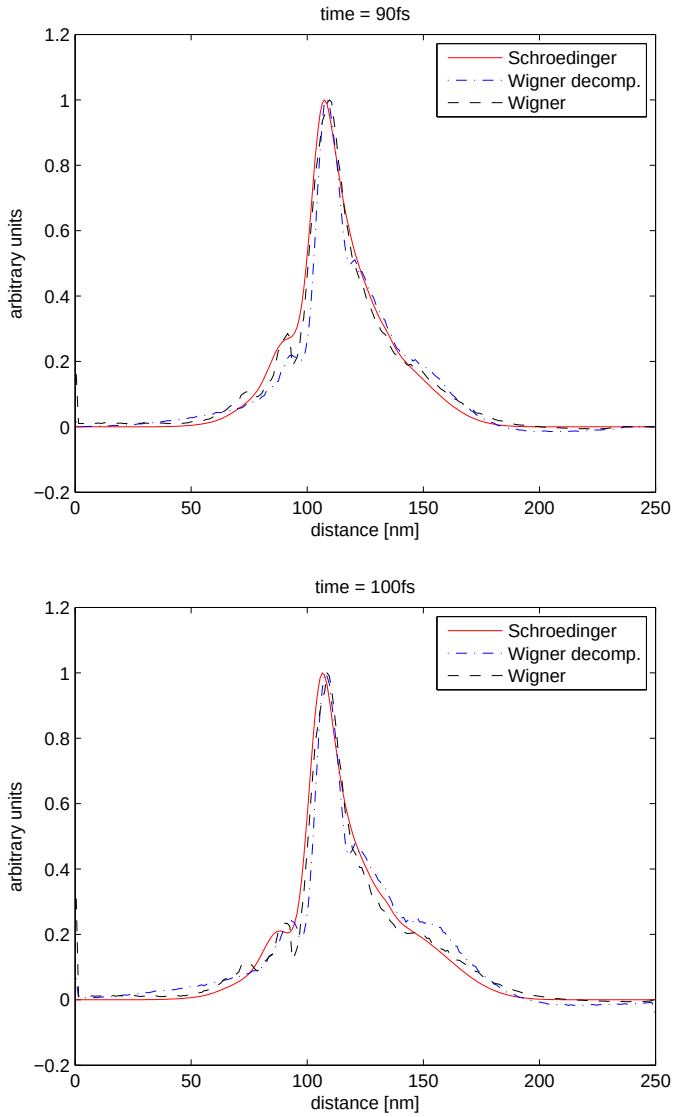

Figure 6: Evolution of a Gaussian wave packet inside a realistic potential at 70fs and 80fs.

neling in diodes. In addition, we show that it is numerically efficient and the solution is in better agreement with the benchmark solution compared to the results obtained with the decomposition technique.

In the Schrödinger formalism, the initial wave packet has the following form

$$\Psi^0(x) = Ae^{-\frac{(x-x_0)^2}{2\sigma^2}}e^{-ik_0x}$$

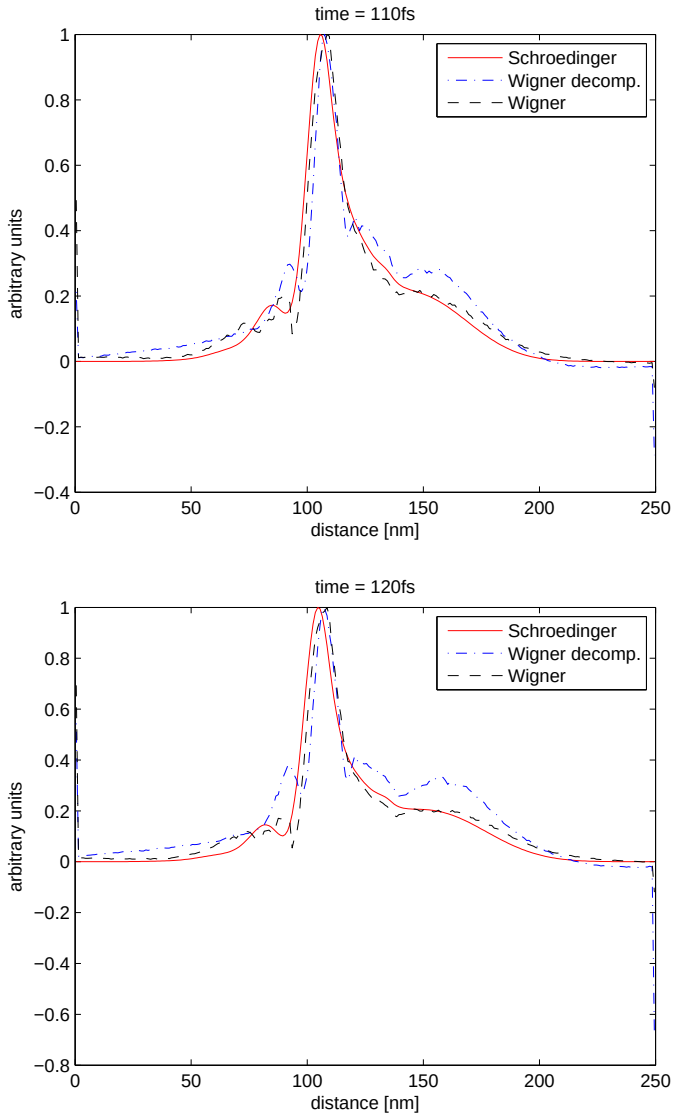

Figure 7: Evolution of a Gaussian wave packet inside a realistic potential at 90fs, 100fs, 110fs and 120fs respectively.

with A a normalization constant, x_0 the initial position, σ the spread of the packet, and k_0 the initial wave vector. Usually, the corresponding Wigner initial conditions are calculated by applying a Wigner-Weyl transform [20], [12]. It is to note that this transform does not take into account the semi-discrete nature of the phase-space and thus must be modified accordingly. It is possible to

obtain a semi-discrete Wigner-Weyl which reads

$$f_W(x, n\Delta k, t) = \frac{1}{L_C} \int_{-\frac{L_C}{2}}^{+\frac{L_C}{2}} dx' e^{-in\Delta k x'} \rho(x + \frac{x'}{2}, x - \frac{x'}{2}, t), \tag{13}$$

where the function $\rho = \rho(x, y, t)$ is the density matrix. The Wigner initial condition now reads

$$f_W^0(x, n\Delta k) = A' e^{-\frac{(x-x_0)^2}{\sigma^2}} \int_{-\frac{L_C}{2}}^{+\frac{L_C}{2}} dx' e^{-\frac{x'^2}{\sigma^2} - i2(n\Delta k - k_0)x'} \tag{14}$$

A' is a normalization constant. The semi-discrete initial conditions are now in integral form and have to be integrated numerically. For our purposes, we use a Gaussian quadrature technique.

4.1. Results

Fig. 1 shows the potential profile (black continuous) decomposed into two components, a slowly varying one (classical, blue dot dashed) and a rapidly varying one (quantum, red dashed). The initial Gaussian wave packet is evolved in that potential profile, until a final time equal to 120fs is reached. This represents a very long final time for such a situation which is useful to show the excellent accuracy of the full WMC. The three models (full WMC, decomposed potential technique, and Schrödinger) are compared in Figs 2, 3, 4, 5, 6, and 7. In particular, Figs.2 and 3 show the evolution of the wave packet at 10fs, 20fs, 30fs and 40fs. While the agreement between the three models seems to be good up to 30fs, differences start to appear at 40fs. Indeed the result of the potential decomposition technique (blue dot dashed line) starts to diverge from the solution of the discretized Schrödinger equation (red continuous line) and the result of the full WMC model (black dashed line). On the contrary, quantitative agreement still holds for the result of the full WMC method and the Schrödinger equation. Figs. 4 and 5 show the further evolution of the wave packet at 50fs, 60fs, 70fs, and 80fs. The differences between the models become now more pronounced. The results of the full WMC method is still in agreement with the solution of the discretized Schrödinger equation. Finally Figs.6 and 7 reports the evolution of the system at 90fs, 100fs, 110fs, and 120fs. The agreement between the solutions of the discretized Schrödinger equation and the full WMC model is excellent even for such long simulation times. Instead, the solution obtained with the decomposition technique agrees only qualitatively. Furthermore, the numerical resources exploited by the full WMC method are of the same order as those of the potential decomposition technique, since it exploits the annihilation technique [10].

5. The simulator and hardware

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 [15]. 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 has been to develop a full quantum time-dependent nanodevice simulator including phonon scattering effects. The code is entirely developed in C and optimized to get the best performance from the hardware. It can run on parallel machines using of the OpenMP standard library. The results of the present version are posted on the nano-archimedes website, dedicated to the simulation of nanodevices [16].

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 280c with dual Intel Xeon X5560 @ 2.8Ghz (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 20Gbps line speed. The theoretical peak performance is 3.23 Tflops.

6. Conclusions

In this paper the concept of potential decomposition has been described and modified for the case of a semi-discrete phase-space occuring in the time-dependent signed particle Wigner Monte Carlo method. In particular, we discussed the possible choices for the parameters q_c and n_k, which produce a smooth classical component. Both methods, with and without decomposition, were compared against the solution of the Schrödinger equation. The numerical experiment chosen for the comparisons consists of a Gaussian wave packet tunneling through a realistic, precalculated, source-to-drain potential profile. We have shown that the results of the full WMC technique are in excellent agreement with the solution of the Schrödinger equation even for very long final simulation times, unlike, when coupled to a potential decomposition. In this numerical experiment, the Wigner Monte Carlo technique has proved to be reliable, applicable to technologically relevant situations, and reasonable in terms of demand on resources. The full WMC method does not require the use of a potential decomposition. It performs excellent calculations without any extra numerical burden.

7. Acknowledgments

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