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## A sensitivity study of the Wigner Monte Carlo method



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### ABSTRACT

Recently a Wigner Monte Carlo technique exploiting the concept of signed particles has been developed for time dependent, multi-dimensional simulations of quantum mechanical effects in the ballistic regime. This method is based on the introduction of a semi-discrete phase-space which involves a free parameter  $L_C$  defining the discretization of the space of momenta. A systematic study to understand how the quality and reliability of the solution is influenced by this parameter is necessary. In this work, we analyze the sensitivity of the Wigner Monte Carlo method on  $L_C$ . To this aim, three quality measures are introduced based on a comparison with the Schrödinger equation (considered as a benchmark model in this work). We show that, essentially, the Wigner Monte Carlo method is not affected by the choice of  $L_C$ . Indeed, a large range of valid choices is available which demonstrates the robustness and reliability of the method.

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### 1. Introduction

Quantum mechanics was born as a necessity to explain experiments which are not comprehensible in terms of classical physics [1]. During the development of this theory, several equivalent formalisms eventually appeared, with their respective advantages and disadvantages, among which we cite the work of Schrödinger [2], Wigner [3] and, more recently, Keldysh [4]. Over the years, the Schrödinger equation has become the standard formalism of quantum mechanics. In this formalism, the evolution of a system is described by means of a complex wave function  $\Psi = \Psi(\mathbf{x})$  defined over the position  $\mathbf{x}$ , with no direct connection to any physical object. In order to make predictions, one recurs to the Born rule which states that only the square of the modulus of a wave function has a statistical interpretation [5]. The Schrödinger equation is relatively easy to treat mathematically, especially if compared to other existing formalisms. Furthermore, the principle of superposition is easy to explain in this context.

In his attempt to find quantum corrections to classical statistical mechanics [3], E. Wigner formulated a rather different (but completely equivalent) approach to quantum mechanics where a physical system is described by means of a more intuitive (quasi) distribution function defined over the phase-space,  $f_W = f_W(\mathbf{x}, \mathbf{p}, t)$  (with  $\mathbf{p}$  the momentum and  $t$  the time). While this formalism sounds very attractive, it constitutes an incredible mathematical challenge from both theoretical and numerical perspectives. Indeed, the Wigner equation is a partial integro-differential equation which unknown is defined on a multi-dimensional phase-space. These mathematical difficulties, eventually, prevented any analytical approach to the model. Despite the complexity of the Wigner equation, early numerical studies started to appear in the field of self-consistent simulations of semiconductor devices, based on finite difference techniques [6]. Very quickly it became clear that the diffusion term  $\mathbf{v} \cdot \nabla_{\mathbf{x}} f_W$  cannot be treated by such technique (where  $\mathbf{v} = \frac{\mathbf{p}}{m}$ ). Indeed, it is known that the Wigner function oscillates rapidly in the phase-space causing severe problems in the numerical calculation of the derivatives [7].

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Recently, several new approaches, based on Monte Carlo (MC) techniques, have been proposed which avoid the problems connected to the diffusion term. Initially, ensemble MC techniques were developed [8,9] and a special class based on the concept of particle affinity started to appear [10–13]. In particular, the technique presented in [13] has proved to be quite successful. By using the concept of particle affinity, a real number in the range  $[-\infty, +1]$  assigned to every particle, a whole range of physical phenomena occurring in semiconductor devices have been explained [14–16]. Then, an MC method based on the concept of signed particles was introduced [17]. This method relies on the Iterative MC technique [18,19], a time-dependent approach which can deal with general initial and boundary conditions. In particular, the signed particle Wigner MC method is formulated in a semi-discrete phase-space which introduces a free parameter  $L_C$  (sometimes called the coherence or cut-off length). This parameter has both a physical interpretation and a computational connotation. Physically speaking, it introduces the non-local effects of feeling the boundaries of the domain at distance (we are in the ballistic case, so no phonon is involved in the process). Computationally speaking, it defines the discretization of the wave-space. Thus, a systematic and thorough study is necessary in order to understand how the solution can be affected by the choice of this parameter.

In this work, we perform a variance-based sensitivity analysis of  $L_C$  in the context of the Wigner MC method. The ultimate goal of this investigation is to show that this method is robust and reliable and can, thus, be utilized for practical calculations with confidence. Indeed we show, by comparing against the Schrödinger model, that the quality of the solutions obtained by means of the signed particle Wigner MC method is not influenced by a particular choice of  $L_C$  as long as it belongs to an educated range (that is suggested below). In order to accurately perform this investigation, we utilize the typical tools of sensitivity analysis and introduce three different indicators to measure the quality of the solutions. The indicators are based on the cosine similarity, the 2-norm and the  $\infty$ -norm respectively, giving different perspectives on the problem. When utilized together, they provide a complete picture on the subject. Indeed, given two multi-dimensional real vectors (in our case describing the probability density defined over a one-dimensional domain), the cosine similarity gives us a judgment on their respective orientation, the 2-norm provides information on the relative directions and magnitudes and, finally, the  $\infty$ -norm describes the component on which these two vectors have a maximum departure. For every generated random value of  $L_C$  we perform a simulation starting from the same initial conditions corresponding to an electron wave packet in Gallium Arsenide (GaAs) material with a potential barrier provided by a material, such as Aluminum Gallium Arsenide (AlGaAs), with a different Fermi level. This is repeated for a big enough number of samples (in our case 512) and the three indicators are calculated at every simulation by comparison with the solution obtained from the Schrödinger equation. Eventually, we show that, if the free parameter  $L_C$  is chosen in an educated range, the solution calculated by the Wigner MC method is not noticeably affected, i.e. a strong indication of robustness and reliability.

## 2. The Wigner Monte Carlo method

In this section, we briefly sketch the Wigner MC method. The interested reader is suggested to read [17–19] for a complete description.

In a one-dimensional (1D) space and continuous phase-space the Wigner equation reads

$$\frac{\partial f_W}{\partial t} + \frac{p}{m} \frac{\partial f_W}{\partial x} = Q_W[f_W], \quad (1)$$

where  $f_W = f_W(x, p, t)$  is the unknown quasi-distribution function defined over the phase-space  $(x, p)$ ,  $m$  is the mass of a charge (usually an electron),  $Q_W$  is a functional defined as

$$Q_W[f_W](x, p, t) = \int dp' V_W(x, p - p', t) f_W(x, p', t),$$

and the Wigner potential is defined as

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

By introducing a free parameter  $L_C$  describing the discretization of the space of momenta  $\Delta p = \frac{\hbar\pi}{L_C}$ , the Wigner equation can be rewritten accordingly [17]. In particular, the space of momenta is now expressed in terms of multiples of the quantity  $\Delta p$  and a momentum is denoted by an integer  $M$  with  $p = M\Delta p$ . One should note that for every  $L_C$  the discretization of the momentum space changes accordingly, in other words the number and length of cells vary. Thus, in this semi-discrete phase-space, the Wigner equation reads

$$\frac{\partial f_W}{\partial t}(x, M) + \frac{M\Delta p}{m} \frac{\partial f_W}{\partial x}(x, M) = \sum_{N=-\infty}^{+\infty} V_W(x, M - N) f_W(x, N), \quad (3)$$

where the semi-discrete Wigner potential is formulated accordingly

$$V_W(x, M, t) = \frac{1}{i\hbar^2 L_C} \int_{-L_C/2}^{L_C/2} dx' e^{-i\frac{M\Delta px'}{\hbar}} \left[ V(x + x', t) - V(x - x', t) \right].$$

By applying the Iterative MC method [18,19] to the semi-discrete Wigner equation (3), it is possible to simulate the time-dependent quantum dynamics of the system [17]. A quantity  $\gamma = \gamma(x)$ , obtained from the positive part of the Wigner potential, is introduced and a particle generation process is given, where all particles carry a sign. During its flight, an initial particle creates a pair of new particles, one positive and the other negative. In particular, if initially the parent particle has a sign  $s$ , position  $x$  and momentum  $M$ , it generates, two new particles with signs  $s, -s$  and momenta  $M' = M + N, M' = M - N$  respectively, at the current position of the parent particle, with a given rate depending on the Wigner potential. After creation, the parent particle continues its flight until a given time  $T$  and the new pair of particles is evolved in turn. All signed particles evolve over field-less Newtonian trajectories and contribute to the values of the physical averages only by their sign. The evolution of the whole system in time is carried only by generation and annihilation of field-less Newtonian particles which replace the acceleration due to Newtonian forces [17]. This method is intrinsically three-dimensional and has been validated with success against one-dimensional, two-dimensional benchmark tests and technologically relevant situations [17,20,21].

### 3. Sensitivity analysis and indicators

In sensitivity analysis it is assumed that a mathematical model is given in terms of a function model [22]. Given a  $n$ -dimensional vector of input parameters  $\mathbf{x} = (x_1, x_2, \dots, x_n)$  selected in a space  $U^n = [a_1; b_1] \times [a_2; b_2] \times \dots \times [a_n; b_n]$  ( $a_i, b_i$  are real numbers and  $a_i < b_i$  for  $i = 1 \dots n$ ) with a joint probability density function  $p(\mathbf{x}) = p(x_1, x_2, \dots, x_n)$ , the model returns an  $m$ -dimensional output vector  $\mathbf{u} = (u_1, u_2, \dots, u_m)$ , where

$$\mathbf{u} = f(\mathbf{x}). \tag{4}$$

The output vector  $\mathbf{u}$  can be considered as a random vector since it is defined in terms of the random input vector  $\mathbf{x}$ . In general, models are characterized by multiple input parameters but, in our particular case, we are interested only in the free parameter  $L_C$ . Thus, the space of input parameters  $U^n$  reduces to a 1D space  $[a; b]$  where the (real) values  $a$  and  $b$  are specified in the next section (with  $a < b$ ). Finally, in the aim of a sensitivity study of the Wigner MC model  $f = f(x)$ , an indicator that measures the influence of a given input parameter must be introduced. In this work, we introduce three different indicators to have a complete overview of the dependence of  $f$  on  $L_C$ . Every indicator gives a different perspective on the problem and sheds light on the interpretation of the results. For our purpose, we exploit the concepts of cosine similarity, euclidean norm (also known as the 2-norm) and maximum norm (also known as the  $\infty$ -norm or supremum norm). In order to define these indicators, we fix a simulation context (see next section) and use the solution of the Schrödinger equation as a benchmark. We denote by  $\mathbf{u}$  the solution of the Wigner model and by  $\mathbf{v}$  the solution of the Schrödinger model. In both cases they represent the probability of finding a particle in a given discretized 1D domain described by a mesh with  $N_x$  cells. Thus, the solutions  $\mathbf{u}$  and  $\mathbf{v}$  can be seen as two vectors with  $N_x$  (real) components. Given a value for  $L_C$ , an output vector  $\mathbf{u} = \mathbf{u}(L_C)$ , and the solution of the Schrödinger equation  $\mathbf{v}$ , it is now possible to define an indicator.

The first indicator, based on the cosine similarity, is introduced as

$$I_{cos}(L_C) = I_{cos}[\mathbf{u}(L_C), \mathbf{v}] = \frac{\mathbf{u} \cdot \mathbf{v}}{|\mathbf{u}||\mathbf{v}|}, \tag{5}$$

where the operation  $\cdot$  is the scalar product and  $|\mathbf{u}|$  is the modulus of the vector  $\mathbf{u}$ . Strictly speaking, this indicator is not a metric as, for example, the non-negativity axiom is violated. Indeed  $I_{cos}$  can be negative for vectors which point in opposite directions in the  $N_x$ -dimensional space of output vectors. In any case, it is a good indicator of similarity between two vectors. Indeed, when two vectors point in the same direction and have comparable moduli the value of  $I_{cos}$  is close to 1, when they are orthogonal then  $I_{cos} = 0$  and when they are opposite then  $I_{cos} = -1$ . In this work, we use this indicator as a starting point for our analysis. In this perspective, one expects that, if the Wigner MC method is not too sensitive on the parameter  $L_C$  (given in a certain range), then  $I_{cos}(L_C)$  should be close to 1 for every random value  $L_C$ .

The second indicator we use is based on the Euclidean norm and reads

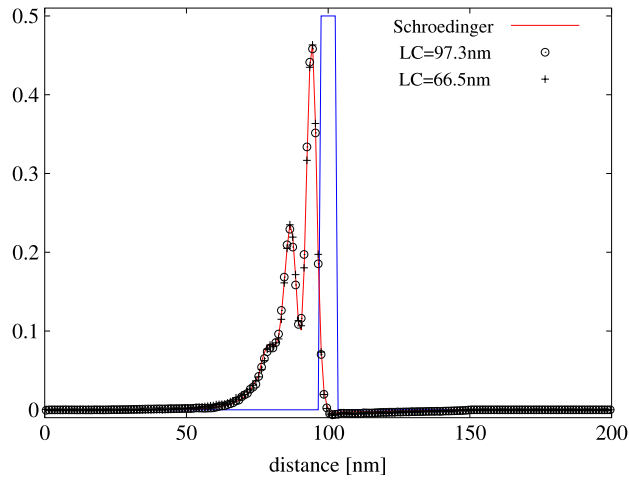
$$I_2(L_C) = I_2[\mathbf{u}(L_C), \mathbf{v}] = |\mathbf{u}(L_C), \mathbf{v}|_2 = \sqrt{\sum_{i=1}^{N_x} (u_i - v_i)^2}, \tag{6}$$

where  $u_i$  and  $v_i$  are the  $i$ th component of the vectors  $\mathbf{u}$  and  $\mathbf{v}$  respectively. This indicator is a metric and can be considered as the distance between the Wigner vector  $\mathbf{u}(L_C)$  and the Schrödinger solution  $\mathbf{v}$ . It is a clear indication of the quality of the computed solution compared to the benchmark solution. The lower the value of  $I_2(L_C)$ , the better the quality of the solution.

Finally, one can exploit the  $\infty$ -norm to define a further indicator

$$I_\infty(L_C) = I_\infty[\mathbf{u}(L_C), \mathbf{v}] = |\mathbf{u}(L_C), \mathbf{v}|_\infty = \max_{i=1 \dots N_x} |u_i - v_i|. \tag{7}$$

This indicator is a metric too. For our purpose, we use the value  $I_\infty$  as an indication of the maximum distance the Wigner solution can have from the benchmark solution in a point of the simulation domain.



**Fig. 1.** Comparison of probability densities of a wave-packet interacting with a potential barrier at 40 fs. The (red) continuous line represents the solution calculated with the Schrödinger equation while the  $\circ$  and  $+$  curves represent Wigner solutions with  $L_C = 97.3$  nm and  $L_C = 66.5$  nm respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

### 4. Numerical experiments

In order to perform a significant sensitivity analysis of the Wigner MC method, we focus our attention on the following standard and practical situation. A Gaussian wave packet moves in a GaAs crystal towards a potential barrier positioned in the center of the domain and miming the presence of an AlGaAs thin layer. The domain length  $L_x$  is 200 nm long, and the barrier is 6 nm thick with an energy equal to 0.3 eV (see Fig. 1, blue continuous segments in the center). The corresponding initial Wigner function reads

$$f_W^0(x, p) = A e^{-\frac{(x-x_0)^2}{\sigma^2}} e^{-(p-p_0)^2 \sigma^2}, \tag{8}$$

where  $A$ ,  $p_0$ ,  $x_0$  and  $\sigma$  are, respectively, a constant of normalization, the initial momentum, the initial position, and the initial dispersion of the wave packet. The parameters defining the packet are chosen such that it collides with the potential barrier in a relatively short time. The initial momentum has a value equal to  $4 \cdot 10^8 \text{ } \hbar m^{-1}$ , the initial position of the center of the wave packet is at 68.5 nm, and the value for  $\sigma$  is equal to 10 nm. The solution is evolved until a final time equal to 40 fs. Finally, a set of 512 random  $L_C$  samples is uniformly generated in the interval  $[\frac{L_x}{10}; \frac{9L_x}{10}]$ . The reason for such interval comes from the fact that, in the Wigner MC method, the parameter  $L_C$  completely defines the discretization of the momentum space. In other words, once a value for  $L_C$  is selected then a corresponding length and number of cells for this space are fixed through the relations (see [17])

$$\Delta p = \frac{\hbar\pi}{L_C},$$

$$N_p = \left[ \frac{L_C}{2\Delta x} \right]_{int},$$

where  $\Delta x$  is the length of cells in the spatial domain,  $[\cdot]_{int}$  is the integer part of a real number, and  $N_p$  is the number of cells in one direction of the momentum space. Furthermore, one should note that the parameter  $L_C$  cannot be too small or too large since, in the first case, the virtual particles would simply not feel the non-local effects due to the environment, while in the second case the solution could rapidly deteriorate due to a too small  $\Delta p$  [17]. Thus, the intervals  $(0; \frac{L_x}{10})$  and  $(\frac{9L_x}{10}; L_x]$  are not taken into account since they correspond to a very coarse mesh in the momentum-space in the first case, and to an extremely refined mesh in the second case. Obviously, the definition of such interval strongly depends on the simulation that is performed and other equally convenient intervals may be suggested for different numerical situations.

For each generated value of  $L_C$  a simulation is performed with the same initial conditions and the solutions are stored until a set of 512 output vectors  $\mathbf{u}_i$  (corresponding to the probability density defined over the meshed domain) is generated. For clarity, two examples for two different values of  $L_C$  are shown in Fig. 1 along with the benchmark solution (Schrödinger). At that point, the indicators  $I_{cos}$ ,  $I_2$  and  $I_\infty$  are applied on the previously computed arrays  $\mathbf{u}_i$ . A graphical representation of the indicators  $I_{cos}$ ,  $I_2$  and  $I_\infty$ , applied to the set of values  $L_C$ , is reported in Figs. 2–4 respectively. Finally, for the sake of completeness, Table 1 shows the respective mean values, standard deviations and variances. In particular, Fig. 2 shows the cosine similarities between the set of Wigner solutions and the Schrödinger solution. The mean value for the set of  $I_{cos}$  is equal to 0.99904 while the standard deviation is  $4.71e-04$ . This is a first clear indication that the Wigner solutions are very

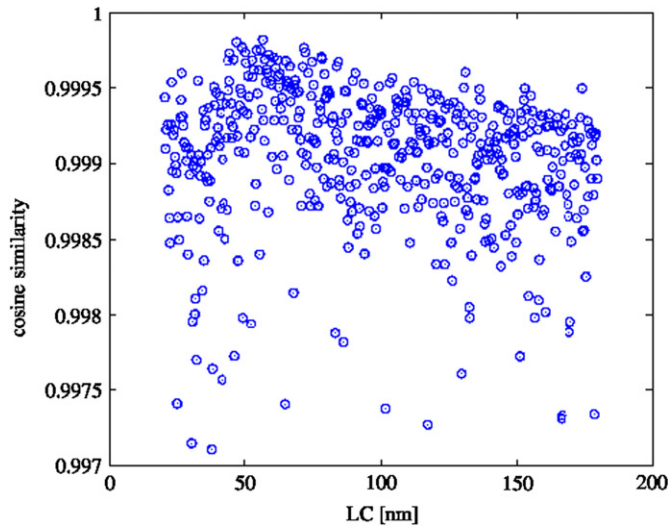


Fig. 2. Cosine similarities for a set of 512  $L_C$  samples.

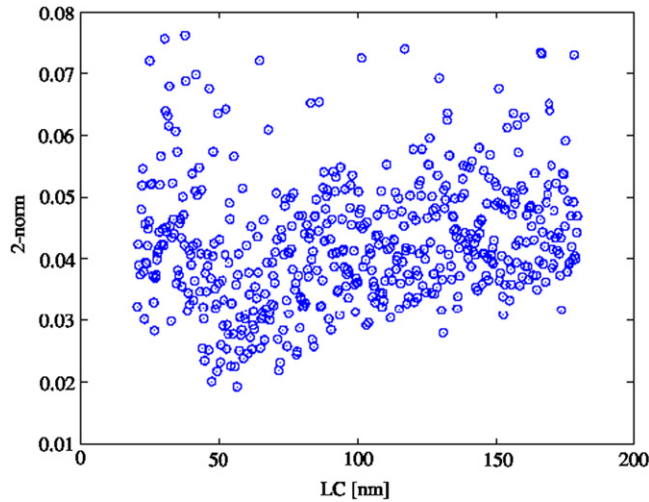


Fig. 3. 2-norms for a set of 512  $L_C$  samples.

**Table 1**  
Mean value, standard deviation and variance for the indicators  $I_{cos}$ ,  $I_2$  and  $I_\infty$ . The statistics is performed over a set of 512 samples in the range  $[\frac{L_c}{10}; \frac{9L_c}{10}]$ .

	Mean value	Stand. deviat.	Variance
$I_{cos}$	0.99904	4.7088e-04	2.2173e-07
$I_2$	0.042597	0.010119	1.0239e-04
$I_\infty$	0.017833	0.0050076	2.5076e-05

similar to our benchmark, whatever the value of  $L_C$  in the proposed range. In Fig. 3 the Euclidean norm in function of  $L_C$  is shown. In this case, the mean value is equal to 0.042, another clear indication that the Wigner solutions are not so distant from the benchmark. Finally, Fig. 4 shows the values for the indicator  $I_\infty$ . Even in this case, good agreement between the generated Wigner solutions and the Schrödinger benchmark is found.

The good agreement shown by the three different (and independent) indicators brings us to the conclusion that the Wigner MC method is essentially not sensitive to the choice of the free parameter  $L_C$  as long as it is chosen in a well educated range. Thus, it is a robust and reliable method.

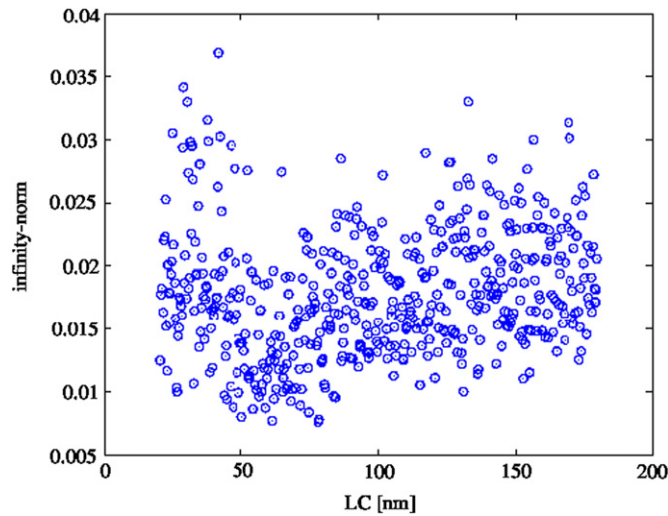


Fig. 4.  $\infty$ -norm for a set of 512  $L_C$  samples.

## 5. Conclusions

In this work, we introduced an MC technique to simulate the Wigner equation, a formalism based on the concept of a phase-space and equivalent to the Schrödinger model. This MC method introduces a semi-discrete phase-space that relies on the choice of a free parameters  $L_C$ . We investigated the sensitivity of the computed solution on the choice for  $L_C$  in the range  $\left[\frac{L_x}{10}; \frac{9L_x}{10}\right]$ , where  $L_x$  is the total length of the domain. The indicators utilized for such study are  $I_{\cos}$ ,  $I_2$  and  $I_\infty$  based on the concept of cosine similarity, Euclidean norm and supremum norm respectively. They rely on the comparison of the Wigner solutions with the benchmark Schrödinger equation. We found that, in spite of the quite large range of possible choices for the parameter  $L_C$ , there is very good quantitative agreement between the Wigner MC method and the Schrödinger equation. Therefore, one can safely conclude that the Wigner MC method is a robust and reliable technique which can be utilized to simulate full quantum, time-dependent and multi-dimensional mechanical effects.

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