

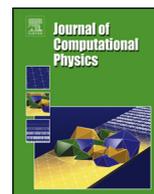


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The many-body Wigner Monte Carlo method for time-dependent ab-initio quantum simulations



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ABSTRACT

The aim of ab-initio approaches is the simulation of many-body quantum systems from the first principles of quantum mechanics. These methods are traditionally based on the many-body Schrödinger equation which represents an incredible mathematical challenge. In this paper, we introduce the many-body Wigner Monte Carlo method in the context of distinguishable particles and in the absence of spin-dependent effects. Despite these restrictions, the method has several advantages. First of all, the Wigner formalism is intuitive, as it is based on the concept of a quasi-distribution function. Secondly, the Monte Carlo numerical approach allows scalability on parallel machines that is practically unachievable by means of other techniques based on finite difference or finite element methods. Finally, this method allows *time-dependent* ab-initio simulations of strongly correlated quantum systems. In order to validate our many-body Wigner Monte Carlo method, as a case study we simulate a relatively simple system consisting of two particles in several different situations. We first start from two non-interacting free Gaussian wave packets. We, then, proceed with the inclusion of an external potential barrier, and we conclude by simulating two entangled (i.e. correlated) particles. The results show how, in the case of negligible spin-dependent effects, the many-body Wigner Monte Carlo method provides an efficient and reliable tool to study the time-dependent evolution of quantum systems composed of distinguishable particles.

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1. Introduction

Traditionally, ab-initio simulations are known to be an incredibly difficult task to achieve. Indeed, they require immense computational resources. On the other hand, such calculations allow the development of tools which can drastically improve many aspects of human life. They may assist the design of new drugs, new materials or even enable the development of new information processing technologies, just to mention some of the infinite possibilities. It is, thus, not surprising that a very early interest has been shown in this direction and big efforts have been made, since then, to develop reliable and efficient techniques to simulate the quantum many-body problem.

The term *ab-initio* first appeared in [1] with the meaning of simulations based on the *first principles of quantum mechanics*. Today, many approaches to ab-initio simulations exist. The simplest method one can think of is the Hartree–Fock method (also known as the self-consistent field method) [2,3] which is based on the assumption that the many-body quantum wave-function can be expressed in terms of a Slater determinant [4] (in case of a system of fermions). More sophisticated

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approaches known as post-Hartree–Fock methods also exist, among which we have, for example, the configuration interaction method [5], the Møller–Plesset method [6], etc. Another interesting class of post-Hartree–Fock methods is represented by the so-called quantum Monte Carlo methods which aim is to handle the multi-dimensional integrals arising from the quantum many-body problem by means of Monte Carlo techniques (variational, diffusion, etc.) [7–9]. In any case, whatever the method is, they all have one thing in common: they rely on our capability of calculating the stationary wave-function of the many-body Schrödinger equation [10]. In this perspective, other equivalent formalisms of quantum mechanics, such as the Wigner model [11], seem to be not common in the ab-initio community, to the best of our knowledge.

This work introduces the use of the many-body *time-dependent* Wigner Monte Carlo (WMC) method in ab-initio calculations for the particular case of distinguishable particles and negligible spin-dependent effects. This can be considered as a first attempt to use a phase-space formulation of quantum mechanics in ab-initio simulations for strongly correlated systems. Despite the mentioned limitations, this brings several advantages. First of all, it is based on the iterative Monte Carlo (MC) method for solving linear and non-linear equations (both integral and algebraic) [12,13] which is known to scale very well on parallel machines [14]. This opens the way towards the time-dependent simulation of complex quantum systems hardly approachable in the context of finite difference or finite element discretization techniques. Secondly, being the many-body Wigner equation a formulation of quantum mechanics in terms of a phase-space, it represents a more intuitive approach to explain quantum mechanics. Indeed the main unknown of this model is a quasi-distribution function (see, for example, [15] and [16] for the description of hydrogen and closed-shell atoms). Finally, general boundary conditions (BCs) can be applied. For chemical systems, the most commonly used are reflective (equivalent to the closed-box assumption) and absorbing BCs (which are time-irreversible and thus in agreement with the requirements in [17]). The case of open BCs is still an open problem and it is not contemplated in this work [18].

During the last decade several MC methods to simulate the single-particle Wigner equation, which avoid the problems introduced by finite difference or finite elements methods (see for example [19]), were developed [20–24]. One of them introduces the concept of signed (virtual) particles, generated by the Wigner potential, and it is a full quantum, multi-dimensional, time-dependent approach [24]. This method exploits the notions of energy quantization and indistinguishable particles which are entangled with the concepts of Newtonian trajectories, particle ensemble, and particle annihilation. Very recently, it has been applied with success to ab-initio simulations in the context of density functional theory [25].

In this work, we present a generalization of the signed particle one-body Wigner MC method to the many-body Wigner equation for distinguishable particles in the absence of spin-dependent effects. We validate our approach by studying the time-dependent evolution of a system containing two charged particles (electrons, no spin involved), with and without an external potential. The results show that the WMC method is an intuitive, reliable and scalable tool which allows time-dependent, ab-initio, simulations of the many-body Wigner equation. This paves the way towards ab-initio WMC simulations of strongly correlated quantum systems.

2. The many-body Wigner Monte Carlo method

The many-body Wigner formulation of quantum mechanics [11] describes a system of n interacting particles in terms of a quasi-distribution function $f_W = f_W(\mathbf{x}; \mathbf{p}; t)$, where $(\mathbf{x}; \mathbf{p}; t) = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n; \mathbf{p}_1, \mathbf{p}_2, \dots, \mathbf{p}_n; t)$, \mathbf{x}_i is the position and \mathbf{p}_i is the momentum of the i -th particle respectively ($i = 1, 2, \dots, n$). The pure state Wigner function is related to the solution of the many-body Schrödinger equation $\Psi = \Psi(\mathbf{x}; t)$ via the (invertible) Wigner–Weyl transform:

$$f_W(\mathbf{x}; \mathbf{p}; t) = \frac{1}{(\hbar\pi)^{d \cdot n}} \int d\mathbf{x}' e^{-\frac{i}{\hbar} \sum_{k=1}^n \mathbf{x}'_k \cdot \mathbf{p}_k} \times \Psi\left(\mathbf{x} + \frac{\mathbf{x}'}{2}; t\right) \Psi^*\left(\mathbf{x} - \frac{\mathbf{x}'}{2}; t\right), \quad (1)$$

where $d = 1, 2, 3$ is the dimensionality of space, and $\int d\mathbf{x}' = \int d\mathbf{x}'_1 \int d\mathbf{x}'_2 \dots \int d\mathbf{x}'_n$ ($\mathbf{x} \pm \frac{\mathbf{x}'}{2}$) = $(\mathbf{x}_1 \pm \frac{\mathbf{x}'_1}{2}, \mathbf{x}_2 \pm \frac{\mathbf{x}'_2}{2}, \dots, \mathbf{x}_n \pm \frac{\mathbf{x}'_n}{2}; t)$. Analogously, in the case of mixed states, a similar relation can be defined in terms of the many-body density matrix $\rho = \rho(\mathbf{x}; \mathbf{y}; t)$

$$f_W(\mathbf{x}; \mathbf{p}; t) = \frac{1}{(\hbar\pi)^{d \cdot n}} \int d\mathbf{x}' e^{-\frac{i}{\hbar} \sum_{k=1}^n \mathbf{x}'_k \cdot \mathbf{p}_k} \rho\left(\mathbf{x} + \frac{\mathbf{x}'}{2}; \mathbf{x} - \frac{\mathbf{x}'}{2}; t\right).$$

By applying the transform (1) to the many-body Schrödinger equation, one obtains the many-body Wigner equation:

$$\frac{\partial f_W}{\partial t}(\mathbf{x}; \mathbf{p}; t) + \sum_{k=1}^n \frac{\mathbf{p}_k}{m_k} \cdot \nabla_{\mathbf{x}_k} f_W = \int d\mathbf{p} f_W(\mathbf{x}; \mathbf{p}; t) V_W(\mathbf{x}; \mathbf{p}; t), \quad (2)$$

where $\int d\mathbf{p} = \int d\mathbf{p}_1 \int d\mathbf{p}_2 \dots \int d\mathbf{p}_n$, m_k is the mass of the k -th particle, and the function $V_W = V_W(\mathbf{x}; \mathbf{p}; t)$, known as the Wigner potential or kernel, is defined over the phase-space and reads:

$$V_W(\mathbf{x}; \mathbf{p}; t) = \frac{i}{\pi^{dn} \hbar^{dn+1}} \int d\mathbf{x}' e^{-\frac{2i}{\hbar} \sum_{k=1}^n \mathbf{x}'_k \cdot \mathbf{p}_k} \left[V\left(\mathbf{x} + \frac{\mathbf{x}'}{2}; t\right) - V\left(\mathbf{x} - \frac{\mathbf{x}'}{2}; t\right) \right].$$

The function $V = V(\mathbf{x}; t)$ is the potential acting over the particles, which in the general case may vary in time. For example, for a molecular many-body problem, in the Born–Oppenheimer approximation, it reads (in atomic units):

$$V(\mathbf{x}; t) = - \sum_{i,j=1}^N \frac{Z_j q^2}{|\mathbf{x}_i - \mathbf{x}_j|} + \frac{1}{2} \sum_{i \neq j}^N \frac{q^2}{|\mathbf{x}_i - \mathbf{x}_j|} - U(\mathbf{x}; t),$$

where the first term represents the superposition of Coulombic potentials due to the nuclei (which atomic number is Z_j for the j -th nucleus), the second term is the Hartree potential (i.e. the electron–electron interactions) and the last term is an eventual external potential (e.g. a potential barrier, an applied electric field, etc.).

In this context, our objective consists of solving equation (2) in a specified domain along with given initial and boundary conditions. This, of course, represents an incredible mathematical and numerical challenge. In order to achieve such a goal, we proceed to the generalization of the WMC method depicted in [24] to its many-body counterpart.

As a first step, we reformulate the many-body Wigner equation in a semi-discrete phase-space with a continuous spatial variable \mathbf{x} and a discretized momentum space \mathbf{p} described in terms of a *quantum* $\Delta \mathbf{p} = \frac{\hbar \pi}{L_C}$ (L_C specifies the mesh for the momentum discretization and has the units of a length). The many-body Wigner equation now reads:

$$\frac{\partial f_W}{\partial t}(\mathbf{x}; \mathbf{M}; t) + \sum_{k=1}^n \frac{\mathbf{M}_k \Delta \mathbf{p}}{m_k} \cdot \nabla_{\mathbf{x}_k} f_W = \sum_{\mathbf{M}=-\infty}^{+\infty} f_W(\mathbf{x}; \mathbf{M}; t) V_W(\mathbf{x}; \mathbf{M}; t), \tag{3}$$

with $\mathbf{M} = (\mathbf{M}_1, \mathbf{M}_2, \dots, \mathbf{M}_n)$, $\sum_{\mathbf{M}=-\infty}^{+\infty} = \sum_{\mathbf{M}_1=-\infty}^{+\infty} \sum_{\mathbf{M}_2=-\infty}^{+\infty} \dots \sum_{\mathbf{M}_n=-\infty}^{+\infty}$, and

$$V_W(\mathbf{x}; \mathbf{M}; t) = \frac{i}{\pi^{dn} \hbar^{dn+1}} \int d\mathbf{x}' e^{-\frac{2i}{\hbar} \sum_{k=1}^n \mathbf{x}'_k \cdot \mathbf{M}_k \Delta \mathbf{p}} \left[V\left(\mathbf{x} + \frac{\mathbf{x}'}{2}; t\right) - V\left(\mathbf{x} - \frac{\mathbf{x}'}{2}; t\right) \right].$$

Note that, now, the momentum of the i -th particle is expressed as a set of d integers $\mathbf{M}_i = (M_1^i, \dots, M_d^i)$ and $\mathbf{M}_i \Delta \mathbf{p} = (M_1^i \Delta p_1, \dots, M_d^i \Delta p_d)$ where $\Delta \mathbf{p} = (\Delta p_1, \dots, \Delta p_d)$.

We can now rewrite Eq. (3) in an integral form. To this purpose, we define the following function γ :

$$\gamma(\mathbf{x}) = \sum_{\mathbf{M}=-\infty}^{\infty} V_W^+(\mathbf{x}; \mathbf{M}), \tag{4}$$

where V_W^+ is the positive part of V_W , i.e. it takes the values of V_W if $V_W > 0$ and 0 otherwise. Thus, Eq. (3) can be rewritten by adding and subtracting the term $\gamma(\mathbf{x})$.

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

$$\Gamma(\mathbf{x}; \mathbf{M}; \mathbf{M}') = V_W^+(\mathbf{x}; \mathbf{M} - \mathbf{M}') - V_W^+(\mathbf{x}; -(\mathbf{M} - \mathbf{M}')) + \gamma(\mathbf{x}) \delta_{\mathbf{M}, \mathbf{M}'}. \tag{5}$$

We also assume that the evolution of an initial condition $f_i(\mathbf{x}; \mathbf{M})$ starts at time 0. By following the method in [24], it is possible to rewrite the semi-discrete many-body Wigner equation in the form of a Fredholm integral equation of second kind:

$$f_W(\mathbf{x}; \mathbf{M}; t) - e^{-\int_0^t \gamma(\mathbf{x}(y)) dy} f_i(\mathbf{x}(0); \mathbf{M}) = \int_0^t dt' \sum_{\mathbf{M}'=-\infty}^{+\infty} \int d\mathbf{x}' f_W(\mathbf{x}'; \mathbf{M}'; t') \Gamma(\mathbf{x}'; \mathbf{M}; \mathbf{M}') e^{-\int_{t'}^t \gamma(\mathbf{x}(y)) dy} \theta(t - t') \delta(\mathbf{x}' - \mathbf{x}(t')) \theta_D(\mathbf{x}'). \tag{6}$$

In order to ensure the explicit appearance of the variables $\mathbf{Q} = (\mathbf{x}; \mathbf{M}; t)$ and $\mathbf{Q}' = (\mathbf{x}'; \mathbf{M}'; t')$, the kernel has been augmented by the θ and δ functions exactly as in [24]. Following the generalization of the signed particle MC method, one can express the many-body expectation value of the physical quantity $A = A(\mathbf{Q})$ at a moment τ as:

$$\langle A \rangle(\tau) = \int dt \int d\mathbf{x} \sum_{\mathbf{M}=-\infty}^{\infty} f_W(\mathbf{x}; \mathbf{M}; t) A(\mathbf{x}; \mathbf{M}) \delta(t - \tau) = \int d\mathbf{Q} f_W(\mathbf{Q}) A_\tau(\mathbf{Q}). \tag{7}$$

One can realize that, formally speaking, the equations so far recovered are in the very same shape as the ones obtained in the single-particle WMC method. This suggests that it is possible to follow exactly the same procedure described [24] and express the expectation value (7) as a Liouville–Neumann series to depict a signed particle MC method for the many-body Wigner.

Indeed, it is straightforward to show that the zeroth order term of the series reads:

$$\langle A \rangle_0(\tau) = \int_0^\infty dt' \int d\mathbf{x} \sum_{\mathbf{M}'=-\infty}^{\infty} f_i(\mathbf{x}; \mathbf{M}') e^{-\int_0^{t'} \gamma(\mathbf{x}(y)) dy} A(\mathbf{x}(t'), \mathbf{M}') \delta(t' - \tau),$$

and the mathematical Monte Carlo theory for solving integrals suggests us to consider part of the integrand as a product of conditional probabilities (MC multi-dimensional integration). If f_i is normalized to unity, one generates random points $(\mathbf{x}; \mathbf{M}')$ at the initial time 0. These initialize the particle trajectories $\mathbf{x}(y)$ and the exponent gives the probability for the particle to remain over the trajectory provided that the out-of-trajectory event rate is γ . This probability filters out these particles, such that the randomly generated out-of-trajectory time is less than τ . If the particle remains in the same trajectory till time τ , it has a contribution to $\langle A \rangle_0(\tau)$ equal to $f_i(\mathbf{x}, \mathbf{M}')A(\mathbf{x}(\tau), \mathbf{M}')$, otherwise it does not contribute at all. Thus, $\langle A \rangle_0(\tau)$ is estimated by the mean value obtained from the N initialized particles.

In the same way, one can show that the first order term of the many-body Liouville–Neumann series reads:

$$\begin{aligned} \langle A \rangle_1(\tau) = & \int_0^\infty dt' \int d\mathbf{x} \sum_{\mathbf{M}'=-\infty}^\infty f_i(\mathbf{x}, \mathbf{M}') \{ \gamma(\mathbf{x}(t')) e^{-\int_0^{t'} \gamma(\mathbf{x}(y)) dy} \} \\ & \times \theta_D(\mathbf{x}') \int_{t'}^\infty dt \sum_{\mathbf{M}=-\infty}^\infty \left\{ \frac{\Gamma(\mathbf{x}'; \mathbf{M}; \mathbf{M}')}{\gamma(\mathbf{x}(t'))} \right\} \{ e^{-\int_{t'}^t \gamma(\mathbf{x}'(y)) dy} \} A(\mathbf{x}'(t); \mathbf{M}; t) \delta(t - \tau), \end{aligned}$$

and, again, a physical interpretation can be given. Now, a particle is initialized at $(\mathbf{x}, \mathbf{M}', 0)$ which follows the trajectory until time t' given by the probability density in the first curly brackets. Then, the particle phase-space position is $\mathbf{x}' = (\mathbf{x}(t'); \mathbf{M}'; t')$ and the evolution continues if the particle is still in the simulation domain (otherwise the contribution is zero). A similar interpretation can be given to the term in the next curly bracket which brings the particle from \mathbf{M}' to \mathbf{M} (locally in space at the time t'). Thus, at moment t' the particle initializes the trajectory $(\mathbf{x}'; \mathbf{M})$ and, with the probability given by the exponent in the last curly brackets, remains over the trajectory until time τ .

The first three terms of the Liouville–Neumann series show how to continue with higher order terms [24]. Indeed, one observes that the expansion of $\langle A \rangle$ actually branches, and the total value is given by the sum of all branches. We can, thus, equivalently talk in terms of three appearing particles even for the many-body WMC method (note that by particle we mean simply a mathematical point defined in a nd -dimensional phase-space), in other words:

$$\frac{\Gamma(\mathbf{x}; \mathbf{M}; \mathbf{M}')}{\gamma(\mathbf{x})} = \left\{ \frac{V_W^+(\mathbf{x}, \mathbf{M} - \mathbf{M}')}{\gamma(\mathbf{x})} \right\} - \left\{ \frac{V_W^-(\mathbf{x}, \mathbf{M} - \mathbf{M}')}{\gamma(\mathbf{M})} \right\} + \{\delta_{\mathbf{M}, \mathbf{M}'}\}. \quad (8)$$

According to the last term, the initial parent particle survives and a couple of new signed particles are generated with the first two probabilities. In other words, we generate the first many-body momentum state $\mathbf{M} - \mathbf{M}' = \mathbf{L}$ with probability:

$$\frac{V_W^+(\mathbf{x}, \mathbf{L})}{\gamma(\mathbf{x})},$$

and, with the same probability, we generate another value, say \mathbf{L}' , for the second state $\mathbf{M}' - \mathbf{M} = \mathbf{L}'$ exactly as it happens for the single-particle MC method [24]. In the same way, by exploiting the term $\Gamma(\mathbf{x}; \mathbf{M}; \mathbf{M}')$, it is possible to depict a MC algorithm for the integration of the many-body semi-discrete Wigner equation (3). After any free flight the initial particle creates two new particles with opposite signs and momentum offset (around the initial momentum) equal to $+\mathbf{L}$ and $-\mathbf{L}$ with $\mathbf{L} = \mathbf{M} - \mathbf{M}'$. The initial particle and the created couple represent three contributive terms to the many-body Liouville–Neumann series.

One should note that our proposed method is a MC method which implies high scalability of the algorithm. In particular, in our method, the scalability does not depend on the number of particles involved in the many-body problem. Indeed, at every time step, the solution is constructed by an ensemble of field-less Newtonian particles which are independent from each other. This represents an important advantage especially for complex and realistic systems where the number of involved bodies can be quite relevant.

3. Numerical validation

In order to validate our proposed signed particle MC method for the many-body Wigner equation, we perform numerical experiments involving several instances of a two-body system. This is a relatively simple and reasonable system from which to start. All experiments happen in a four-dimensional phase-space (x_1, x_2, p_1, p_2) and, consequently, every particle is represented by a four-dimensional set of coordinates. In the first experiment we simulate a two-body problem consisting of two independent Gaussian wave packets moving in the same direction with the same group velocity (see Fig. 1). This is an important benchmark problem since we know that, in this situation, the solution consists of two independent waves moving at the same pace. The second experiment consists of the same initial conditions but, this time, a potential barrier in the middle of the spatial domain is introduced (see Fig. 2). In this case, one expects that, if the two packets are independent and, while the first packet interacts with the potential barrier, the second one does not feel it at all. Finally, in the last experiment we study the dynamics of a two-body Wigner function corresponding to two strongly correlated (entangled) wave packets. Mathematically speaking, the correlation between the two packets is introduced by an initial quasi-distribution function which cannot be expressed in terms of product of two independent wave packets. This situation can be handled

only by a full many-body approach such as the one introduced in this work. Indeed it is well known that it would be impossible to simulate correctly such a system by a method based on approximations such as the ones introduced in the density functional theory [25].

The two-body model. For the sake of clarity, we report below the corresponding one-dimensional two-body Wigner equation used in all numerical experiments:

$$\begin{aligned} & \frac{\partial f_W}{\partial t}(x_1, x_2; p_1, p_2; t) + \frac{p_1}{m} \frac{\partial f_W}{\partial x_1} + \frac{p_2}{m} \frac{\partial f_W}{\partial x_2} \\ & = \int dp'_1 \int dp'_2 f_W(x_1, x_2; p_1 + p'_1, p_2 + p'_2; t) V_W(x_1, x_2; p'_1, p'_2), \end{aligned} \quad (9)$$

where m is the mass of a free electron and

$$\begin{aligned} V_W(x_1, x_2; p_1, p_2) &= \frac{i}{\pi^2 \hbar^3} \int dx'_1 \int dx'_2 e^{-\frac{2i}{\hbar}(x'_1 p_1 + x'_2 p_2)} \\ & \times [V(x_1 + x'_1, x_2 + x'_2) - V(x_1 - x'_1, x_2 - x'_2)]. \end{aligned}$$

In the first two experiments, we assume that the two electrons are initially in independent states. This allows us to start from an initial Wigner quasi-distribution function expressed in terms of the product of two Gaussian states:

$$f_W^0(x_1, x_2; p_1, p_2) = N e^{-\frac{(x_1 - x_1^0)^2}{\sigma^2}} e^{-\frac{(x_2 - x_2^0)^2}{\sigma^2}} e^{-(p_1 - p_1^0)^2 \sigma^2} e^{-(p_2 - p_2^0)^2 \sigma^2}, \quad (10)$$

where N is a normalization constant, x_1^0 and x_2^0 are the spatial center of the first and second wave-packet respectively, p_1^0 and p_2^0 are the momentum center of the first and second wave-packet respectively, and σ is the spread of both packets.

In the last experiment, we simulate two strongly entangled electrons which initial conditions read:

$$\begin{aligned} f_W^0(x_1, x_2; p_1, p_2) &= N_1 e^{-\frac{(x_1 - x_1^0)^2}{\sigma^2}} e^{-(p_1 - p_1^0)^2 \sigma^2} \\ & + N_2 e^{-\frac{(x_2 - x_2^0)^2}{\sigma^2}} e^{-(p_2 - p_2^0)^2 \sigma^2} \\ & + N_{12} e^{-(x_1 - x_1^0)^2 \sigma_e^2} e^{-(x_2 - x_2^0)^2 \sigma_e^2} \\ & \times e^{-\frac{|p_1 - p_1^0|}{2\sigma_e}} e^{-\frac{|x_2 - x_2^0|}{2\sigma_e}} \\ & \times 2 \sin\left(\frac{p_1 - p_1^0}{\sigma_e}\right) \\ & \times 2 \sin\left(\frac{p_2 - p_2^0}{\sigma_e}\right), \end{aligned} \quad (11)$$

where N_1 , N_2 and N_{12} are normalization constants and x_1^0 , x_2^0 , p_1^0 , p_2^0 have the same meaning as above.

Finally, the total electron probability density $n(x, t)$ is calculated as follows:

$$n(x, t) = \int dp [f_W^1(x, p, t) + f_W^2(x, p, t)], \quad (12)$$

where $f_W^1(x, p, t) = \int dx_2 \int dp_2 f_W(x, x_2; p, p_2; t)$ and $f_W^2(x, p, t) = \int dx_1 \int dp_1 f_W(x_1, x; p_1, p; t)$.

Two-body free wave-packet. In this experiment, the initial conditions (10) are imposed to the two-body Wigner equation (9), with $p_1^0 = p_2^0 = \Delta p = 6\frac{\hbar p}{L_C}$, $L_C = 50$ nm, $\sigma = 10$ nm, and no external potential is included. This is an important benchmark since, in this case, the solution is known to behave as two independent spreading Gaussian wave-packets moving in the same direction with the same group velocity. The results obtained by applying the many-body Wigner MC method are shown in Fig. 1 for times equal to 0 fs, 10 fs, 20 fs, 30 fs and 40 fs, respectively. In this case, the MC method provides smooth solutions as expected by an optimal MC method [14] and the computed solution is correct.

Two-body wave-packet in external field. The aim of this numerical experiment is to analyze the dynamics of two initially independent wave-packets interacting with an external potential. The initial conditions are the same as in the previous experiment (10) and a potential barrier with energy 0.3 eV and thickness 6 nm is placed in the center of the spatial domain. The results are shown in Fig. 2 and the corresponding function $\gamma = \gamma(x_1, x_2)$ is shown in Fig. 3. The function $g_W(x; p) = \int dx_2 \int dp_2 f_W(x, x_2, p, p_2) + \int dx_1 \int dp_1 f_W(x_1, x, p_1, p)$ at 20 fs is shown in Fig. 5. It is interesting to compare this figure with Fig. 4. Indeed, this time one expects the left wave-packet colliding with (and eventually tunneling through) the potential barrier, while the right wave-packet simply evolves as an independent Gaussian wave packet.

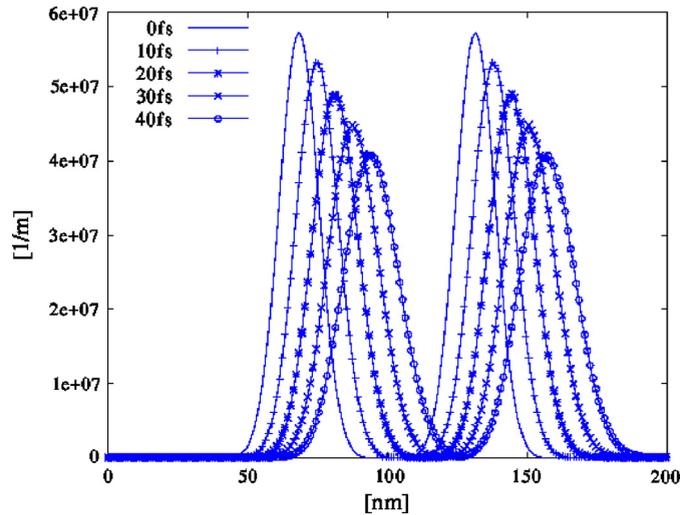


Fig. 1. Two-body time-dependent probability density in function of time. The continuous, "+", "*", "x" and "o" curves correspond to 0 fs, 10 fs, 20 fs, 30 fs and 40 fs respectively.

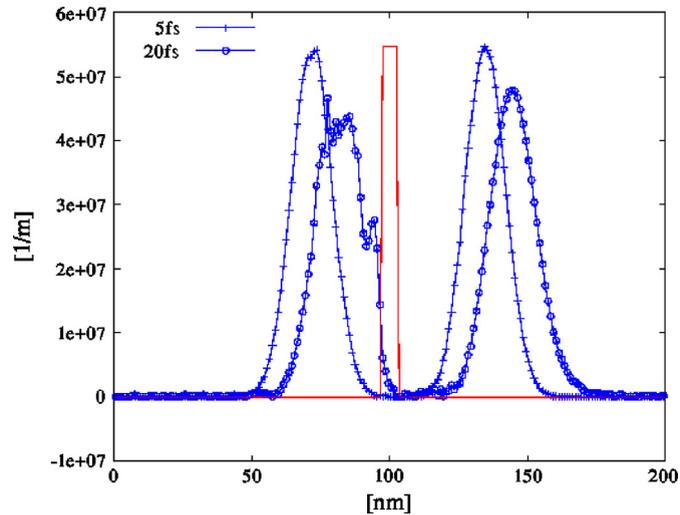


Fig. 2. Two-body time-dependent probability density in function of time, in the presence of a potential barrier at 5 fs and 20 fs respectively.

Two-body entangled wave-packet. We conclude this section by simulating an entangled system consisting of a two-body wave-packet which cannot be expressed by a product of two independent wave-packets (11). It is a well-known fact that such entangled systems can be simulated correctly only by a full many-body approach. Indeed the density functional theory, while being very successful for non-strongly correlated system, completely fails to describe entangled systems. The aim of this experiment is to show that our many-body WMC method based on signed particles can handle naturally such kind of system. The results are shown in Fig. 6, Fig. 7, and Fig. 8 for times equal to 0 fs, 20 fs and 40 fs respectively. These figures give a pretty clear insight on how two entangled wave packets evolve in time. In Fig. 6 the initial conditions are reported. One clearly sees the two packets along with their entanglement (between the two packets). Fig. 7 and Fig. 8 show how the system evolves in time. On one hand, the packets behave in phase-space as two Gaussians spreading in space and momenta. On the other hand, the entanglement evolves along with these packets accordingly keeping them correlated.

4. Software and hardware

The results presented in this section have been obtained using the HPC cluster installed at the Institute of Information and Communication Technologies (IICT) 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 @ 2.8 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

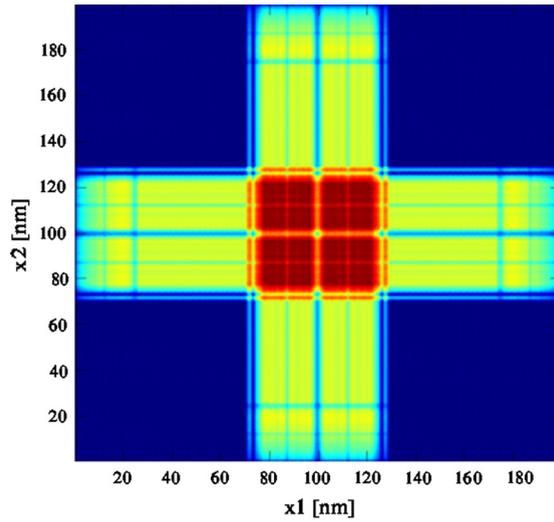


Fig. 3. Plot of the function $\gamma = \gamma(x_1, x_2)$ at 0 fs for a two-body wave packet interacting with an external potential barrier (see Fig. 2).

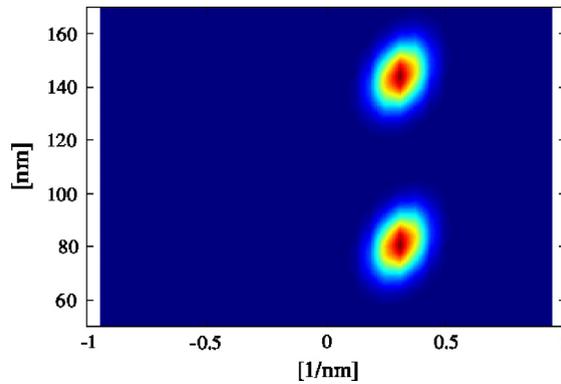


Fig. 4. Plot of the function $\int dx_2 \int dp_2 f_W(x_1, x_2, p_1, p_2) + \int dx_1 \int dp_1 f_W(x_1, x_2, p_1, p_2)$ at 20 fs for a free two-body wave-packet.

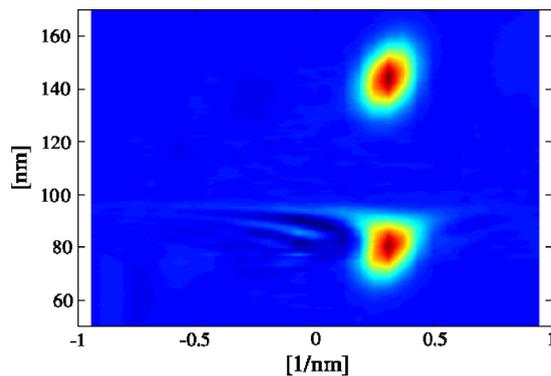


Fig. 5. Plot of the function $\int dx_2 \int dp_2 f_W(x_1, x_2, p_1, p_2) + \int dx_1 \int dp_1 f_W(x_1, x_2, p_1, p_2)$ at 20 fs for a two-body wave-packet interacting with a potential barrier.

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 [26]. 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 develop a full quantum simulator. The code is entirely developed

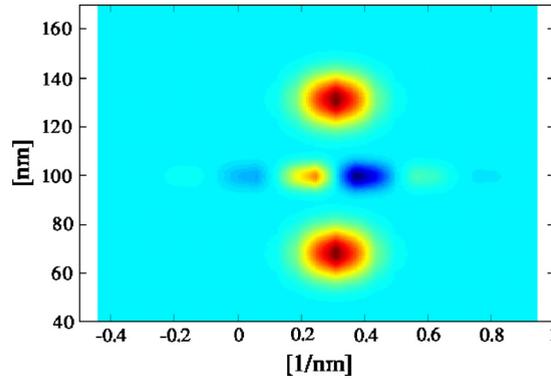


Fig. 6. Initial configuration of the function $\int dx_2 \int dp_2 f_W(x_1, x_2, p_1, p_2) + \int dx_1 \int dp_1 f_W(x_1, x_2, p_1, p_2)$ for two entangled wave-packets.

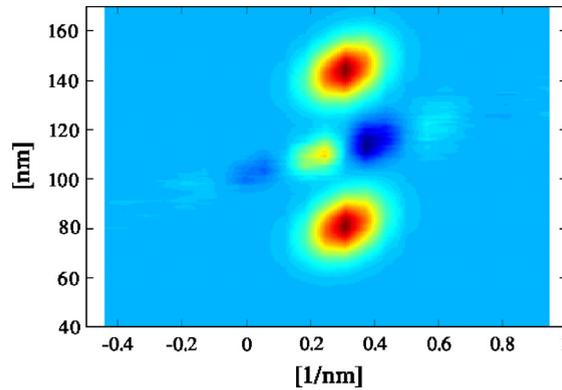


Fig. 7. Plot of the function $\int dx_2 \int dp_2 f_W(x_1, x_2, p_1, p_2) + \int dx_1 \int dp_1 f_W(x_1, x_2, p_1, p_2)$ corresponding to two entangled wave-packets at 20 fs.

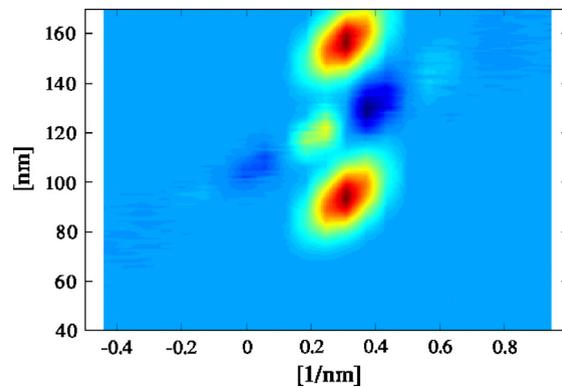


Fig. 8. Plot of the function $\int dx_2 \int dp_2 f_W(x_1, x_2, p_1, p_2) + \int dx_1 \int dp_1 f_W(x_1, x_2, p_1, p_2)$ corresponding to two entangled wave-packets at 40 fs.

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 (see [27]).

5. Conclusions

In this work we presented a Monte Carlo method for the time-dependent many-body quantum problem restricted to distinguishable particles in the absence of spin-dependent effects. It is based on the resolution of the many-body Wigner equation (2), which is a generalization of the Monte Carlo method for the single-particle Wigner equation presented in [24]. The many-body Wigner model is equivalent to the many-body Schrödinger equation. Indeed, an invertible Wigner–Weyl transform (1) is available to go from one formalism to another. However the Wigner approach to quantum mechanics has a first important advantage: the problem is described by an intuitive quasi-distribution function $f_W = f_W(\mathbf{x}_1, \dots, \mathbf{x}_n; \mathbf{p}_1, \dots, \mathbf{p}_n; t)$, with n being the number of particles. Furthermore, our proposed numerical method is based on the iterative Monte Carlo

method which represents a second important advantage: it scales very well on parallel machines [13,14] and scalability does not depend on the number of bodies involved. It is well-known that, in terms of scalability, Monte Carlo based methods often outperform numerical approaches based on finite differences or finite elements. This allows time-dependent ab-initio simulation of strongly correlated particles.

In order to validate the proposed approach, we performed three different numerical experiments. The first experiment is a benchmark test involving independent traveling Gaussian wave-packets. The results presented in Fig. 1 and Fig. 4 show clearly that our many-body Monte Carlo gives the correct solution. Indeed, the total probability density depicts two spreading and moving waves as expected. The second experiment involves the same kind of initial conditions but, this time, an external field consisting of a potential barrier is introduced in the middle of the spatial domain (see Fig. 2). In this case, one expects the left wave-packet to interact with the barrier while the right one just to behave as a traveling Gaussian packet. The results reported in Fig. 2 and Fig. 5 show that our method provides the correct solution even in the presence of an external potential. Finally, we simulated a system consisting of two entangled particles. This kind of system can be correctly handled only by a genuine many-body approach. The results are shown in Fig. 6, Fig. 7, and Fig. 8, where the evolution of the system as a whole is reported at three different times. It is clear how the entanglement evolves along with the wave-packets.

The presented results show that our signed particle Monte Carlo method for the time-dependent simulation of many distinguishable quantum particles in the absence of spin-dependent effects is reliable and efficient. It represents a new TCAD (Technology Computer Aided Design) tool which can be used by physicists and chemists for time-dependent simulations of complex correlated quantum systems.

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