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On a full Monte Carlo approach to quantum mechanics

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HIGHLIGHTS

- We compute the Wigner kernel by means of stochastic approaches.
- We exploit Monte Carlo integration techniques based on importance sampling.
- The stochastically computed Wigner kernel is utilized in the context of signed particles for the time dependent simulation of quantum systems.
- Single- and Many-body quantum systems are simulated successfully.

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ABSTRACT

The Monte Carlo approach to numerical problems has shown to be remarkably efficient in performing very large computational tasks since it is an embarrassingly parallel technique. Additionally, Monte Carlo methods are well known to keep performance and accuracy with the increase of dimensionality of a given problem, a rather counterintuitive peculiarity not shared by any known deterministic method.

Motivated by these very peculiar and desirable computational features, in this work we depict a full Monte Carlo approach to the problem of simulating single- and many-body quantum systems by means of signed particles. In particular we introduce a stochastic technique, based on the strategy known as importance sampling, for the computation of the Wigner kernel which, so far, has represented the main bottleneck of this method (it is equivalent to the calculation of a multi-dimensional integral, a problem in which complexity is known to grow exponentially with the dimensions of the problem). The introduction of this stochastic technique for the kernel is twofold: firstly it reduces the complexity of a quantum many-body simulation from non-linear to linear, secondly it introduces an embarassingly parallel approach to this very demanding problem.

To conclude, we perform concise but indicative numerical experiments which clearly illustrate how a full Monte Carlo approach to many-body quantum systems is not only possible but also advantageous. This paves the way towards practical time-dependent, first-principle simulations of relatively large quantum systems by means of affordable computational resources.

1. Introduction

In his 1777 pioneering essay known as *L'aiguille de Buffon* (Buffon's needle) [1], the french mathematician Georges-Louis Leclerc comte de Buffon poses, for the first time, the following problem: *supposing one drops a needle onto a floor made of*

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parallel and uniform strips of wood, what is the probability that the needle lies across a line between two strips? He demonstrated that the solution is equal to $\frac{2l}{\pi t}$, where l is the length of the needle and t is the distance between each strip. As pointed out later on by the Marquis Pierre-Simon de Laplace (1886), this approach can be utilized as a practical method to compute the value of the number π. In fact, by repeatedly throwing a needle onto a lined sheet of paper, and by counting the number of intersected lines, one can eventually estimate the value of π, a perfect instance of a Monte Carlo method. Afterwards, in 1949, with the advent of computational resources, intensive applications started to be developed in the Manhattan project by J. von Neumann, E. Fermi, G. Kahn and S.M. Ulam [2]. The legend says that the name *Monte Carlo* was eventually suggested by N. Metropolis in honor of Ulam's uncle who was a well-known gambler.

Nowadays in computational mathematics, by *Monte Carlo* or *stochastic* methods one intends a broad class of methods which approximate the solution of a given problem by performing random sampling of a certain random variable in which mathematical expectation coincides with a desired functional of the solution [3]. With the increase of available computational resources, this very particular approach to applied problems has eventually turned out to be very fruitful, representing one the most powerful numerical tool in applied mathematics, physics, chemistry and engineering, especially when deterministic methods hopelessly break down. In fact, unlike their deterministic counterpart, Monte Carlo methods do not require any additional regularity of the solution and it is always possible to control their accuracy in terms of the probability error. Furthermore, another important advantage consists in very high efficiency when dealing with very and extremely large computational problems such as, for instance, multi-dimensional numerical integration, the resolution of very large linear systems, the simulation of partial integro-differential equations in highly dimensional spaces, etc. Last but not least, Monte Carlo methods are embarassingly efficient on parallel machines (embarassingly parallel methods). In consequence, these methods have rapidly found a wide range of applications in an extensive class of scientific and technological disciplines. Nowadays, Monte Carlo algorithms exist for a plethora of different computational problems (in both contexts of simulations and numerical solvers) and it is practically impossible to specify a complete list. Of course, this does not mean that Monte Carlo methods always outperform their deterministic counterparts. In fact there are situations where, for instance, a finite difference method can provide a better solution than a stochastic method. This happens for example when a subspace of rare events in the space of solutions cannot be probed with sufficient accuracy by a Monte Carlo approach. In any case, in this paper we focus on the use of stochastic methods in order to understand what advantages they can provide in a very particular situation (described below).

One of the most significant and computationally demanding problem in applied physics is represented by the simulation of many-body quantum systems approached by first principles only [4], a somehow elusive and daunting task and, yet, of paramount importance for our comprehension of the way Nature works along with the (consequent) development of new technologies. Many methods certainly exist, based on the many different approximations introduced. For instance among the simplest ones, the Hartree–Fock or self-consistent field method [5,6] is based on expressing the many-body wave-function for Fermions in terms of Slater determinants [7]. More sophisticated approaches, known as post-Hartree–Fock methods, have been developed as well among which one has, e.g., the configuration interaction method [8], the Møller–Plesset method [9], various variants of quantum Monte Carlo methods [10–12], etc. In particular, the reader should note that, although different formulations of quantum mechanics are available nowadays [13–15], all mentioned methods rely on the ability of computing *wave-functions* in the Schrödinger formalism [16]. Recently, a new formulation of quantum mechanics has been suggested which is based on the concept of signed particles [17]. This novel theoretical framework describes time-dependent quantum systems by means of ensembles of field-less point-like particles provided with a position, a momentum and a *sign*. This is not the first time that classical particles augmented with some *quantum* variable are utilized to approach quantum systems (see Ref. [18]). For instance, there is a long history in the development of techniques to solve the Wigner equation which are based on the concept of *particle quantum affinity* [19–23] (inspired by the pioneering works [24,25]), a real valued variable in the range $(-\infty, 1]$.

It has been shown that the signed particle formulation, when restricted to a finite and semi-discrete phase-space, coincides with the signed particle Wigner Monte Carlo method [26], a numerical approach which lately has been extensively validated in the case of both single- and many-body problems, therefore proving to be a very promising tool [27–29]. This formulation is based on a set of three postulates which completely defines the evolution of a quantum system. These rules dictate how an ensemble of particles evolves, one particle at a time. The advantages of such an approach have been thoroughly discussed previously (see, for example, Refs. [17,26]) and mainly consist of (1) being intuitive and, therefore, easy to implement, and (2) embarassingly parallelizable as signed particles are independent from each other. The only bottleneck is, thus, represented by the numerical computation of the Wigner kernel which, in essence, coincides with the integration of a multi-dimensional integral. Usually, the kernel can be calculated analytically only in a few (oversimplified) cases and one must resort to numerical techniques.

In this paper, we focus on the problem of *numerically* computing the (highly multi-dimensional) Wigner kernel. Although, so far, this problem has been successfully approached by means of deterministic methods (e.g. see Ref. [30]), the authors firmly believe that stochastic techniques can be applied. Therefore, we introduce the usage of an *importance sampling technique* [31] to compute the Wigner kernel in the context of signed particles and show how this introduces crucial advantages, especially in terms of efficiency and complexity. Indeed, it is well known that a *crude Monte Carlo method* has already a rate of convergence which does not depend on the dimensions of a given integral, therefore making the Monte Carlo approach to multi-dimensional integration the only practical method for the treatment of the Wigner kernel, especially when a substantial number of bodies is involved in the simulation of a given quantum system [3]. It is certainly possible