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A cellular automaton for the signed particle formulation of quantum mechanics

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HIGHLIGHTS

- This paper discusses about the possibility of reformulating quantum mechanics, in particular the signed particle formulation, in terms of cellular automata.
- In more details, we present one instance of a cellular automaton which can reproduce (up to a certain accuracy) the simulation of quantum systems.

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ABSTRACT

Recently, a new formulation of quantum mechanics, based on the concept of signed particles, has been suggested. In this paper, we introduce a cellular automaton which mimics the dynamics of quantum objects in the phase-space in a time-dependent fashion. This is twofold: it provides a simplified and accessible language to non-physicists who wants to simulate quantum mechanical systems, at the same time it enables a different way to explore the laws of Physics. Moreover, it opens the way towards hybrid simulations of quantum systems by combining full quantum models with cellular automata when the former fail. In order to show the validity of the suggested cellular automaton and its combination with the signed particle formalism, several numerical experiments are performed, showing very promising results. Being this article a preliminary study on quantum simulations in phase-space by means of cellular automata, some conclusions are drawn about the encouraging results obtained so far and the possible future developments.

1. Introduction

Inspired by the increasing availability of computational resources provided by the advent of modern electronics, in the 1950s several researchers started to suggest independently a series of precursor algorithms which, today, would be defined as *cellular automata* (in the following we use the acronym CA for both singular and plural cases). But the concept of CA truly emerged in a clearly defined and formal way only with the work of J. Von Neumann [1] and the contribution of S. Ulam (who suggested the use of a discrete space for the states of a CA).

Despite their apparent simplicity, the concept of CA constitutes a powerful model for the study of non-linear complex systems and has been applied to, for instance, the study of biological and artificial life systems [2], the simulation of the Navier–Stokes equation [3] and the creation of random number generators [4]. The simplicity, of course, is only illusory as CA can contain many rules with very complex outcomes. As a matter of fact, CA have been successfully implemented for the

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modelization of epidemics, cancer spreading, financial market and lattice gases [5–8]. The Reader should note that, albeit these exciting achievements, the question of whether a CA can simulate physical systems in an *exact* fashion still remains an open (and fascinating) problem [9,10].

Recently, a new formulation of quantum mechanics based on the concept of signed particles has been introduced [11]. This novel theory approaches the problem of simulating quantum systems time-dependently by utilizing ensembles of classical field-less particles. These point-like objects are provided with a position, a momentum, and a *sign*, and allow the simulation of complex quantum systems by means of relatively small computational resources. It has been shown that, when restricted to finite domains and semi-discrete phase-spaces, this formalism coincides with the signed particle Wigner Monte Carlo method [12], a numerical approach which has been extensively validated in the case of both single- and many-body problems (e.g. Refs. [13–16]), proving to be very promising.

In particular, the signed particle 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. In this work, we introduce a CA implementation of this novel formalism by transforming the three postulates into rules defining a new CA. This is threefold: first, it provides a relatively simple language for non-experts which, moreover, gives the opportunity to utilize all theoretical results already known for CA, second it might allow the study of the laws of Nature on a different (and most likely complementary) level [17], finally it offers a new numerical tool for the study of quantum systems.

Finally, the Reader should note that, although this is certainly not the first time that such an approach is proposed in the field of quantum mechanics (see for example the — incomplete — list of papers [18–29]), to the best of our knowledge it seems that these attempts are mainly based on the Schrödinger formalism defined in the space of normalized complex functions. The approach proposed in this paper, instead, exploits the definition of a discretized phase-space (in other words a grid of cells) on which a CA acts in order to evolve a given quantum system in time.

This article is organized as follows. In the next section we shortly introduce the three postulates of the signed particle formulation of quantum mechanics giving the physical picture provided by this novel formalism. We then convert these postulates into a set of rules which completely define a (stochastic) CA. Afterwards, we show the validity of the defined CA by performing numerical experiments which highlight the strengths and weaknesses of this new approach. Furthermore, we introduce a novel technique exploiting CA which extends the simulation capabilities of the signed particle formulation when the number of particles increases exponentially. Finally, we conclude with a discussion on the possible future developments in this direction.

2. The signed particle formulation and its cellular automaton

In this section, we start by introducing the complete set of postulates which defines the *signed particle formulation* of quantum mechanics [11] and shortly discuss the physical picture provided by this novel approach (for the interested Reader, a practical implementation is available [30]). We then proceed with the definition of a *cellular automaton* which can simulate time-dependent quantum systems by evolving its current state only. A simple classification is also provided which highlights some of its mathematical properties. The numerical experiments comparing the two approaches are presented and discussed in the next section.

2.1. Signed particle postulates

The signed particle formulation of quantum mechanics consists of the following set of postulates.

Postulate I. *Physical systems can be described by means of (virtual) Newtonian particles, i.e. provided with a position* $\mathbf{x}$ *and a momentum* $\mathbf{p}$ *simultaneously, which carry a sign which can be positive or negative.*

Postulate II. *A signed particle, evolving in a potential* $V = V(\mathbf{x})$*, behaves as a field-less classical point-particle which, during the time interval* $\mathrm{d}t$*, creates a new pair of signed particles with a probability* $\gamma(\mathbf{x}(t))\,\mathrm{d}t$ *where*

$$\gamma(\mathbf{x}) = \int_{-\infty}^{+\infty} \mathcal{D}\mathbf{p}' V_W^+(\mathbf{x};\mathbf{p}') \equiv \lim_{\Delta\mathbf{p}'\to 0^+} \sum_{\mathbf{M}=-\infty}^{+\infty} V_W^+(\mathbf{x};\mathbf{M}\Delta\mathbf{p}'), \tag{1}$$

and $V_W^+(\mathbf{x};\mathbf{p})$ *is the positive part of the quantity*

$$V_W(\mathbf{x};\mathbf{p}) = \frac{i}{\pi^d \hbar^{d+1}} \int_{-\infty}^{+\infty} \mathrm{d}\mathbf{x}'\, \mathrm{e}^{-\frac{2i}{\hbar}\mathbf{x}'\cdot\mathbf{p}} \left[V(\mathbf{x}+\mathbf{x}') - V(\mathbf{x}-\mathbf{x}')\right], \tag{2}$$

known as the Wigner kernel (in a d-dimensional space) [31]. If, at the moment of creation, the parent particle has sign s, position $\mathbf{x}$ *and momentum* $\mathbf{p}$*, the new particles are both located in* $\mathbf{x}$*, have signs* $+s$ *and* $-s$*, and momenta* $\mathbf{p}+\mathbf{p}'$ *and* $\mathbf{p}-\mathbf{p}'$ *respectively, with* $\mathbf{p}'$ *chosen randomly according to the (normalized) probability* $\frac{V_W^+(\mathbf{x};\mathbf{p})}{\gamma(\mathbf{x})}$.

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