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Combining neural networks and signed particles to simulate quantum systems more efficiently

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HIGHLIGHTS

- This work presents a new technique which drastically reduces the computational requirements to simulate time-dependent quantum systems.
- This new technique is based on the use of an appropriately tailored neural network combined with the signed particle formulation of quantum mechanics.
- The introduced neural network is able to compute efficiently and reliably the Wigner kernel without any training as its entire set of weights and biases is specified by analytical formulas.
- This work offers an alternative way to study the laws of Physics which might shed new light.

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ABSTRACT

Recently a new formulation of quantum mechanics has been suggested which describes systems by means of ensembles of classical particles provided with a sign. This novel approach mainly consists of two steps: the computation of the Wigner kernel, a multi-dimensional function describing the effects of the potential over the system, and the field-less evolution of the particles which eventually create new signed particles in the process. Although this method has proved to be extremely advantageous in terms of computational resources – as a matter of fact it is able to simulate in a time-dependent fashion many-body systems on relatively small machines – the Wigner kernel can represent the bottleneck of simulations of certain systems. Moreover, storing the kernel can be another issue as the amount of memory needed is cursed by the dimensionality of the system. In this work, we introduce a new technique which drastically reduces the computation time and memory requirement to simulate time-dependent quantum systems which is based on the use of an appropriately tailored neural network combined with the signed particle formalism. In particular, the suggested neural network is able to compute efficiently and reliably the Wigner kernel without any training as its entire set of weights and biases is specified by analytical formulas. As a consequence, the amount of memory for quantum simulations radically drops since the kernel does not need to be stored anymore as it is now computed by the neural network itself, only on the cells of the (discretized) phase-space which are occupied by particles. As its is clearly shown in the final part of this paper, not only this novel approach drastically reduces the computational time, it also remains accurate. The author believes this work opens the way towards effective design of quantum devices, with incredible practical implications.

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1. The need for efficient quantum TCAD

About a century ago, in order to understand a series of experiments involving small physical objects such as electrons, atoms and molecules, a peculiar theory was conceived, known today as *quantum mechanics*. This remarkable theoretical framework consists of a distinct set of rules which can (in a broad sense) explain and predict the observed features of what we call a *quantum system*. The implications of such theory are not only of philosophical importance, they also have a huge relevance in applied fields such as electronics and nanoelectronics. In fact, as today semiconductor devices have active lengths in the range of a few tens of nanometers, quantum effects are dominant and classically designed complementary metal–oxide–semiconductor (CMOS) transistors do not operate reliably any longer.

Presently, we are entering in the post-CMOS era. Although this might sound like the end of a very successful period for the semiconductor industry, one should also recognize the exciting opportunities the development of drastically different devices might bring [1,2]. In particular, we now expect that devices should not work *despite* the presence of quantum effects, but *because* of them, bringing new features barely conceivable just a decade ago. As an instance, a new class of silicon based devices exploiting single buried phosphorus atoms [3,4] has been suggested, and exciting experimental results have recently appeared [5], which could, one day, become practical implementations of *quantum computing* devices. While it is clear, from a theoretical perspective, that incredible speedup (to use a mild expression) could be achieved with these suggested quantum technologies, how to actually build scalable quantum devices and circuits is still an important open problem (for the sake of clarity, we hereafter refer to the *gate* paradigm of quantum computing).

Sadly, in spite of the plethora of drastically different experimental platforms suggested (exploiting photons, electrons, ionized atoms, etc.), what precise *scalable* architecture to make use of for practical purposes remains unclear and, thus, design capabilities to investigate various possible systems are *acutely desirable*. In practice, though, the theoretical comprehension of quantum particle dynamics in such experimental devices is still in its infancy since this new paradigm comes with incredible challenges. For meaningful simulations, a mathematical model should be time-dependent, fully quantum, capable of including lattice vibrations and, finally, able to deal with open leads (i.e. the presence of contacts).

Recently a new formulation of quantum mechanics based on the concept of particles with a sign has been suggested by the author of this work [6], which is known as the *signed particle formulation* (its numerical discretization is, instead, known as the *Wigner Monte Carlo method* [7]). Despite its recent appearance, this novel formalism has been thoroughly validated in both the single- and many-body cases, showing to be uncommonly advantageous in terms of computational resources. As a matter of facts, it has allowed the time-dependent simulation of quantum many-body systems on relatively small machines in both the density functional theory (DFT) and first-principle frameworks [8,9]. Even daunting situations such as systems of indistinguishable Fermions have been simulated without any particular computational necessity [10].

Very interestingly, being the signed particle formulation based on *classical* particles, the inclusion of elastic and inelastic scattering terms, e.g. coming from the vibrations of the lattice, is practically trivial. As a matter of fact, the author of this work has been able to easily extend this formalism to the presence of phonons (i.e. the quantization of the lattice vibrations) in a silicon substrate, clearly showing that this recent theory is capable of accurately tackling very complex situations [11]. As a practical instance, a *three-dimensional wave packet moving in a semiconductor substrate* in the presence of a Coulombic potential and various phonon scattering events has been successfully simulated (at different temperatures) and in the presence of both reflective and absorbing boundary conditions, a quite daunting task in other more standard approaches. More recently, the same approach has also been applied to the study of *resilience of entanglement in quantum systems* in the presence of environmental noise, showing to be a very promising candidate to the development of technology computer aided design (TCAD) software for the development of quantum computing devices [12]. To the best of the author knowledge, this is the only formulation of quantum mechanics which can tackle such problems by means of relatively affordable computational resources.

In spite of these successes, one issue still needs to be addressed though: the computation of the multi-dimensional function known as the *Wigner kernel*, a quantity which represents the effects of the potential over the signed particles and corresponding to the computation of a multi-dimensional integral, can be in some cases a critical point, especially in the presence of time-dependent potentials. In this particular situation, this numerical computation becomes not only time consuming but also memory demanding.

In recent times, Artificial Neural Networks (ANNs) have been applied to broader and broader sets of applications with immense success. For example, ANNs have been constantly improved and utilized to recognize individual objects in high-resolution photographs, as well as in speech recognition with impressive results. Spectacular outcomes have been reported in the field of pedestrian detection with superhuman performances. Constantly, ANNs have grown in complexity along with the problems they can solve. Generally speaking, ANNs have shown to excel in tasks where information is complex and voluminous, clearly showing to be a powerful tool. It is therefore not surprising to see a drastic raise of interest coming from the scientific community [13]. In particular, these impressive results achieved by ANNs have inspired the author to seek for neural networks which could ease the computation of the Wigner kernel.

Consequently, in this paper we depict an ANN capable of computing the multi-dimensional Wigner kernel for a given many-body quantum system described by its potential in the configuration space. The suggested ANN does not make any difference between time-dependent and time-independent potentials and can, thus, be applied to these two different situations without limitations. Moreover, a very interesting peculiarity of the network presented in this work consists of the fact that it does not require any training process. In practice, the weights and biases needed to define it are computed