

# The Signed Particle Formulation of Quantum Mechanics: A Parallelization Scheme

K.G. Kapanova\*, I.T. Dimov, J.M. Sellier

\*IICT, Bulgarian Academy of Sciences, Acad. G. Bonchev str. 25A, 1113 Sofia, Bulgaria,  
kapanova@parallel.bas.bg, kkapanova@gmail.com

**Keywords:** quantum mechanics, signed particles formulation, Wigner Monte Carlo, parallelization scheme

## 1 Introduction

Classical mechanics, introduced by I. Newton, improved by L. Euler and furthered by J.L. Lagrange and P.S. Laplace has been a serving as a powerful paradigm for the coherent description of phenomena. While the paradigm has been able to answer many questions about the world around us, it has failed to provide explanations of many experiments, performed in the last 100 years. Therefore, the field of quantum mechanics was developed in order to provide a sufficient way to explain phenomena. As with the classical mechanics, there are many formalisms in quantum as well. Currently, the standard quantum mechanics approach is the mathematical formulation provided by E. Schroedinger [1], although alternative formulations exists – like E. Wigner [2], R. Feynman [3], L.V. Keldysh [4], K. Husimi [5], D. Bohm [6], [7].

At the outset, one may say those models are radically different, but there are in fact mathematically and experimentally equivalent. Looked from the mathematical perspective – there is a transform between any two formulations, and experimentally, one could prove the predictions made by these theories are all exactly the same. Furthermore, due to the same set of predictions provided, one may consider them as complementary.

In 2015, a new formulation of quantum mechanics was proposed by one of the authors of this paper [8]. This formalism describes quantum objects in terms of classical particles by suggesting a new interpretation of the mathematical Wigner Monte Carlo method extended to infinite domains and non-discretized phase spaces [9] which is able to simulate the time-dependent single- and many-body Wigner equation [10], [11]. This formalism uses the

adfa, p. 1, 2011.

© Springer-Verlag Berlin Heidelberg 2011

method uses signed particles provided with a position and momentum, while preserving the Heisenberg principle of uncertainty. The dynamics of the system is expressed in terms of creation, evolution and annihilation of signed particles only.

The reader should note that when we restrict this formulation to final domain and to semi-discrete phase spaces, we obtain the well-known Wigner Monte Carlo method [13]. This formulation deals with single- as well as many-body cases and approaches problems in a time-dependent fashion from first principles of Physics.

In this paper we introduce a computationally convenient parallelization scheme based on the ensemble of particles which do not need any communication. In the next section we introduce the signed particle formulation of quantum mechanics while in the third section we provide the parallelization method we have employed for the task.

## 2 The signed particle formulation of Quantum Mechanics

In this section we introduce the three postulates of the signed particle formulation which we parallelize in this work.

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

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

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

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

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

known as the Wigner kernel (in a  $d$ -dimensional space) [2]. If, at the moment of creation, the parent particle has sign  $s$ , position  $x$  and momentum  $p$ , the new particles are both located in  $x$ , have signs  $+s$  and  $-s$ , and momenta  $p+p'$  and  $p-p'$  respectively, with  $p'$  chosen randomly according to the (normalized) probability  $\frac{V^+(x;p)}{\gamma(x)}$ .

**Postulate III.** Two particles with opposite sign and same phase-space coordinates  $(x, p)$  annihilate.

Firstly, we assign initial conditions to the system by means of an ensemble of signed particles and compute the gamma function. Then particles are evolved using formula (2) iteratively. For every particle in the ensemble, we compute free flight, create new signed particles pairs, equivalent to the recursive application of the operator  $\hat{S}$  defined in [8]. Finally we have an annihilation step, which is important in situations where the number of signed particles may increase indefinitely (although this is not always the case, e.g. the trivial situation in which the function gamma is identically zero).

### 3 Parallelization Scheme

Recently a parallelization scheme for the Wigner Monte Carlo method has been proposed in [12], which is based on the decomposition of the spatial domain. In this section we propose a computationally convenient alternative achieved through the following.

It is well known that virtual signed particles represent different configurations of the system in the phase space [13]. As such they are independent mathematical objects which are evolved by iteratively applying postulate II. Therefore this suggests that the original ensemble can be divided in subsets among CPUs and evolved without any communication.

Of course, one should remember that all environmental variables describing the potential involved in the simulation have to be copied on every CPU. In order to show the applicability and efficiency of the proposed algorithm we show in fig. 1 the parallel speedup and efficiency curve (the system consists of wave packet impinging on energetic barrier) [14].

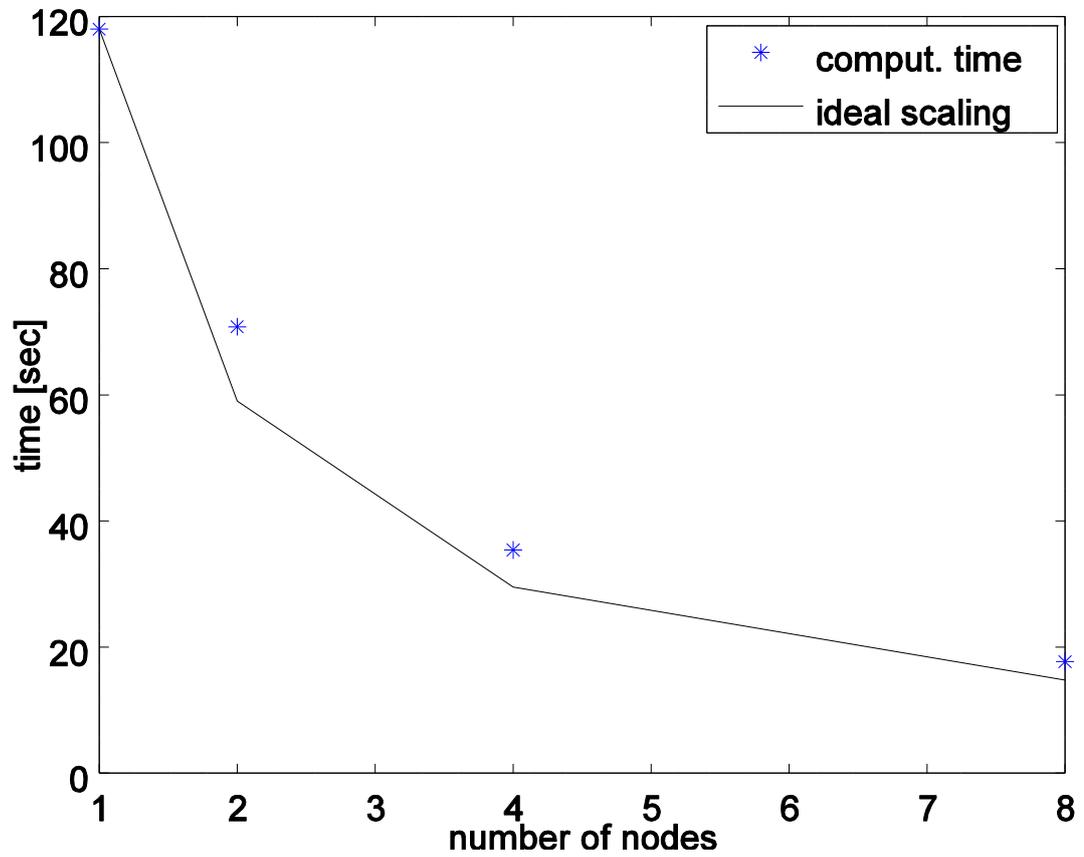


Fig. 1

#### 4 References

1. E. Schroedinger, Quantisierung als Eigenwertproblem, Annalen der Physik 385, (1926) 437-490.
2. E. Wigner, On the Quantum Correction for Thermodynamic Equilibrium, Phys. Rev. 40 (1932) 749.
3. R.P. Feynman, Space-Time Approach to Non-Relativistic Quantum Mechanics, Rev. of Mod. Phys. 20, (1948) 367.
4. L.V. Keldysh, Zh. Eksp. Teor. Fiz., Sov. Phys. JETP 20, (1965).
5. K. Husimi, Some Formal Properties of the Density Matrix, Nippon Sugaku-Buturigakkwai Kizi Dai 3 Ki, Vol. 22, No. 4. (1940), pp. 264-314.
6. D. Bohm, A Suggested Interpretation of the Quantum Theory in Terms of Hidden Variables. I, Phys. Rev. 85, 166 (1952).

7. D. Bohm, A Suggested Interpretation of the Quantum Theory in Terms of Hidden Variables. II, *Phys. Rev.* 85, 180 (1952).
8. Jean Michel Sellier, A signed particle formulation of non-relativistic quantum mechanics, *Journal of Computational Physics*, Volume 297, 15 September 2015, Pages 254-265, ISSN 0021-9991, <http://dx.doi.org/10.1016/j.jcp.2015.05.036>
9. J.M. Sellier, M. Nedjalkov, I. Dimov, S. Selberherr, A benchmark study of the Wigner Monte-Carlo method, *Monte Carlo Methods and Applications*, De Gruyter, DOI: 10.1515/mcma-2013-0018, (2014).
10. J.M. Sellier, I. Dimov, A Wigner Monte Carlo Approach to Density Functional Theory, *Journal of Computational Physics* 270, pp. 265-277 (2014).
11. J.M. Sellier, I. Dimov, The Many-body Wigner Monte Carlo Method for Time-dependent Ab-initio Quantum Simulations, *Journal of Computational Physics* 273, pp. 589-597 (2014).
12. Ellinghaus, J Weinbub, M Nedjalkov, S Selberher, and I. T. Dimov. Distributed-memory parallelization of the Wigner Monte Carlo method using spatial domain decomposition, *Journal of Computational Electronics*, Volume 13 (2014), pp. 1-12
13. J.M. Sellier, M. Nedjalkov, I. Dimov, An introduction to applied quantum mechanics in the Wigner Monte Carlo formalism, *Physics Reports*, Volume 577, 12 May 2015, Pages 1-34, ISSN 0370-1573, <http://dx.doi.org/10.1016/j.physrep.2015.03.001>.
14. Jean Michel Sellier, Mihail Nedjalkov, Ivan Dimov, Siegfried Selberherr, "A benchmark study of the Wigner Monte Carlo method", *Monte Carlo Methods Appl.*, De Gruyter, DOI 10.1515/mcma-2013-0018, (2014)