Quantum Mechanics and Signed Particles, A New Formulation Has Come into Existence

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Abstract

Quantum mechanics represents a puzzling problem since almost a century now. Indeed, in the standard approach utilized by mainstream scientists, systems are described by means of wave-functions, a still enigmatic concept. Recently a new and promising approach has been introduced which relies on the novel concept of signed particles. This novel formulation is built on an unusual interpretation of the Wigner equation, a relatively unfamiliar model equivalent to the standard approach. The new theory provides a singular physical picture in terms of particles interacting with external forces by means of creation of pairs of signed particles. The approach therefore reduces to statistical calculations over an ensemble of signed particles which allow intuitive, and computationally convenient, time-dependent simulations for both single- and many-body quantum problems. As a matter of fact, and despite its relatively recent appearance, this approach has already proven to be a very versatile and valuable tool in many different contexts touching the realms of Physics, Chemistry and Nanotechnologies. This article wants to be a short introduction to this exciting topic which comes with incredible promises for theoretical, applied Science and technology.

Introduction

Quantum mechanics was created to explain a series of experimental observations in the realm of elementary particles, atoms and molecules, which classical mechanics had no hope to explain. The physical evidences for baffling phenomena such as particle-wave duality and energy quantization were puzzling a whole community of scientists. In spite of these difficulties, eventually a successful set of rules was created, able to theoretically reproduce and predict the observed features of quantum systems. Shortly, this is how quantum mechanics was born.

This remarkable achievement was in great part made possible thanks to the application of an equation provided by E. Schrödinger, summarizing the description of quantum systems in terms of probability amplitudes or wave-functions, a revolutionary concept at that time and still an enigmatic concept today. A physical (and heuristic) interpretation to this equation was provided by M. Born, nowadays known as the standard or Copenhagen interpretation. This theory remains, to this day, the most utilized approach to the study and comprehension of quantum systems.

But this is a rather incomplete story. As a matter of fact, right after the birth of the Schrödinger equation, other formulations of quantum mechanics appeared which greatly helped in shedding light on aspects that were hardly understandable otherwise. Among these alternatives, the work of E. Wigner stands out, being an intuitive model which provides a direct connection between classical and quantum physics, due to its strong similarities with classical statistical mechanics, and describing systems in terms of (quasi) distribution functions, a concept experimentalists are quite familiar with [1], [2].

Based on a rather unconventional interpretation of the Wigner approach to quantum mechanics, a peculiar and promising new formulation involving *signed* particles has recently come into existence [2]. This novel theory provides a set of few rules which, applied recursively, allows time-dependent simulations of single- and many-body problems, considered to be one of the most computationally demanding problem in Physics. The theory offers significant advantages in terms of intuitiveness, computational implementation and parallelization. In fact, despite its relatively recent appearance, this approach has already proven to be a very versatile and valuable tool for scientists. It has already been utilized to explain, e.g., the appearance of quantum decoherence in silicon material, and the appearance of Fermi (or exchange-correlation) holes for indistinguishable electrons, two daunting problems in the standard approach. This paper introduces, from a simplified (but still accurate) perspective the signed particle formulation of quantum mechanics. These are exciting times for quantum mechanics, and the signed particle formulation promises to revolutionize, once again, our understanding of the quantum world.

The Signed Particle Formulation

The signed particle formulation consists of a set of three rules given below (which can be seen either as a physical interpretation of the Wigner equation or as a generalization of the Wigner Monte Carlo method to an infinite domain and non-discretized phase-space).

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

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

$$\gamma(\vec{x}) = \lim_{\Delta\vec{p}\to 0} \sum_{M=-\infty}^{+\infty} V_W^+(\vec{x}; M\Delta\vec{p})$$

and $V_W^+(\vec{x};\vec{p})$ is the positive part of the quantity known as the Wigner kernel. If, at the moment of creation, the parent particle has sign s, position $\vec{x}$ and momentum $\vec{p}$, the new particles are both located in $\vec{x}$, have signs $+s$ and $-s$, and momenta $\vec{p}+\vec{p}'$ and $\vec{p}-\vec{p}'$ respectively, with $\vec{p}'$ chosen randomly according to the (normalized) probability

$$\frac{V_W^+(\vec{x};\vec{p})}{\gamma(\vec{x})}.$$

This rule can be simplified by saying that a particle interacts with an external potential by simply creating a new pair of signed particles randomly (although the randomness is given by an explicit mathematical expression) at the same position of the parent particle.

Rule III. Two particles with opposite sign and same phase-space coordinates annihilate.

The physical picture offered by this set of rules is rather peculiar and different than any other mathematical formulation of quantum mechanics. Quantum systems are now described by means of ensembles of Newtonian field-less particles which now carry a sign and interact with an external potential by means of creation and annihilation events only. When a pair of particles is created, one is in an experimentally reachable state (positive sign), and the other in a non-reachable state (negative sign) [3]. This new view point is relatively easy to grasp and allows the inclusion of quite complex effects in a natural way when it is time to simulate quantum systems in a realistic context.

This rather atypical picture actually can recover typical quantum phenomena historically described by the standard approach. Let us now see a few examples.

The tunneling effect [2]. Tunneling is a typical quantum effect which cannot be explained in terms of classical mechanics. It represents one of the foundational experimental evidence for the need of a quantum theory. This experiment shows that material particles can tunnel through potential barriers, even though the initial particle energy is classically not sufficient. Fig. 1 shows that such experimental observation can be reproduced by the signed particle formulation.

Entangled particles [4]. It is a well-known fact that two entangled particles can be simulated correctly only by a full many-body approach. Indeed, methods such as the density functional theory, while being very successful for non-strongly correlated system, completely fail to describe entangled systems. Fig. 2 shows that the many-body version of the signed particle formulation can handle naturally such kind of systems.

The exclusion principle [5]. By pinching two electrons with same energy against each other a lower probability is developed in the central area of the phase-space, preventing the two particles to be in the same position with the same energy. Fig. 3 proofs the presence of the Pauli exclusion principle which, essentially, states that two particles with the same spin cannot be in the same orbital at the same time.

Conclusions

In this article, the signed particle formulation of quantum mechanics has been introduced which consists of a set of three rules that completely describe the time evolution of quantum systems. Successful applications of the new approach to quantum tunneling, entangled particles and identical electrons have been shown. Clearly, still a lot remains to be explored from both a theoretical and computational point of view. For instance, the definition of the function $\gamma = \gamma(\vec{x})$ does not prevent the divergence of the series and further mathematical investigation is needed. At the moment, for practical purposes, the series is truncated over a finite phase-space. Furthermore, the classical limit of the new theory is still under analysis. Despite of all, the author thinks that, based on the promising results reported in this and other articles, it is a very exciting time for those scientists who want to use an alternative approach to the standard formulation of quantum mechanics.

Computational Aspects

The code utilized to simulate the examples reported in this article is nano-archimedes [6], a GNU package available on-line under GPL. The reader is strongly encouraged to download it in order to duplicate the results shown. This code is entirely developed in C and optimized to get the best performance from the hardware. It can run on both serial and parallel machines exploiting the OpenMP standard library.

The results presented in Figs. 2 and 3 have been obtained using the HPC cluster deployed at the Institute of Information and Communication Technologies 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 X5560 @ 2.8 Ghz and 32 GB RAM. All these servers are interconnected via non-blocking DDR Infiniband interconnect at 20Gbps line speed. The theoretical peak performance is 3.23 Tflops.

References and Notes

1. E. Wigner, On the quantum correction for thermodynamic equilibrium, Phys. Rev. 40, 749 (1932).
2. J.M. Sellier, M. Nedjalkov, I. Dimov, An introduction to applied quantum mechanics in the Wigner Monte Carlo formalism, Physics Reports 577, 1-34, (2015).
3. D. Leibfried, T. Pfau, C. Monroe, Shadows and mirrors: reconstructing quantum states of atom motion, Physics Today, April (1998).
4. J.M. Sellier, I. Dimov, The many-body Wigner Monte Carlo method for time-dependent ab-initio quantum simulations, Journal of Computational Physics 273, 589-597 (2014).
5. J.M. Sellier, I. Dimov, On the simulation of indistinguishable Fermions in the many-body Wigner formalism, Journal of Computational Physics 280, 287-294 (2015).
6. www.nano-archimedes.com

Acknowledgments

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Figures and Tables

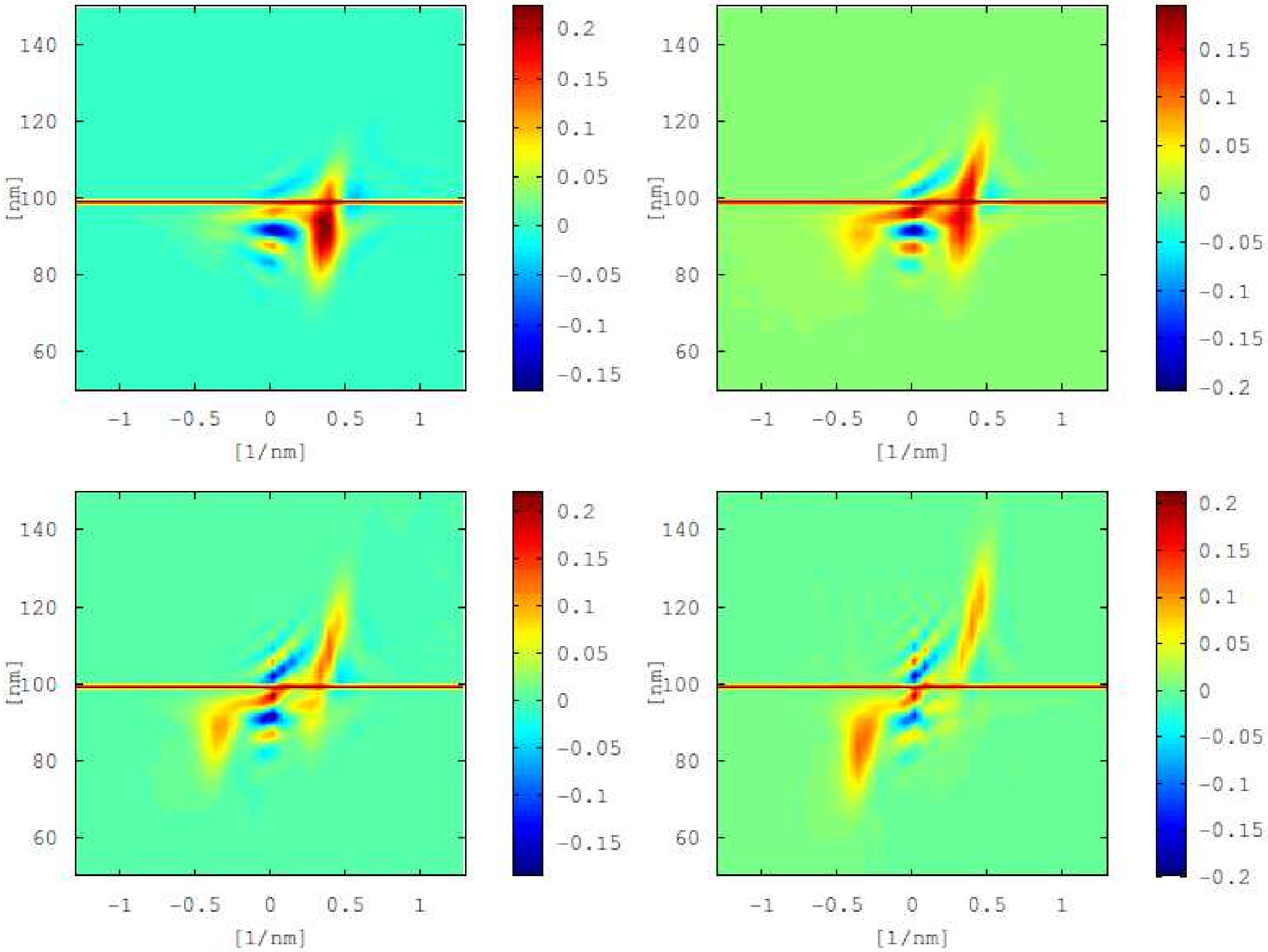

Figure 1. Quantum tunneling effect at different times. A Gaussian wave packet travels towards a potential barrier (symbolized by a red line). The dynamics is shown in the phase-space. Part of the wave-packet is reflected (lower part of the plot) while the other part tunnels through the barrier (upper part of the plot).

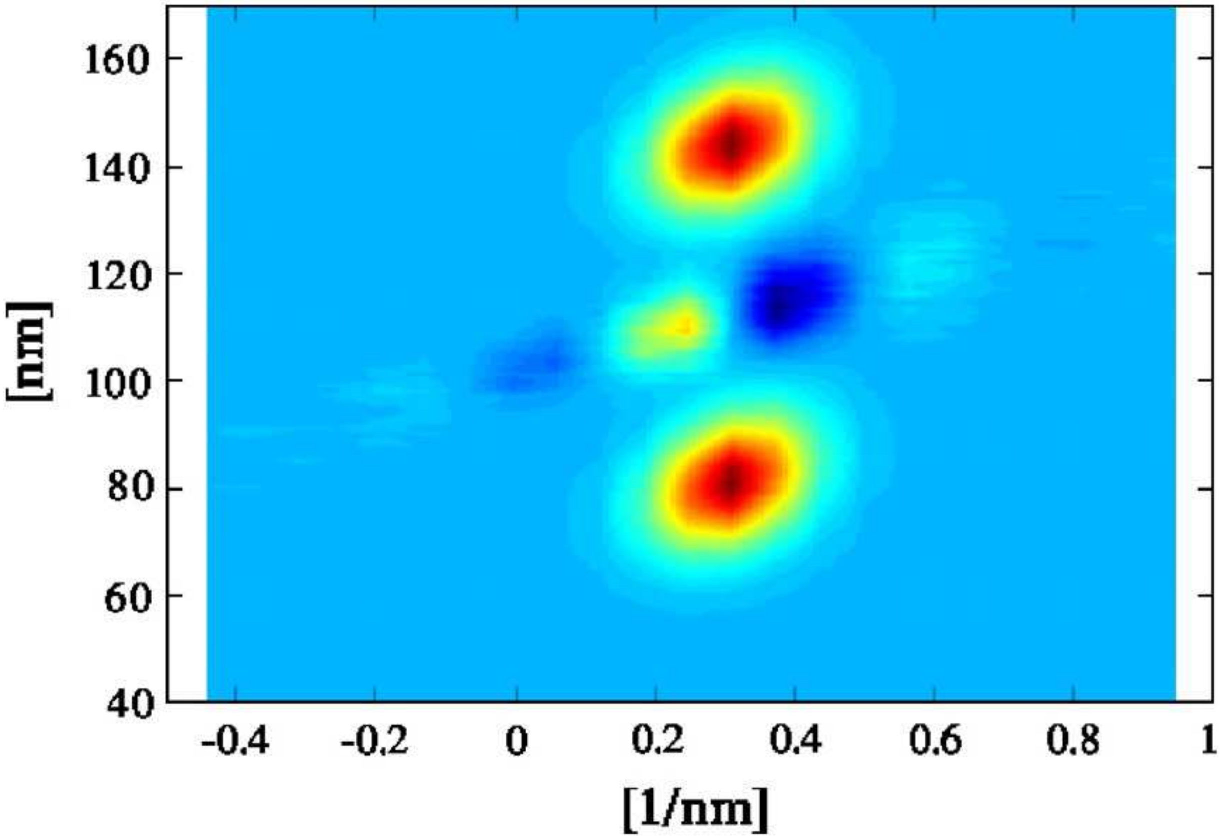

Figure 2. Simulation of two entangled Gaussian wave-packets. The reduced quasi-distribution function is shown at time 20 fs. A rotation in the phase-space of both packets and entanglement (oscillations between the packets) is clearly observable.

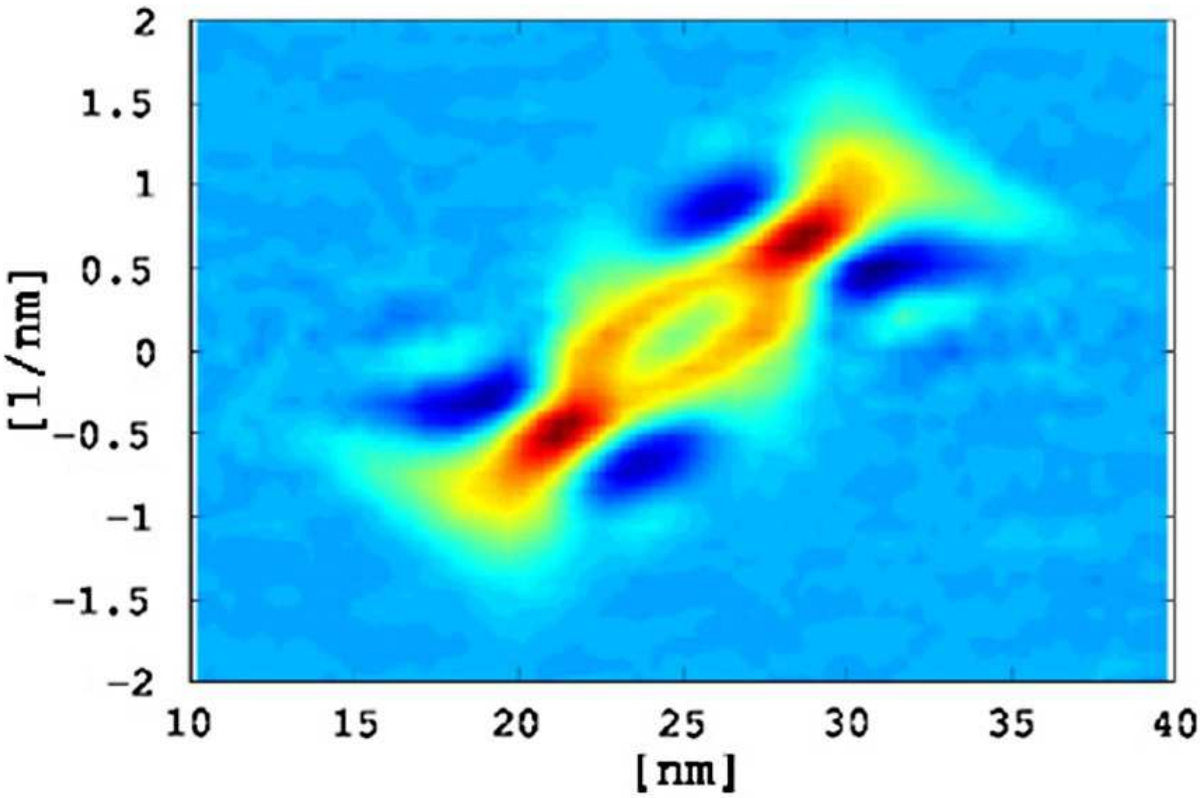

Figure 3. Simulation of two indistinguishable Fermions (electrons) squeezed one against the other while having the same energy. The formation of a Fermi (or exchange-correlation) hole at time 2.5 fs is clearly visible. This is a strong evidence of the presence of the Pauli exclusion principle.