Signed Particles and Quantum Similarity

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Introduction

The concept of molecular quantum similarity is a rather subjective notion which depends on the definition of a molecular descriptor. Recently, a new definition of quantum similarity has been proposed based on the concept of quasi-distribution functions [1]. This novel approach exploits the Wigner formulation of quantum mechanics which belongs to the class of phase-space formalisms and has been implemented in the framework of the Wigner Monte Carlo method [1].

On the other hand, a new formulation of quantum mechanics has been presented which is based on the intuitive concept of classical particles provided with a sign which describes the experimental reachability of a particular configuration of a system [2]. Being the particles contemporarily provided with a position and a momentum, this formalism belongs to the class of phase-space formulations of quantum mechanics.

In this paper, we show that it is possible to combine these two approaches to compute quantum similarities of different systems in a amount of details which is barely possible by other approaches. In the next section, we provide the postulates of the signed particle formulation of quantum mechanics and describe how to compute similarities in this novel context.

Signed Particles and Quantum Similarity

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).

Postulate 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.

Postulate 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.

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

The physical picture offered by this set of rules is rather peculiar. Quantum systems are described by ensembles of classical field-less particles which carry a sign and interact with a given 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) [2]. This new view point is relatively easy to grasp and intuitive. As a matter of fact, it allows the inclusion of complex effects (such as

phonon scattering, dispersive backgrounds, energy bands, etc.) in a natural way [2]. It is clear that quasi-distribution functions of given systems can be easily reconstructed by these ensemble of particles. Indeed, by taking into account the sign of every single particle one re-obtains the Wigner quasi-distribution of the system [2].

On the other hand, a new definition of quantum similarity based on the utilization of quasi-distribution functions has been provided in [1] which reads:

$$d_{AB}^{n}(t) = \left(\int d\mathbf{x} \int d\mathbf{p} \left| f_{W}^{A}\left(\mathbf{x};\mathbf{p};t\right) - f_{W}^{B}\left(\mathbf{x};\mathbf{p};t\right) \right|^{n} \right)^{\frac{1}{n}},$$

with n an integer (usually taken equal to 1). It is trivial to see that, by simulating quantum systems by means of the signed particle formulation, one can reconstruct the quasi-distribution function of two given systems and, therefore, compute their similarity.

References

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