Positive definite phase space quantum mechanics

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Abstract

Still today the discussion about the foundations, physical interpretation, and real scope of quantum mechanics has never ceased. It would be wrong to dismiss these issues as mere philosophical problems, because questions of consistency and interpretation are not devoid of practical utility.

We present the foundations and main properties of a *positive definite phase space quantum mechanics*. A new quantization procedure is proposed as well. This new interpretation/formulation eliminates conceptual and technical difficulties from quantum mechanics: (**i**) many paradoxes typical of the wave-particle duality, EPR experiments, macroscopic superpositions, and collapse of wavefunctions disappear; (**ii**) the elimination of the wavefunctions from quantum theory is in line with the procedure inaugurated by Einstein with the elimination of the ether in the theory of electromagnetism; (**iii**) it is useful in considering the classical limit, can treat mixed states with ease, and brings certain conceptual issues to the fore; (**iv**) confirms the ensemble interpretation of the wavefunctions, derives its statistical interpretation, corrects the temporal dependence of the old wavefunctions, and considers pure classical states –localizable states– beyond the Hilbert space; (**v**) the quantum equation of motion is of the Liouville kind and star-products are not needed, simplifying the formalism; and (**vi**) eliminates the hypothetical external quantum field of the pilot wave interpretation, solving its problems on the status of probability, and correcting well-known inconsistencies of the Bohm potential.

Finally, we offer some perspectives on future developments and research in progress.

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1 Introduction

Since its very born, about ninety years ago, quantum mechanics has acquired a prominent place among the physical theories. However, this place is a very curious one. At the one hand, there is no doubt that quantum mechanics can be considered one of the most useful physical theories. At the other hand, the discussion about its foundations, its physical interpretation, and its real scope has never ceased [1–7].

For instance, still today there is not agreement among experts on if the wavefunction fully describes the behavior of a single particle or only describes the associated ensemble [8, 9]. Another example is found on the relationship with classical mechanics. P. A. M. Dirac stated his belief on that classical mechanics may be regarded as the limiting case of the ordinary quantum mechanics when Planck constant $\hbar$ tends to zero [10]. But forty-five years latter Robert B. Griffiths recognizes that «*showing that classical physics is a limiting case of quantum physics is a nontrivial task which, despite considerable progress, is not yet complete*» [11]. More recently, Ulf Klein affirms «*that classical mechanics cannot be regarded as the limiting case of quantum mechanics for* $\hbar \to 0$» [12].

It would be wrong to dismiss these issues as mere philosophical problems, because questions of consistency and interpretation in quantum mechanics are not devoid of practical utility. Leslie E. Ballentine gives a detailed account of an incident that took place at a physics conference in 1956, where the participants expended considerable effort debating the size and coherence length of the wave packets associated to the individual electrons involved in an interference experiment; Ballentine shows how the confusion would be avoided if a different interpretation had been used and reports similar situations that occurred more recently [8].

When orthodox quantum mechanics is applied in an unfamiliar setting –such as it is happening at the present time in the new fields of quantum computation, quantum cosmology, and nanotechnology–, its unresolved conceptual difficulties are a serious impediment to physical understanding. Consider quantum cosmology: what interpretation would be used to study the early instants of the universe? According to Hug Everett III [4], John Archibald Wheeler [5], Max Tegmark, and other proponents of the many-world interpretation, the universe is fully described by the deterministic Schrödinger equation. In the opposite side, Griffiths [11], Murray Gell-Mann, J. B. Hartle, R. Omnès, and other proponents of the consistent histories interpretation, consider that the time evolution of any isolated quantum system [13] is fundamentally stochastic, with the deterministic evolution arising only in the special case in which the relevant probability is one.

The conceptual landscape briefly touched above becomes still more complex after noticing that many formulations of quantum mechanics have been developed besides the different interpretations and that some formulations cannot be applied to certain problems. Daniel F. Styer et al. [14] review the wavefunction, matrix, path integral, Wigner & Moyal, density matrix, second quantization, variational, Hamilton & Jacobi formulations, and pilot wave formulations –although the latter is best characterized as an interpretation [6]–.

The aim of this paper is to present a new interpretation/formulation of quantum mechanics that eliminates the main conceptual and technical difficulties associated to existent formulations and interpretations.

The following section presents the quantum Liouvillian phase space which is at the foundation of this quantum mechanics. Sections 3 and 4 show how the wavefunction formulation can be derived as a special case for a specific kind of phase space ensembles. A simple quantization procedure is proposed which relies on a new quantization rule that emphasizes that quantum effects are stochastic corrections to the classical momentum. In the following section, we extend the discussion to mixed states, obtaining the density matrix formulation as another special case of this new quantum mechanics.

The section 6 confirms the commutative character of the phase space of this quantum mechanics and demonstrates how this phase space generates the non-commutativity of the HILBERT space and its associated HEISENBERG uncertainty principle. The section 7 compares this new quantum mechanics with the existent formulations and interpretations emphasizing its main advantages. Finally, we offer some perspectives on future developments and research in progress.

2 The quantum Liouvillian phase space

Consider a phase space (p, x) of $6N$ dimensions with *implicit* time-parametrization; here $p = (p_1, p_2, ...p_N)$ and $x = (x_1, x_2, ...x_N)$ are momenta and positions, respectively, of the N-particle system. Dynamical observables of a system are associated to functions in this phase space $\mathbb{O} = \mathbb{O}(p, x; t)$

The state of a system is given by the state function $\sigma = \sigma(p, x; t)$. This state is positive definite

$$\sigma \geq 0 \tag{1}$$

and normalizable

$$\int \sigma \, \mathrm{d}p \, \mathrm{d}x \equiv \int \int \cdots \int \sigma \, \mathrm{d}p_1 \, \mathrm{d}x_1 \, \mathrm{d}p_2 \, \mathrm{d}x_2 \cdots \mathrm{d}p_N \, \mathrm{d}x_N = 1. \tag{2}$$

Therefore $\sigma \, \mathrm{d}p \, \mathrm{d}x$ represents the probability of finding at time t a representative point in the volume element $\mathrm{d}p \, \mathrm{d}x$ of the phase space. The existence of a pure probability interpretation of the phase space quantum state σ is one the advantages over the old WIGNER & MOYAL formulation of quantum mechanics, as we will see below in the section 7.

The total change in the state function $\sigma(p, x; t)$ follows from the total differential

$$\frac{\mathrm{d}\sigma}{\mathrm{d}t} = \frac{\partial \sigma}{\partial t} + \sum_{j=1}^{N} \left(\frac{\partial \sigma}{\partial p_j} \frac{\mathrm{d}p_j}{\mathrm{d}t} + \frac{\partial \sigma}{\partial x_j} \frac{\mathrm{d}x_j}{\mathrm{d}t} \right). \tag{3}$$

We will only consider conservative systems, $\mathrm{d}\sigma / \mathrm{d}t = 0$, in this work, in whose case the equation of motion for the state reduces to

$$\frac{\partial \sigma}{\partial t} = -i \hat{L} \sigma, \tag{4}$$

with the Liouvillian operator

$$\hat{L} \equiv -i \sum_{j=1}^{N} \left(\frac{\partial H}{\partial p_j} \frac{\partial}{\partial x_j} - \frac{\partial H}{\partial x_j} \frac{\partial}{\partial p_j} \right), \tag{5}$$

where $H = H(p, x; t)$ denotes the phase space Hamiltonian.

Dynamical observables associated to the phase space function $\mathbb{O}(p, x; t)$ for a system in a given state σ are computed according to

$$\langle \mathbb{O} \rangle = \int \mathbb{O}(p, x; t)\, \sigma(p, x; t)\, \mathrm{d}p\, \mathrm{d}x. \tag{6}$$

In the following three sections, we will show how the generalized equation of motion (4) and the averages (6) for dynamical observables reduce to those of the wavefunction and density matrix formulations under a well-defined set of conditions.

3 The Schrödinger equation as a special case

By simplicity we will consider here the six-dimensional phase space associated to one-particle systems, but the generalization to a many-particle system is direct. We start from the quantum Liouville equation (4) and take into account a semi-mixed state

$$\sigma = \rho(x; t) \delta_{\mathrm{D}}(p; t) \tag{7}$$

using a phase space Hamiltonian

$$H(p, x; t) = \frac{p^2}{2m} + H_{\mathrm{Q}}(x; t). \tag{8}$$

By separating variables and using the identity $\delta_{\mathrm{D}}(p; t) = \delta_{\mathrm{D}}(p - p(t))$, we obtain from (4) the continuity equation in configuration space

$$\frac{\partial \rho}{\partial t} = -\nabla \left[\frac{p(t)}{m} \rho \right] \tag{9}$$

plus the quantum Hamiltonian equation

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = -\nabla H_{\mathrm{Q}}. \tag{10}$$

By using a generalization of the Hamilton & Jacobi formulation of classical mechanics –see appendix–, the last equation can be substituted by a generalized Hamilton & Jacobi equation for the semi-mixed Hamiltonian $H = H(p(t), x; t)$

$$\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{2m} + H_{\mathrm{Q}} = 0. \tag{11}$$

The independent real equations (9) and (11) can be written again as a single equation. For that purpose, one can introduce a complex function

$$\Psi \equiv \sqrt{\rho} \exp\left(\frac{iS}{\hbar} \right). \tag{12}$$

With this definition of Ψ, the system of equations (9) and (11) is equivalent to

$$i\hbar\frac{\partial\Psi}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + H_{\mathrm{Q}} + \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}\right)\Psi. \tag{13}$$

This is the SCHRÖDINGER equation of quantum mechanics if the Q-Hamiltonian verifies

$$H_{\mathrm{Q}} \equiv V - \frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}}. \tag{14}$$

The generalization to many-particle systems is direct. Therefore the fundamental quantum LIOUVILLE equation (4) for a many-particle system with a quantum Hamiltonian

$$H \equiv \sum_j^N \frac{p_j^2}{2m_j} + V - \sum_j^N \frac{\hbar^2}{2m_j}\frac{\nabla_j^2\sqrt{\rho}}{\sqrt{\rho}} \tag{15}$$

reduces to the many-particle SCHRÖDINGER equation of the wavefunction formulation of quantum mechanics when the state is given by (7).

4 Observables and quantum averages

By introducing the state (7) into the equation (6) for the phase space average we obtain

$$\langle \mathbb{O} \rangle = \int \mathbb{O}(p(t), x; t)\, \rho(x; t)\, \mathrm{d}x. \tag{16}$$

We will show that this equation provides the same quantum averages that the wavefunction formulation of quantum mechanics. For phase space functions that do not depend on the momentum, such as the potential V in (14) or the position x, the demonstration is direct

$$\langle \mathbb{O} \rangle = \int \mathbb{O}(x; t)\, \rho(x; t)\, \mathrm{d}x = \int \Psi^*(x; t)\, \mathbb{O}(x; t)\, \Psi(x; t)\, \mathrm{d}x, \tag{17}$$

where the polar representation (12) has been used. For phase space functions that do not depend on the position, such as the kinetic energy in (8) or the momentum $p(t)$, the demonstration requires the use of the identity

$$p(t) = \frac{i\hbar\nabla\sqrt{\rho}}{\sqrt{\rho}} - \frac{i\hbar\nabla\Psi}{\Psi}, \tag{18}$$

which is obtained by applying the operator $(-i\hbar\nabla)$ to (12). By using this identity, the phase space average of the momentum $p(t)$ gives

$$\langle p(t) \rangle = \int p(t)\, \rho(x; t)\, \mathrm{d}x = \int \Psi^*(x; t)\, (-i\hbar\nabla)\, \Psi(x; t)\, \mathrm{d}x, \tag{19}$$

in agreement with the wavefunction formulation of quantum mechanics. Notice that the third integral involving the term $i\hbar\nabla\sqrt{\rho}/\sqrt{\rho}$ vanishes; this can be shown either by direct integration or by considering that the operator $(-i\hbar\nabla)$ is Hermitian and the integral of $p(t)$ is real, which implies that the imaginary term from the third integral cancels out.

The quantum average of the kinetic energy cannot be obtained from $p(t)^2/2m$, because this is a classical kinetic term, not the proper quantum kinetic term. For obtaining the quantum kinetic term we must consider a generalization of the identity (18). The result of applying n-times the operator $(-i\hbar\nabla)$ to (12) is

$$\tilde{p}^n(t) \equiv \frac{(-i\hbar\nabla)^n\Psi}{\Psi} = p^n(t) + \frac{(-i\hbar\nabla)^n\sqrt{\rho}}{\sqrt{\rho}}. \tag{20}$$

The above definition can be taken as the basis of a *quantization rule*

$$p^n(t) \to \tilde{p}^n(t). \tag{21}$$

By substituting $p^n(t)$ in the classical expressions by $\tilde{p}^n(t)$ we will obtain the correct quantum generalizations. By using this rule we can obtain the quantum average of any phase space function that depends on the momentum. For instance, the average kinetic energy is found to be

$$\langle K(t)\rangle = \int \frac{\tilde{p}^2(t)}{2m}\,\rho(x;t)\,\mathrm{d}x = \int \Psi^*(x;t)\,\frac{(-i\hbar\nabla)^2}{2m}\,\Psi(x;t)\,\mathrm{d}x \tag{22}$$

in complete agreement with the quantum average using wavefunctions and operators. The consideration of a phase space function that depends on both momentum and position provides the next equivalence

$$\langle\mathbb{O}\rangle = \int \mathbb{O}(\tilde{p}(t),x;t)\,\rho(x;t)\,\mathrm{d}x = \int \Psi^*(x;t)\,\mathbb{O}(-i\hbar\nabla,x;t)\,\Psi(x;t)\,\mathrm{d}x \tag{23}$$

where the use of the quantization rule is made explicit. Notice that this new approach explains the physical origin and the role of the position $\hat{x} \equiv x$ and momentum operators $\hat{p} \equiv -i\hbar\nabla$ in the wavefunction formulation [15].

The quantization rule explains the physical origin and role of the term $-\hbar^2\nabla^2\sqrt{\rho}/2m\sqrt{\rho}$ in (14) as a quantum correction to the classical kinetic Hamiltonian. Comparison of $\tilde{p}(t)$ with the average (19) provides further insight on the physical nature of the correction term $-i\hbar\nabla\sqrt{\rho}/\sqrt{\rho}$ in (20) as a kind of *quantum* fluctuation [16] over the average $p(t) = \langle\tilde{p}(t)\rangle$

$$\tilde{p}(t) = p(t) + \delta p(t). \tag{24}$$

Evidently $\langle\delta p(t)\rangle = 0$ but, in general, $\langle\delta p(t)\delta p(t)\rangle \neq 0$ and the quantum correction to the classical $\langle p^2(t)/2m\rangle$ is found to be a statistical covariance. Notice that the *quantum* fluctuation $\delta p(t)$ depends on the shape of the state ρ in the configuration space, but not in its magnitude –a rescaling $\rho \to \lambda\rho$ leaves unchanged the fluctuation–. The dependence with the shape is logarithmic and reveals a link with *quantum* information

$$-i\hbar\frac{\nabla\sqrt{\rho}}{\sqrt{\rho}} = -\frac{i\hbar}{2}\nabla\ln\rho. \tag{25}$$

5 Mixed states

In the section 3, we obtained the equation of SCHRÖDINGER for quantum systems described by a semi-mixed state (7). In this section we consider a more general kind of quantum systems in the mixed state

$$\sigma = \rho(x;t)\xi(p;t) = \sum_{\beta}^{s} w_\beta \, \rho(x;t)\delta_{\mathrm{D}\beta}(p;t), \tag{26}$$

where the constants w_β denotes the density or weight of the state β in the total ensemble and $\delta_{\mathrm{D}\beta}(p;t) = \delta_{\mathrm{D}}(p - p_\beta(t))$.

Notice that the mixed state (26) can be written in the form $\sigma = \sum_\beta^s w_\beta \sigma_\beta$, which implies that the quantum LIOUVILLE equation (4) splits into s equations of motion, one for each σ_β. By repeating the procedure in the section 3 we will obtain now that the whole dynamics of (26) is equivalent to a set of s weighted SCHRÖDINGER equations of motion

$$i\hbar \frac{\partial \Psi_\beta}{\partial t} = \left(-\frac{\hbar^2}{2m}\nabla^2 + V \right)\Psi_\beta, \tag{27}$$

with weights w_β and wavefunctions $\Psi_\beta \equiv \sqrt{\rho}\, \exp(iS_\beta/\hbar)$. Notice that the w_β are not amplitudes and the dynamics described by the above set of s equations *cannot* be reproduced by a single SCHRÖDINGER equation for a *hypothetical* superposition $\Phi = \sum_\beta^s c_\beta \Psi_\beta$. We are dealing with a non-linear problem outside the scope of the wavefunction theory.

The above set of s equations can be reduced to a single equation by introducing the concept of density matrix $D(x,x';t) \equiv \sum_\beta^s w_\beta \Psi_\beta(x;t)\Psi_\beta^*(x';t)$. By differentiating $D(x,x';t)$ and taking into account the equation of motion for each Ψ_β and its conjugate Ψ_β^*, we can derive the ordinary equation of motion for the density matrix

$$i\hbar \frac{\partial D(x,x';t)}{\partial t} = \sum_s H(x,s;t)D(s,x';t) - \sum_s D(x,s;t)H(s,x';t). \tag{28}$$

As is well-known, when all the weights are zero except one $D(x,x';t) = \Psi(x;t)\Psi^*(x';t)$ the density matrix equation is equivalent to the SCHRÖDINGER equation for $\Psi(x;t)$.

By repeating the procedure in the section 4 but now for the mixed state (26) and taking into account the set of s wavefunctions Ψ_β with weights w_β we obtain an extension of the average equivalence (23) beyond the wavefunction theory

$$\langle \mathbb{O} \rangle = \sum_\beta^s w_\beta \int \mathbb{O}(\tilde{p}_\beta(t), x; t)\, \rho(x;t)\, \mathrm{d}x = \sum_\beta^s w_\beta \int \Psi_\beta^*(x;t)\, \mathbb{O}((-i\hbar\nabla), x; t)\, \Psi_\beta(x;t)\, \mathrm{d}x \tag{29}$$

where the use of the quantization rule is again made explicit. By using the definition of the density matrix, the last integral can be rewritten in the well-known trace form, which completes the demonstration of equivalence with the density matrix formalism.

The generalization of the entire treatment in this section to the many-particle case is direct. Therefore, the fundamental quantum LIOUVILLE equation (4) for a many-particle system with Hamiltonian (15) and the phase space averages (6) reduce to the many-particle equation and averages, respectively, of the density matrix formulation of quantum mechanics when the state is given by (26).

6 Derivation of the uncertainty principle

Evaluation of $[p,x] = px - xp = 0$ confirms the commutative character of the phase space (p,x) of this quantum mechanics. It remains to be demonstrated that this phase space generates the characteristic non-commutativity associated to the HILBERT space.

By using the definition (20) for $\tilde{p}$ and the position $\hat{x} \equiv x$ and momentum operators $\hat{p} \equiv -i\hbar\nabla$ derived in the section 4, we obtain

$$[\tilde{p}, x] = \frac{1}{\Psi}\left(\hat{p}\hat{x} - \hat{x}\hat{p}\right)\Psi = [\hat{p}, \hat{x}] = -i\hbar. \tag{30}$$

In the right-hand side we recognize the HEISENBERG uncertainty principle for the operators. By introducing the decomposition (20)

$$[\hat{p}, \hat{x}] = [p, x] - i\hbar\left[\frac{\nabla\sqrt{\rho}}{\sqrt{\rho}}, x\right] = -i\hbar, \tag{31}$$

which implies that the origin of the uncertainty is the δp correction to the momentum p.

7 Advantages over other interpretations/formulations

The advantages of this new approach are numerous. First of all, many paradoxes typical of the wave-particle duality disappear. On the one hand, in fact, it becomes possible to express the correlations between two distant particles in terms of the product of two probabilities independent from each other. All the speculations on the nature of hypothetical superluminal signals between the particles become, therefore, meaningless. On the other hand, the long time debated question about the meaning of the superposition of state vectors for macroscopic objects may also be set as equally baseless because (14) reduces to the classical potential for a massive body and the dynamics is entirely classical. From a conceptual point of view, the elimination of the wavefunctions from quantum theory is in line with the procedure inaugurated by EINSTEIN with the elimination of the ether in the theory of electromagnetism.

Secondly, this new approach eliminates the conventional hybrid procedure of describing the dynamical evolution of a system, which consists of a first stage in which the theory provides a deterministic evolution of the wavefunction Ψ –notice that the matrix, second quantization, variational, density matrix, and pilot wave formulations also use wavefunctions for several motives [14]–, followed by a hand-made construction of the physically meaningful probability distributions. If the probabilistic nature of the microscopic phenomena is fundamental, and not simply due to our ignorance as in classical statistical mechanics, why would it be impossible to describe them in probabilistic terms from the very beginning? This new approach substitutes the unobservable wavefunction by the observable state function σ.

Thirdly, a direct comparison with the existent formulations and interpretations reveals that this new positive definite phase space quantum mechanics puts together many advantages in a single formalism.

For instance, like the Wigner & Moyal formulation, the new approach is useful in considering the classical limit; like the density matrix formulation, the new approach can treat mixed states with ease, so it is of special value in statistical physics; like the pilot wave formulation, the new approach brings certain conceptual issues to the fore.

A more detailed comparison reveals further advantages. The obtaining of the Schrödinger formalism using the semi-mixed state (7) confirms that the wavefunction Ψ describes an ensemble [9], instead of a single system, and settles this old controversy [1, 3, 8, 12]. The modern statistical interpretation of quantum mechanics eliminates many paradoxes such as the Schrödinger cat paradox or the collapse of the wavefunction [8]. Furthermore, the statistical interpretation of the wavefunction emerges, in a natural way, from the physical meaning of the phase space state: $|\Psi|^2 = \int \sigma(p, x; t)\, \mathrm{d}p$.

Notice that the $6N$ dimensional phase space structure generates a wavefunction $\Psi = \Psi(x; t)$ which lives in a configuration space of $3N$ dimensions. The temporal dependence of the wavefunction Ψ is *implicit*. The abandon of the old time-explicit dependence $\psi = \psi(t, x)$ allows a consistent description of mechanical systems. However, it is needed to emphasize that we derive the correct time-*implicit* dependence of the wavefunction from the underlying phase space structure, whereas the modern $\Psi(x; t)$ are postulated in recent treatments of quantum mechanics [17]. Moreover, the Dirac bra-ket formalism can reproduce the old wavefunctions $\psi(t, x) = \langle x|\psi(t)\rangle$, but cannot reproduce the modern $\Psi(x; t)$.

As shown in the sections 4 and 5, the phase space position x associated to this new approach is transformed into the position operator $\hat{x}$ in the wavefunction formalism, whereas the time t continues being the evolution parameter in both –there is not operator for t–. The incorrect time-explicit dependence of the old $\psi(t, x)$ is partially responsible for the difficulties and inconsistencies of the old relativistic quantum mechanics. The new approach presented here can be extended to include relativistic effects, providing us a consistent relativistic quantum mechanics, but this extension will be made elsewhere.

We have shown that the density matrix formalism can be obtained by generalizing the semi-mixed state (7) to the mixed state (26). But what does happen if we consider instead a pure state $\sigma = \delta_{\mathrm{D}}(x; t)\delta_{\mathrm{D}}(p; t)$? The first consequence is that the quantum correction term in the Q-Hamiltonian (14) vanishes for a massive system [18] *leaving a purely classical description*. The second consequence is that the pure classical state σ cannot be reproduced by any wavefunction. Indeed, according to ordinary quantum mechanics, a system is in a definite position only when $\Psi = \delta_{\mathrm{D}}(x; t)$, but then the wavefunction density is $|\Psi|^2 = \delta_{\mathrm{D}}(x; t)\delta_{\mathrm{D}}(x; t)$. Apart from disagreeing with the correct density $\rho = \int \sigma(p, x; t)\, \mathrm{d}p = \delta_{\mathrm{D}}(x; t)$, the Dirac wavefunctions are not normalizable in the Hilbert space. These results complement Klein's recent findings on the $\hbar \to 0$ limit of the ordinary quantum mechanics. Notice that, unlike the ordinary quantum mechanics [12], the new approach developed here contains classical mechanics as a limiting case.

The old Wigner & Moyal formulation introduces pseudo phase space functions from a Fourier transform of the Hilbert space functions [14, 19–21]. This pseudo phase space inherits the non-commutativity associated to the Hilbert space and, as a consequence, the resulting state –the Wigner function– takes on negative values and cannot be interpreted as a genuine probability distribution; moreover, products in the ordinary phase space are substituted by star-products in the pseudo phase space structure.

The resulting equation of motion in this pseudo phase space structure is not of the LIOUVILLE kind and involves both quadratic and higher order derivatives in the potential V, making its solution very difficult. The pseudo phase space structure implies that the WIGNER functions cannot be localized and a strict reduction to the pure classical limit fails: no WIGNER function can reproduce the pure state $\sigma = \delta_{\mathrm{D}}(x;t)\delta_{\mathrm{D}}(p;t)$.

This contrasts with the new approach developed here. We start from a genuine phase space and obtain the HILBERT space representation as a particular case. The new quantum states (7) and (26) are positive definite and can be interpreted as genuine probability distributions; in fact, the statistical interpretation of both wavefunctions and density matrices is obtained from the new probability distributions. The resulting equation of motion in this new approach is a LIOUVILLE equation (4) with a purely quantum term (14) added to the classical Hamiltonian. The new states strictly reduce to pure classical states, $\sigma = \delta_{\mathrm{D}}(x;t)\delta_{\mathrm{D}}(p;t)$, outside of the HILBERT space.

The purely quantum term in (14) closely resembles the BOHM potential in the pilot wave interpretation [6, 14], but there are fundamental differences between both. In the pilot wave interpretation, the BOHM potential is assumed to be generated by a hypothetical external quantum field, the ψ-field [6], that guides the particle's motion through a supplementary set of quantum Newtonian equations. The dynamics of this hypothetical ψ-field is described by the old SCHRÖDINGER wave-like equation.

In the new approach developed here, the purely quantum term depends on $\rho = \int \sigma(p, x; t)\, \mathrm{d}p$. This is a projection of the phase space state σ into the configuration space; there is no external field here. Additionally, we obtain the SCHRÖDINGER equation of motion (13) for $\Psi(x;t)$ from the LIOUVILLE equation (4) for semi-mixed states (7). Therefore, the equation (13) is an equivalent equation of motion –within the range of validity of (7)– for the N-particle system; again there is no external field here. Notice that $\psi = \psi(t, x)$ [6, 14] and, therefore the pilot-wave interpretation has the same difficulties than the old wavefunction formulation regarding the role of time. The problem of the status of probability in the pilot wave formulation –the identification of the wavefunction as amplitude of a probability density for the position– is still unsolved today. However, the interpretation of ρ as the probability density for the position is completely natural.

Moreover, the analysis of the purely quantum term showed that it has a kinetic origin (24), not a potential origin, eliminating the well-known inconsistencies of the BOHM potential of the pilot wave formulation. This new approach produces a fresh quantization rule (21), whereas the pilot wave formulation assumes a SCHRÖDINGER equation, which has to be first derived outside of the pilot wave interpretation. Finally, the purely quantum term in (14) vanishes for pure classical states $\sigma = \delta_{\mathrm{D}}(x;t)\delta_{\mathrm{D}}(p;t)$, whereas the wavefunctions of the pilot wave interpretation cannot reproduce such classical states, as shown above –see also the criticism made in [8] to the classical limit of the pilot wave interpretation–.

8 Perspectives and final remarks

In this work, we have only considered conservative systems, $\mathrm{d}\sigma/\mathrm{d}t = 0$. A generalization of the equation of motion (4) for dissipative systems will be considered in a future work.

We have also avoided a discussion of spin, relativistic effects, quantum fields, and second quantization. The introduction of relativistic effects or the treatment of quantum fields can be achieved directly, in analogy with existent interpretations/formulations; however, in the spirit of the present work, we hope to offer a new and deep discussion that eliminates current difficulties and paradoxes in the existent interpretations/formulations. For instance, we are developing a new approach to second quantization that predicts the properties of bosons such as the photon from first principles, without the need of *ad hoc* renormalization and regularization procedures; we get rid of the unphysical bare photons and only need to consider them during comparisons with the ordinary quantum field theory, because the latter theory is built over such unphysical objects.

As shown in the section 5, the equation of motion (4) and the averages (6) for mixed states (26) reproduce the density matrix formalism. It is possible to consider a generalization of the density matrix formalism that works also for pure classical states $\sigma = \delta_{\mathrm{D}}(x;t)\delta_{\mathrm{D}}(p;t)$. This generalization provides an alternative matrix representation to the scalar positive definite phase space quantum mechanics developed here. The matrix representation is a homomorphism to the scalar complex representation introduced by the quantization rule (21). This alternative matrix representation seems to be very useful for relativistic and spin corrections; for instance, it is the natural arena for the use of the PAULI spin matrices.

As discussed in previous sections, the quantization rule (21) introduces a quantum correction term in the Hamiltonian (14) that closely resembles the BOHM potential. In recent years, this 'potential' –see discussion about its correct physical interpretation in the section 7– has been applied to physicochemical problems such as the study of chemical reactivity dynamics and quantum chaos [22], definition of atoms in molecules and solids [23], proton affinity [24], and others. These successful applications are inherited by the positive definite phase space quantum mechanics developed here.

The theory of Atoms in Molecules (AIM) [25] is an interpretative theory which aims to recover chemical insight from modern high-resolution electron densities ρ. These densities may be of experimental origin or derived from quantum theory. AIM defines two important cornerstones of chemistry: the atom and the bond. AIM addresses the topology of ρ and the topology of its Laplacian $\nabla^2\rho$. The impression that AIM encompasses two separate parts is a consequence of historical developments and its present incomplete state. In the longer term AIM might be expanded into a complete topological theory of many if not all chemically relevant scalar properties. It is interesting that the expansion of the quantum correction term in (14) yields

$$-\frac{\hbar^2}{2m}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} = -\frac{\hbar^2}{4m}\left[\frac{\nabla^2\rho}{\rho} - \frac{1}{2}\left(\frac{\nabla\rho}{\rho}\right)^2\right] \tag{32}$$

where the chemically relevant quantities ρ, $\nabla\rho$, and $\nabla^2\rho$ appear in a unified fashion.

All the topics mentioned in this section will be considered elsewhere.

Summarizing: We present the foundations and main properties of a *positive definite phase space quantum mechanics*. An innovative quantization procedure is proposed as well. This new interpretation/formulation eliminates conceptual and technical difficulties from quantum mechanics: (**i**) many paradoxes typical of the wave-particle duality, EPR experiments, macroscopic superpositions, and collapse of wavefunctions disappear; (**ii**) the elimination of the wavefunctions from quantum theory is in line with the procedure inaugurated by EINSTEIN with the elimination of the ether in the theory of electromagnetism; (**iii**) it is useful in considering the classical limit, can treat mixed states with ease, and brings certain conceptual issues to the fore; (**iv**) confirms the ensemble interpretation of the wavefunctions, derives its statistical interpretation, corrects the temporal dependence of the old wavefunctions, and considers pure classical states –localizable states– beyond the HILBERT space; (**v**) the quantum equation of motion is of the LIOUVILLE kind and star-products are not needed, simplifying the formalism; and (**vi**) eliminates the hypothetical external quantum field of the pilot wave interpretation, solving its problems on the status of probability, and correcting well-known inconsistencies of the BOHM potential.

9 Appendix: Generalized Hamilton & Jacobi method

The HAMILTON & JACOBI formulation of classical mechanics finds a generating functional S for the canonical transformation $(p(t), x(t)) \rightarrow (P(t), X(t))$ to a set of constant dynamical quantities $\mathrm{d}P(t)/\mathrm{d}t = \mathrm{d}X(t)/\mathrm{d}t = 0$. Since the HAMILTON equations in the new $P(t)$ and $X(t)$ trivially vanish, the whole dynamics is encoded in the HAMILTON & JACOBI equation

$$\frac{\partial S}{\partial t} + H(p(t), x(t)) = 0. \tag{33}$$

For the derivation of the SCHRÖDINGER equation in the section 3, we need to consider a semi-mixed case (7) where the first HAMILTON equation is substituted by the continuity equation (9) and, therefore, the ordinary HAMILTON & JACOBI equation of above does not apply.

From the semi-mixed state (7), we can obtain the semi-mixed Hamiltonian $H = H(p(t), x; t)$ –notice that it 'lives' somewhat in the middle between the phase space Hamiltonian $H(p, x; t)$ and the observable Hamiltonian $H(p(t), x(t))$–. We use this semi-mixed Hamiltonian to define the following action in configuration space

$$S = S(x; t) \equiv \int \left(p(t) \frac{\mathrm{d}x}{\mathrm{d}t} - H \right) \mathrm{d}t. \tag{34}$$

By taking the gradient of the action yields the relationship between the momentum and the action

$$p(t) = \nabla S, \tag{35}$$

whereas taking the time derivative of the action and using the identity $\mathrm{d}/\mathrm{d}t = \partial/\partial t + v(t)\nabla$ and (35) we obtain the generalized HAMILTON & JACOBI equation

$$\frac{\partial S}{\partial t} + H(p(t), x; t) = 0. \tag{36}$$

By substituting the specific value for $H(p(t), x; t)$ in the above, this is just the equation (11). We will show now how the equation (10) can be replaced by (11).

We start by introducing (35) into (10) and use once again the identity $\mathrm{d}/\mathrm{d}t = \partial/\partial t + v(t)\nabla$; the result is

$$\nabla\left[\frac{\partial S}{\partial t} + \frac{(\nabla S)^2}{m} + H_{\mathrm{Q}}\right] = 0. \tag{37}$$

The integration of this equation is direct; by using (36), the integration constant κ is found to be $\kappa = (\nabla S)^2/2m$ and we arrive to equation (11) finally.

References and notes

[1] Can Quantum-Mechanical Description of Physical Reality be Considered Complete? **1935:** *Phys. Rev. 47(10), 777–780*. EINSTEIN, A.; PODOLSKY, B.; ROSEN, N.

[2] Einstein and the quantum theory **1979:** *Rev. Mod. Phys. 51(4), 863–914*. PAIS, A.

[3] The statistical interpretation of quantum mechanics **1970:** *Rev. Mod. Phys. 42(4), 358–381*. BALLENTINE, L. E.

[4] "Relative State" Formulation of Quantum Mechanics **1957:** *Rev. Mod. Phys. 29(3), 454–462*. EVERETT III, HUGH.

[5] Assessment of Everett's "Relative State" Formulation of Quantum Theory **1957:** *Rev. Mod. Phys. 29(3), 463–465*. WHEELER, JOHN A.

[6] A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. I **1952:** *Phys. Rev. 85(2), 166–179*. BOHM, DAVID.

A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. II **1952:** *Phys. Rev. 85(2), 180–193*. BOHM, DAVID.

[7] Speakable and Unspeakable in Quantum Mechanics **1987:** *Cambridge University Press; Cambridge*. BELL, JOHN S.

[8] Quantum Mechanics: A Modern Development **2000:** *World Scientific Publishing Co. Pte. Ltd.; Singapore*. BALLENTINE, LESLIE E.

[9] The conceptual ensemble associated to a single particle would not be confused with a population of particles, as it is unfortunately made by critics of the statistical interpretation of quantum mechanics.

[10] The principles of quantum mechanics; 4th edition **1958:** *Oxford University Press; Oxford*. DIRAC, P. A. M.

[11] Consistent Quantum Theory **2003:** *Cambridge University Press; Cambridge*. GRIFFITHS, ROBERT B.

[12] What is the limit $\hbar \to 0$ of quantum theory? **2012:** *Accepted for publication in the American Journal of Physics*. KLEIN, ULF.

[13] We prefer the modern and standardized term «*isolated*» instead of the older and inadequate term «*closed*» for referring to systems that cannot interchange energy or matter with the surrounds.

[14] Nine formulations of quantum mechanics **2002:** *Am. J. Phys. 70(3), 288-297.* Styer, Daniel F.; Balkin, Miranda S.; Becker, Kathryn M.; Burns, Matthew R.; Dudley, Christopher E.; Forth, Scott T.; Gaumer, Jeremy S.; Kramer, Mark A.; Oertel, David C.; Park, Leonard H.; Rinkoski, Marie T.; Smith, Clait T.; Wotherspoon, Timothy D.

[15] In the wavefunction formulation the use of operators associated to observables and the specific form of such operators is introduced through postulates.

[16] The quantum fluctuation is an imaginary term, whereas classical fluctuations are real.

[17] The General Formulation of Quantum Mechanics **2003:** *In Handbook of Molecular Physics and Quantum Chemistry, Volume 1 Fundamentals; John Wiley & Sons Ltd.; Wilson, Stephen (Editor-in-chief); Bernath, Peter F. (Associate Editor); McWeeny; Roy (Associate Editor).* McWeeny, R.

[18] The classical kinetic term is proportional to m and survives in the limit $m \to \infty$. The quantum correction term is proportional to $1/m$ and vanishes in the limit. This analysis is in agreement with the interpretation (24) of the quantum correction term as a fluctuation.

[19] On the Quantum Correction For Thermodynamic Equilibrium **1932:** *Phys. Rev. 40(5), 749–759.* Wigner, E.

[20] Quantenmechanik und Gruppentheorie **1927:** *Z. Phys. A-Hadron Nucl. 46(1-2), 1–46.* Weyl, H.

[21] Quantum mechanics as a statistical theory **1949:** *Math. Proc. Cambridge 45(1), 99–124.* Moyal, J.E.

[22] Chemical Reactivity Dynamics and Quantum Chaos in Highly Excited Hydrogen Atoms in an External Field: A Quantum Potential Approach **2002:** *Int. J. Mol. Sci. 3, 338–359.* Chattaraj, P. K.; Maiti, B.

[23] Bader's interatomic surface and Bohmian mechanics **2002:** *Europhys. Lett. 57(1), 20–24.* Site, L. Delle.

[24] Correspondence between the one-electron potential and the Laplacian of the electron density as indicators of proton affinity **1999:** *Chem. Phys. Lett. 301(1–2), 53–58.* Chan, Wai-To; Hamilton, I.P.

[25] Atoms in Molecules **1994:** *Oxford University Press; Oxford.* Bader, R. F. W.