

On the quantum-classical character of the quantum wavefunction of material particles

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ABSTRACT. We show that the quantum wavefunction, interpreted as the probability density of finding a single non-localized quantum particle that evolves according to classical laws of motion, is an intermediate description of a material particle between the quantum and the classical realms. Accordingly, classical and quantum mechanics should not be treated separately, a unified description in terms of the Wigner distribution function being possible. Although defined on classical phase space coordinates, the Wigner distribution function accommodates the non-localization property of quantum systems, and leads to the Schrödinger equation for the quantum wavefunction and to the definition of position and momentum operators.

1 Introduction

Quantum mechanics of material particles differs qualitatively from classical mechanics. In particular, the state of a classical localized particle as determined by position and momentum vectors \mathbf{r} and \mathbf{p} , respectively, is described in quantum mechanics by a vector $|\Psi\rangle$ in the Hilbert space, which in the Schrödinger formalism becomes a non-localized function Ψ of position or momentum. In turn, the classical \mathbf{r} and \mathbf{p} vectors, with Cartesian components x_i and p_i , respectively, become the operators $\hat{\mathbf{r}}$ and $\hat{\mathbf{p}}$ in quantum mechanics, with Cartesian components \hat{x}_i and \hat{p}_i , which act on the quantum state and satisfy the commutation relation

$$[\hat{x}_i, \hat{p}_j] = \hat{x}_i \hat{p}_j - \hat{p}_j \hat{x}_i = i\hbar \delta_{ij}. \quad (1)$$

The meaning of the wavefunction Ψ is not yet clear, but it is an appropriate tool for calculating the outcomes of a measurement of an arbitrary quantum observable.

The aim of this paper is to show that the wavefunction in quantum mechanics is a description of the quantum system that is intermediate between the quantum and the classical world, containing classical parameters in both the equation of motion and the initial conditions. We then argue that the net separation between the classical and quantum mechanical formalism has no sense, the only appropriate description of quantum mechanics being the phase space formalism. The Wigner distribution function provides a suitable link between the quantum and classical aspects of the wavefunction and allows the derivation of the Schrödinger equation and of the form of the position and momentum operators.

2 Quantum aspects the quantum wavefunction

The wavefunction of a quantum particle in the position representation, $\Psi(\mathbf{r})$, satisfies the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\Psi = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(\mathbf{r}, t)\Psi \quad (2)$$

where t is the time coordinate, m is the mass of the particle, and the Hamiltonian operator \hat{H} is obtained by replacing the position and momentum in the classical non-relativistic Hamiltonian $H(\mathbf{r}, \mathbf{p}, t) = \mathbf{p}^2/2m + V(\mathbf{r}, t)$ with the operators \mathbf{r} and $-i\hbar\nabla$, respectively, which act on $\Psi(\mathbf{r})$. Besides the wavefunction, which is commonly considered as quantum, there are two non-classical quantities in (2): the term $i\hbar$ on the left-hand-side and the form of the momentum operator, $\mathbf{p} = -i\hbar\nabla$. Indeed, unlike for a classical free particle starting from the origin of the coordinate system, for which $\mathbf{p} = m\mathbf{dr}/dt$ and \mathbf{p} is parallel to \mathbf{r} , in quantum mechanics \mathbf{p} is normal to the surface $\Psi(\mathbf{r}) = \text{const.}$, in a similar manner as the wavevector in optics is normal to the wavefront. (An operator $\hat{\mathbf{p}} = -i(\lambda/2\pi)\nabla$ canonically conjugate to \mathbf{r} can be also introduced in wave optics [1], the wavelength λ being analogous to $h = 2\pi\hbar$ and t in quantum mechanics being replaced by a spatial coordinate in wave optics.)

The phase space topology of classical and quantum particles are also different. In the one-dimensional case, in which the position is denoted by x and the momentum by p ($\hat{p} = -i\hbar\partial/\partial x$ in quantum mechanics), a classical particle is represented by a point in the two-dimensional (x, p) phase space, with an associated outer product $x \wedge p = (xp - px)/2 = 0$. Since the outer product represents the oriented area of the parallelogram

with sides \hat{x} and \hat{p} [2], a quantum particle, for which $\hat{x} \wedge \hat{p} = i\hbar/2$ according to the commutation relation, is localized in a phase space area $\hbar/2$. (A similar change in the phase space topology occurs in wave optics with regard to ray optics.) The existence of a minimum phase space area bestows to the quantum wavefunction its wave-like behavior and implies the possibility of interference of material particles. This change in phase space topology, which is independent of the wavefunction, is the essence of quantum behavior. The specific form of the wavefunction intervenes only in the uncertainty relation,

$$\Delta x \cdot \Delta p \geq \hbar/2 \quad (3)$$

where $(\Delta x)^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$, a similar relation existing for Δp , with the expectation value of any function of x and p , $f(x, -i\hbar\partial/\partial x)$, calculated as $\langle f(x, -i\hbar\partial/\partial x) \rangle = \int \Psi^*(x, t) f(x, -i\hbar\partial/\partial x) \Psi(x, t) dx$. Of course, when products of x and p are encountered, their order is not arbitrary. The uncertainty in x (p) can be regarded as the spatial extent of the wavefunction in position (momentum).

3 Classical aspects of the quantum wavefunction

In the Schrödinger equation (2), as in any formulation of quantum mechanics, the time coordinate t and the mass m of the quantum particle are classical parameters, with no associated operators. Moreover, the argument \mathbf{r} of the wavefunction and of the potential energy in (2) is not different from the classical position vector. An insightful demonstration that the time coordinate of a quantum system interacting with an environment characterized by semiclassical dynamical variables originates in the classical evolution of the environment and the wavefunction of the quantum system depends on the environmental position variables (although this dependence is not explicit in the Schrödinger equation), can be found in [3].

If the classicality of time, mass and position in (2) is common knowledge, the identification of classical aspects of the wavefunction itself is not. It is the preparation process, which involves the particle source and other filtering devices, that is responsible for the form of the initial quantum state. Then, propagating through the set-up the wavefunction interacts continuously with different parts of the set-up, for example filters and slits, and retains information about them [4,5]. For example, in interference experiments involving slits the wavefunction is projected into a (classical) position state (the position being that of the slit), which

is considered as the initial wavefunction [6]. Analogously, multiple slits generate an initial wavefunction that depends on the (classical) distance between the slits, while detectors that make a determined (classical) angle θ with a slit, measure the momentum eigenstates [6] and determine the final state of the wavefunction.

Moreover, in practically all cases, the engineering of the quantum state of a particle implies interaction with classical fields: the preparation of the states of trapped ion and the transition frequencies between such states depend on classical electric and/or electromagnetic fields, with specific phases and frequencies, and classical time intervals of interaction with these fields [7-10]. In addition, atoms can be trapped, guided, and focused by the forces exerted by intense and inhomogeneous electromagnetic fields with appropriately chosen wavelengths or by current carrying wires, and electrons are manipulated by classical electric and magnetic fields [11]. So, the macroscopic environment influences the wavefunction from its generation up to its detection; the macroscopic world enters the quantum mechanical description through the parameters in the Schrödinger equation (time, position variables, often potential energy expressions) and through boundary conditions (the form of the initial wavefunction), the eigenstates of the observable to be measured (determined by a generally classical measuring apparatus) determining the outcome probabilities of possible measurement results, which test the validity of quantum mechanics. It is hazardous, therefore, to consider the Schrödinger equation as a purely quantum description of the system. One should consider it rather as an intermediate description of a particle between the microscopic (quantum) and macroscopic (classical) realms.

Another argument for the existence of a classical aspect of the wavefunction is based on the misleading assertion that the addition law of classical probabilities is invalidated by quantum interference. The probability of the photon reaching a certain point on the screen when both slits are open is not equal to the sum of probabilities of photons reaching that point when only one of the slits is open, because what must be added are the probabilities of the photon passing through each one of the slit when both are open [12]. When this addition is performed classically we obtain the quantum result, i.e. interference fringes on the screen.

Moreover, the quantum mechanical postulates are intrinsically related to classical measuring devices. In particular, the validity of the postulate, which states that a measurement of an observable described by

an operator always yields one of its eigenvalues, depends on the strength of the interaction between the quantum system and the measuring apparatus; in weak measurements the result can even lie outside the range determined by the operators' eigenvalues [13,14]. The strong measurements, which fulfill the quantum mechanical postulate, are those in which the measuring apparatus behaves classically.

4 Meaning of the quantum wavefunction

In our opinion, the wavefunction is the spatial probability density of finding a single quantum particle, which evolves according to classical laws but differs from a classical particle because it cannot be localized in a phase space area smaller than $\hbar/2$ (smaller than $(\hbar/2)^n$ for an n -dimensional wavefunction or, generally, smaller than a canonical invariant quantum blob [4,15]). In this sense, contrary to the position defended by Schrödinger [16] and de Broglie, who postulated the coexistence of phase-matched particles and guided-waves [17], the wavefunction does not exist as a real entity independent of our knowledge about it, as do, in our opinion, quantum particles. The wavefunction has, however, an epistemological character (as argued by Born [18]) since it can predict the results of future experiments from the knowledge of the present state of the system and the configuration of the measuring set-up.

The dissociation in meaning of the wavefunction from the quantum particle is imposed by experiments (in particular, interference), which show that the wavefunction has a spatial extension that is not compatible with the localized character of the detected quantum particle. The wavefunction cannot represent the quantum particle, whose character does not change even if the wavefunction is modified by canonical transformations. The existence of the minimum phase space area $\hbar/2$ does not mean that the quantum particle has this extent, but that a quantum particle cannot exist unless this phase space area is available. The minimum phase space area should be seen as a sort of self-sustained correlation area, necessary for the stability of the quantum particle.

The wavefunction interpretation as a probability amplitude for a single quantum system as opposed to a parameter with physical meaning only as ensemble average was already defended in [19]. In this reference, the wavefunction of a single particle acquires realistic interpretation through a protective (or weak) measurement during which the wavefunction does not collapse and hence the expectation values of several, even non-commuting observables can be determined. The quantum

wavefunction can then be recovered from measurements of a sufficient number of observables performed on a single system and not on an ensemble of identical copies. Protective measurements can be generalized to determine the density matrix of a single quantum system [20].

As an insight into the meaning of wavefunction, as corresponding to classically moving particles, it was shown that the wavefunction is the probability density of classically propagating particles, classical mechanics describing exactly the propagation of discontinuities in the quantum wavefunction [21]. Further support for the classical propagation law of quantum particles is found in [22], where the evolution laws of quantum observables are derived from the classical Hamilton equations with the only additional assumption of phase space non-commutativity. This result states that the quantum particle differs from the classical one only with regard to phase space localizability.

Because the quantum particle is not point-like, although satisfying classical laws of motion, our interpretation of the wavefunction differs from that in Bohmian quantum mechanics, which implies classical particles that follow trajectories perfectly determined by the classical equation of motion complemented with an additional wavefunction-dependent quantum potential [23]. Another argument toward our interpretation of the wavefunction is that the classical limit of a quantum state is an ensemble of orbits and not just a single orbit [24], as is usually assumed by a superficial interpretation of the Ehrenfest's theorem.

5 Reconciliation of the classical and quantum aspects of the quantum Wavefunction

Mainstream quantum mechanics states that the quantum and classical descriptions of the world are completely different but, as seen in the previous sections, the quantum wavefunction carries information about the classical environment. These points of view can be reconciled using the Wigner distribution function (WDF) formalism of quantum mechanics, which employs classical phase space coordinates. For pure quantum states the WDF is defined as [25]

$$W(x, p; t) = h^{-1} \int \Psi^* \left(x - \frac{x'}{2}; t \right) \Psi \left(x + \frac{x'}{2}; t \right) \exp(-ipx'/\hbar) dx', \quad (4)$$

the phase space formalism being analogous to that of Heisenberg and Schrödinger. Among the properties of the WDF [26-30] we mention that the wavefunction can be recovered (up to a constant factor)

from the WDF through an inverse Fourier transform: $\Psi(x)\Psi^*(0) = \int W(x/2, p) \exp(ipx/\hbar) dp$ and that the quantum probability density is given by: $|\Psi(x)|^2 = \int W(x, p) dp$. The fact that the WDF, although real, is not positive defined, as a classical distribution function, should not be a problem since negative regions of WDF, corresponding to “dark” rays in wave optics, are necessary for interference and diffraction [31]. An alternative set of postulates to that of standard quantum mechanics has been defined in terms of the WDF [4], including an interpretation of the measurement problem that allows the inclusion of classical measuring devices in the phase space formalism of quantum mechanics. This phase space representation provides even a more refined quantum-classical correspondence rule than the Bohr-Heisenberg correspondence principle [32].

Unlike in quantum mechanics, x and p commute in phase space. Nevertheless, the commutation relation is incorporated in the definition of the WDF, as we show below by deriving both the Schrödinger equation and the uncertainty relations from the evolution law of the WDF. To our knowledge, this derivation is performed here for the first time.

The evolution law of the WDF

$$\frac{\partial W}{\partial t} + \frac{p}{m} \frac{\partial W}{\partial x} - \frac{\partial V}{\partial x} \frac{\partial W}{\partial p} = \sum_{n=1}^{\infty} \frac{(\hbar/2i)^{2n}}{(2n+1)!} \frac{\partial^{2n+1} V}{\partial x^{2n+1}} \frac{\partial^{2n+1} W}{\partial p^{2n+1}} \quad (5)$$

is usually derived from the Schrödinger equation (2). However, the process can be reversed, and (2) can be derived from (5), since it can be demonstrated that the Fourier transform of the real-valued WDF over the momentum variable can always be written as [33]

$$Z(x, x'/2; t) = \int W(x, p; t) \exp(ipx'/\hbar) dp = \Psi^*(x-x'/2; t) \Psi(x+x'/2; t). \quad (6)$$

(The demonstration in [33] refers to a classical, positive-definite WDF that satisfies the Liouville equation, i.e. the left-hand-side of (5), but only the real-valuedness of the WDF is necessary to show (6).) In order to derive from (5) the Schrödinger equation, we follow the treatment in [34], but start from different premises: in our case the system is completely described by the quantum WDF (4) instead of a positive-defined phase space probability density for point-like classical particles, which follows the evolution law (5). First, we derive the evolution law for the Wigner-Moyal transformation $Z(x, x'/2; t)$ in (6), which can be

considered as a characteristic function over the momentum space. This equation,

$$\frac{\partial Z}{\partial t} - i \frac{\hbar}{m} \frac{\partial^2 Z}{\partial x \partial x'} + i \frac{x'}{\hbar} \frac{\partial V}{\partial x} Z = - \sum_{n=1}^{\infty} i \frac{x'}{\hbar} \frac{(x'/2)^{2n}}{(2n+1)!} \frac{\partial^{2n+1} V}{\partial x^{2n+1}} Z, \quad (7)$$

can be expressed in the new variables $y = x + x'/2$, $y' = x - x'/2$ as

$$\left[\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial y'^2} \right) - [V(y) - V(y')] \right] Z(y, y'; t) = -i \hbar \frac{\partial}{\partial t} Z(y, y'; t), \quad (8)$$

which is the analog of the Schrödinger equation for the quantum wavefunction. The latter is then finally obtained from (8) and (6). Unlike in [34] the derivation of (8) does not rely on x' being an infinitesimal parameter, which implies the neglect of the right-hand-side of (7).

For the classical phase space coordinates x and p the commutator $[x, p]$ vanishes as applied on the WDF, which means that the WDF is well defined on any phase space point. However, the uncertainties in x and p still satisfy (3) if the expectation value is understood as phase space average. More exactly, defining the phase space expectation value of a function of x and p as $f(x, p) = \int f(x, p) W(x, p) dx dp$ (the WDF is considered normalized) the average phase space values for the position and momentum operators become identical to the expectation values for the operators $\hat{x} = x$ and $\hat{p} = -i\hbar \partial / \partial x$ in standard quantum mechanics, respectively, acting on the quantum wavefunction:

$$\begin{aligned} \bar{x} &= \int \Psi^* \left(x - \frac{x'}{2}; t \right) x \Psi \left(x + \frac{x'}{2}; t \right) \exp(-ipx'/\hbar) dx' dx dp \\ &= \int \Psi^*(x; t) x \Psi(x; t) dx = \langle \hat{x} \rangle \end{aligned} \quad (9)$$

$$\begin{aligned} \bar{p} &= \int \Psi^* \left(x - \frac{x'}{2}; t \right) p \Psi \left(x + \frac{x'}{2}; t \right) \exp(-ipx'/\hbar) dx' dx dp \\ &= \int \Psi^*(x; t) \left(-i\hbar \frac{\partial}{\partial x} \right) \Psi(x; t) dx = \langle \hat{p} \rangle \end{aligned} \quad (10)$$

In general, the expectation value of any function of \hat{x} and \hat{p} can be calculated as a phase space average with the WDF as a weighting function, i.e. as $\langle f(\hat{x}, \hat{p}) \rangle = \overline{f(x, p)} = \int f(x, p) W(x, p) dx dp$.

Equations (9) and (10) can serve to define the non-commutative position and momentum operators. The commutation relation is replaced in the phase space treatment of quantum mechanics by commuting operators that act on an extended distribution function; the quantum parameter \hbar is incorporated in the definition of the WDF through the exponential term in (4), which relates the classical x and p variables through a Fourier transform describing a wave-like object extended in the (x,p) plane. The accommodation of the quantum parameter \hbar does not necessarily require the formalism of quantum operators; it is enough to replace the point-like particles with extended particles. The WDF can thus treat in a unified manner both quantum and classical systems. Moreover, the WDF of quantum systems can be obtained from measurements of its marginal distributions for homodyne observables, which are easily determined experimentally [35].

6 Conclusions

We have argued that the quantum wavefunction is an intermediate description of a material quantum particle between the quantum and classical realms. The quantum wavefunction is in our view a probability density of finding a single quantum particle, which evolves according to classical mechanical laws but is not classical since it cannot be localized in a phase space area smaller than $\hbar/2$ (for one-dimensional systems). Accordingly, a unified description of classical and quantum mechanics is possible in terms of the WDF which, although defined on classical phase space coordinates, includes in its definition the non-localization property of quantum systems and leads to both the Schrödinger equation for the quantum wavefunction and to the definition of position and momentum operators acting on it.

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