To know the quantum mechanical state of a system implies not only statistical restrictions on the results of measurements

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Abstract. Using the one-dimensional Schrödinger equation as an example, it is shown that for any self-adjoint operator it is possible to uniquely predict the value of the corresponding observable (including momentum, kinetic and total energy of the particle) at that spatial point where the particle will be accidentally detected at a given instant of time. It is shown that the Schrödinger formalism ensures the fulfillment of the relations of wave-particle duality, which connect the energy and momentum of a particle with the frequency and wave number of the wave function, for any spatial point and any instant of time.

1. Introduction

The concept of the wave function, as well as the Schrödinger equation, is at the heart of quantum mechanics, and it seems that their role is already well understood. But this is not the case! At the moment, only a small part of those physical properties that the wave function actually possesses is known. And this is the main reason why the question of an adequate physical interpretation of the wave function (and, as a consequence, the Schrödinger equation) remains open to this day.

Thus, in the very first phrase of his famous book [1], John Bell writes “To know the quantum mechanical state of a system implies, in general, only statistical restrictions on the results of measurements.” This traditional, purely “statistical” point of view is based on Born’s interpretation of the wave function and underlies all discussions about its ontological status. But such an interpretation leaves unrevealed those restrictions that the wave function imposes on the results of measurements of physical observables.

In contrast to classical mechanics, where knowing the state of a particle means knowing the values of its position and momentum, in quantum mechanics with Born’s interpretation a fundamentally different situation takes place: knowing the state of a particle does not imply now any restrictions on the values of its position and momentum. All observables are represented in quantum mechanics by the corresponding self-adjoint operators, and this theory tells us that the eigenvalues of an observable are exactly
those values that can be measured. But this restriction follows from the eigenvalues problem and has nothing to do with the state of the particle. And, since quantum mechanics does not predict the results of measuring the observable for a given state, there is reason to believe that they did not exist before the measurement, but arose during this measurement.

All this means that modern quantum mechanics actually deprives the microcosm of its physical reality (see also the recent article [2]). Moreover, this “statistical” point of view makes it impossible to interpret the Schrodinger equation written for the modulus and phase of the wave function. Indeed, only one of them – the continuity equation connecting the probability density and the probability flux density – has received a clear physical interpretation. As regards the second equation, its nature is not yet clear.

At first glance, the Bohm approach [3, 4] stands out against this background (see also de Broglie’s approach [5], the hydrodynamic approaches [6]). Bohm showed that if we introduce into quantum mechanics an additional postulate on the existence of single-particle trajectories, then based on the phase of the wave function, one can determine the momentum of a particle, and on the basis of its modulus, in addition to the probability density, one can determine the ’quantum mechanical potential’, which enters together with the ordinary potential into the second equation for the modulus and phase of the wave function.

Thus, in Bohmian approach, the quantum mechanical state implies not only statistical restrictions on the measurement results. In addition, the equation with a ’quantum mechanical potential’ resembles the equation of motion for a classical particle, and the derivation of this equation could be considered an important achievement of Bohm mechanics, if not for the ’quantum mechanical potential’, the ontological status of which remains unclear. In addition, the prospect of reconciling the postulate about one-particle trajectory with the original postulates of quantum mechanics also remains unclear. As a consequence, Bohm’s finds did not in any way affect the status of the phase (and modulus) of the wave function in the framework of standard quantum mechanics (of course, we have to point out the approach [7] where this phase is connected with the probability current density).

At the same time, as will be shown in this work, the Schrödinger formalism, reformulated for the modulus and phase of the wave function, hides in itself a richer physics than that which has been known until now. And in order to discover these properties, there is no need to introduce any additional postulates, for this we will use the standard formula in quantum mechanics for calculating the average values of observables.

2. Physical meaning of the modulus and phase of the wave function

Let us have the wave function
\[ \psi(x, t) = \sqrt{w(x, t)} e^{i\phi(x, t)}, \]
where $w(x, t)$ and $\phi(x, t)$ are real functions; $\int_{-\infty}^{\infty} w(x, t)dx = 1; w(x, t) \geq 0$. According to Max Born, $w(x, t) = |\psi(x, t)|^2$ is the probability density. In what follows, the function $w(x, t)$, characterizing the corresponding quantum ensemble, will be called the probability field (or, for brevity, the $w$-field).

To clarify the physical meaning of the phase of the wave function, let us introduce, with taking into account the properties of the phase of the plane monochromatic wave $e^{i(kx-\omega t)}$, the functions $k(x, t) = \phi_x(x, t), \omega(x, t) = -\phi_t(x, t)$; (2) for any function $f(x, t)$ let $f_t(x, t) \equiv \partial f(x, t)/\partial t, f_x(x, t) \equiv \partial f(x, t)/\partial x, f_{xx}(x, t) \equiv \partial^2 f(x, t)/\partial x^2$: the function $k(x, t)$ will be called the wave-number field, or the $k$-field, and the function $\omega(x, t)$ will be the frequency field, or the $\omega$-field. Our goal is to clarify the relationship of these wave characteristics of the quantum ensemble with corpuscular ones.

Let’s write the average value of the momentum operator $\hat{p} = -i\hbar \frac{d}{dx}$ in the form

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^*(x, t)\hat{p}\psi(x, t)dx \equiv \int_{-\infty}^{\infty} p(x, t)w(x, t)dx,$$

(3)

where

$$p(x, t) = \frac{\text{Re} (\psi^*(x, t)\hat{p}\psi(x, t))}{\psi^*(x, t)\psi(x, t)} = \frac{\hbar}{w(x, t)}\text{Im} (\psi^*(x, t)\psi_x(x, t)) = \hbar \phi_x(x, t) = \hbar k(x, t).$$

(4)

As is seen, the phase of the wave function $\phi(x, t)$, like the square of the modulus $w(x, t)$, has a clear physical meaning. The standard rule for calculating the expected values of physical quantities uniquely determines the function $p(x, t)$ for a given state, which we will call the momentum field of the ensemble. The relations (4) show that this ‘corpuscular’ characteristic is associated with the wave characteristic in full accordance with the wave-particle duality: $p(x, t) = \hbar k(x, t)$. It also follows from this that in a quantum ensemble, in contrast to the classical one, the coordinate and momentum of a particle are not independent quantities.

Note again, the definition of momentum in terms of the phase of the wave function, similar to the definition (1), also appears in Bohmian quantum mechanics [3]. But in [3] the coordinate $x$ depends on $t$, and the momentum is defined as the momentum of the particle on the trajectory $x(t)$. At the same time, in our approach, the function $p(x, t)$ depends on two independent variables $x$ and $t$, and it is introduced on the basis of the formal for calculating the average value of the momentum (see the first equality in [3]) which is standard in quantum mechanics.

For a quantum ensemble, in addition to the momentum field $p(x, t)$, the kinetic energy field $K(x, t)$ can be defined. For this, we write the average value of the kinetic energy operator $\hat{K} = \hat{p}^2/2m$ in the form

$$\langle K \rangle = \frac{1}{2m} \int_{-\infty}^{\infty} \psi^*(x, t)\hat{p}^2\psi(x, t)dx \equiv \int_{-\infty}^{\infty} K(x, t)w(x, t)dx,$$

(5)
where
\[ K(x, t) = \frac{1}{2m} [p(x, t)]^2 + K_w(x, t); \quad K_w(x, t) = \frac{\hbar^2}{4m} \left[ \frac{1}{2} \left( \frac{w_x(x, t)}{w(x, t)} \right)^2 - \frac{w_{xx}(x, t)}{w(x, t)} \right]. \] (6)

As a consequence, the average value of the total energy of a particle with the Hamiltonian \( \hat{H} = \hat{p}^2 / 2m + V(x) \), where \( V(x) \) is the potential energy of the particle, can be written as
\[ \langle E \rangle = \int_{-\infty}^{\infty} E(x, t) w(x, t) dx; \quad E(x, t) = K(x, t) + V(x). \] (7)

Note that the kinetic energy field \( K(x, t) \) contains two contributions: the first contribution, in a sense, is of a corpuscular nature, and the contribution \( K_w(x, t) \) is of a wave nature. And here it is necessary to underline that the contribution of \( K_w(x, t) \) coincides with the Bohm 'quantum mechanical potential'. But in our approach, this contribution has a different physical meaning.

Obviously, on the basis of the wave function describing the state of a spinless particle, one can introduce a field of any physical quantity \( O \) with the self-adjoint operator \( \hat{O} \):
\[ \langle O \rangle = \int_{-\infty}^{\infty} \psi^*(x, t) \hat{O} \psi(x, t) dx \equiv \int_{-\infty}^{\infty} O(x, t) w(x, t) dx; \quad O(x, t) = \text{Re} \left[ \frac{\psi^*(x, t) \hat{O} \psi(x, t)}{\psi^*(x, t) \psi(x, t)} \right]. \]

So the information inherent in the wave function about the physical properties of quantum ensembles is much richer than previously thought.

In conclusion, we note that in those problems in which the bound stationary states of the particle (corresponding to the eigenvalues of the energy operator from the discrete spectrum) are real, the phase of the wave function is zero. As a consequence, the field of pulses is also equal to zero, and the field of kinetic energy is determined only by the second, 'wave' contribution.

3. The physical meaning of the equations for the modulus and phase of the wave function

Our next step is to get the equations for the (squared) modulus and phase of the wave function. For this, we substitute into the Schrödinger equation
\[ i\hbar \frac{\partial \psi(x, t)}{\partial t} = \hat{H} \psi(x, t) \]
Exp. (1) for \( \psi(x, t) \). As a result, we obtain two (real) equations
\[ w_t + \frac{\hbar}{m} (w_x \phi_x + w \phi_{xx}) = 0, \quad \hbar \phi_t + E = 0. \] (8)
If we now take into account the equalities \( \hbar \phi_x = p \) and \( \phi_x = -\omega \) (see (2) and (4)), then Eqs. (8) take the form
\[ w_t(x, t) + j_x(x, t) = 0, \quad \hbar \omega(x, t) - E(x, t) = 0, \] (9)
where \( j(x, t) = w(x, t)p(x, t)/m \) is the probability flux density, and the function \( E(x, t) \) is determined by Exps. (7) and (6). The first equation in (9) is the well-known equation...
of continuity, and the second, obtained for the first time, relates the particle energy to the frequency of the wave function, which are functions of $x$ and $t$.

Let us now combine the second equation in (9) with the relation (11) -

$$E(x,t) = \hbar \omega(x,t), \quad p(x,t) = \hbar k(x,t).$$

Hence, it can be seen that the Schrödinger formalism guarantees the fulfillment of the wave-particle duality, not only in the case of the de Broglie wave, but also for any wave function satisfying the time-dependent Schrödinger equation. Moreover, Eqs. (10) are fulfilled at every spatial point and at every instant of time.

As is known, the conservation law of the 'number of particles' follows from the continuity equation, according to which the normalization condition $\int_{-\infty}^{\infty} w(x,t)dx = 1$ is fulfilled for any moment of time $t$. To find out which 'conservation law' follows from the equation $\hbar \omega(x,t) - E(x,t) = 0$, we have to differentiate it term by term with respect to $x$ and to write it in the form $p_t + E_x = 0$. Further, taking into account the continuity equation $w_t + j_x = 0$, we obtain

$$\int_{-\infty}^{\infty} (wp_t + pw_t)dx + \int_{-\infty}^{\infty} (wE_x + pj_x)dx = 0.$$  \hspace{1cm} (11)

It is easy to check that $wE_x + pj_x = wV_x + Q_x$, where

$$Q(x,t) = \frac{1}{m} \frac{\hbar^2}{4m} \left( \frac{w_x^2}{w} - w_{xx} \right).$$

Taking into account the Ostrogradsky-Gauss theorem, $\int_{-\infty}^{\infty} Q_xdx = 0$ if the function $Q(x,t)$ is equal to zero at infinity (obviously, this condition is certainly satisfied for Gaussian wave packets). As a result, we obtain the Ehrenfest equation

$$\frac{\partial\langle p \rangle}{\partial t} = -\left\langle \frac{\partial V}{\partial x} \right\rangle.$$  \hspace{1cm} (12)

Note that for a stationary state of a particle in an infinitely deep potential well, the function $Q(x,t)$ is identically equal to a constant that does not depend on the state number.

4. Conclusion

It is shown that the wave function assumes not only statistical limitations on the measurement results. It also predicts the values of physical quantities (to which self-adjoint operators correspond) at any spatial point at which a particle will (accidentally) be found at a given moment in time. In addition, it is shown that at each spatial point and at each moment of time the predicted values of the momentum and total energy of the particle are related, by the relations to underlie the particle-wave dualism, with the wave number and frequency of the wave function, which are determined through its phase.
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