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From probabilities to mathematical structure of quantum mechanics

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ABSTRACT

A large part of the mathematical formalism of quantum mechanics including the probability density, probability density current, uncertainty relations, wave function, momentum operator, kinetic energy, commutation relations and potentials is related to the probabilistic character of quantum measurements. Equations of motion of quantum mechanics can be obtained from the relativistic invariance of the space–time Fisher information. Some properties of potentials and existence of antiparticles are related to the CPT symmetry. Operators representing parallel or serial physical events in experimental setups can be represented by the sum or product of the corresponding operators.

1. Introduction

The aim of this article is to summarize and extend results of our previous investigations [1–7] in which the approach to understanding quantum mechanics can be described by the title of this paper. Due to limited number of pages, the discussion in this paper is made as simple as possible. Somewhat different approach to obtaining the most important laws of physics can be found in Refs. [8,9].

2. Uncertainty relations

Uncertainty relations, one of the fundamental results of quantum mechanics, have been studied in a large number of papers (see e.g. Refs. [10–15,1–5]; for a detailed review, see Ref. [16]). The standard approach to their derivation is based on the wave function ψ. In this section, we will show that uncertainty relations can be obtained directly from the probabilistic description of measurements.

To be more concrete, we discuss measurement of the coordinate x. For the sake of simplicity, we consider the one-dimensional space only.

Results of repeated measurements of the coordinate x can be characterized by the mean values

$$\langle x \rangle = \int x\rho(x,t)\,dx, \tag{1}$$

$$\langle x^2 \rangle = \int x^2\rho(x,t)\,dx, \tag{2}$$

where the integration is carried out over the whole space, $\rho(x,t) \geq 0$ is a normalized probability density

$$\int \rho\,dx = 1 \tag{3}$$

and

$$\lim_{x\to\pm\infty} x^n\rho = 0, \quad n = 0,1,2. \tag{4}$$

Normalization condition (3) and Eq. (4) are assumed to be valid at all times t.

First, we perform integration by parts with respect to the variable x in Eq. (3) and get [3]

$$x\rho|_{x=-\infty}^{\infty} - \int x\frac{\partial\rho}{\partial x}\,dx = 1. \tag{5}$$

Assuming that the first term in this equation equals zero (see Eq. (4)) we obtain the equation

$$\int x\frac{\partial\rho}{\partial x}\,dx = -1. \tag{6}$$

This simple result has interesting consequences.

Putting

$$u = x\sqrt{\rho} \tag{7}$$

and

$$v = \frac{1}{\sqrt{\rho}}\frac{\partial\rho}{\partial x} \tag{8}$$

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we get from the Schwarz inequality

$$(u,u)(v,v) \geq |(u,v)|^2 \tag{9}$$

for $(u,v) = \int u^* v \, dx$ the "uncertainty" relation [1–5,17]

$$\langle x^2 \rangle I \geq 1. \tag{10}$$

Here,

$$I = \int \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 dx \tag{11}$$

is the so-called Fisher information known from mathematical statistics [17,18].

The "uncertainty" relation (10) is independent of the concrete meaning of the variable x. It means that similar relations exist not only in physics but also in any probabilistic theory analogous to that described above.

3. Complex wave function

For physical systems, we must give not only the probability density $\rho(x,t)$ but also some quantity describing the motion of a particle in space.

By analogy with continuum mechanics, it is possible to introduce the probability density current j related to the "velocity" v [3]

$$j = \rho v. \tag{12}$$

The quantities ρ and v can be expressed in terms of two real functions $s_1 = s_1(x,t)$ and $s_2 = s_2(x,t)$ as follows:

$$\rho = e^{-2s_2/\hbar}, \tag{13}$$

$$v = \frac{1}{m} \frac{\partial s_1}{\partial x}. \tag{14}$$

Here, $\hbar$ is the Planck constant and m is the mass of the particle. The last equation has a form analogous to that between the velocity v and momentum p in classical mechanics $v = p/m$, where $p = (\partial S/\partial x)$ and S is the classical Hamilton action.

Then, introducing the complex wave function $\psi(x,t)$

$$\psi = e^{(is_1 - s_2)/\hbar}, \tag{15}$$

we get two basic formulae of quantum mechanics for the probability density

$$\rho = |\psi|^2 \tag{16}$$

and probability density current [3]

$$j = \frac{\hbar}{2mi} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right). \tag{17}$$

We see that instead of ρ and j, the state of the system can be described by the functions s_1 and s_2 or, equivalently, the complex wave function ψ (see also Refs. [1–5]). From this point of view, the complex wave function is a very useful mathematical representation which carries all necessary information and has further mathematical advantages discussed below.

According to Eqs. (12)–(14), the probability density ρ and probability density current j do not change if the function s_1 is replaced by $s_1 + \alpha$, where α is a real constant. It agrees with quantum mechanics where the wave functions ψ and $\psi \exp(i\alpha)$ give the same physical state.

By analogy with the classical momentum $p = mv$ we can introduce also the momentum operator $\hat{p} = -i\hbar(\partial/\partial x)$ having the property

$$p = mv = \frac{\partial s_1}{\partial x} = \frac{\Re(\psi^* \hat{p} \psi)}{\rho} \tag{18}$$

in agreement with the discussion given above. According to this equation, the mean momentum can be calculated as

$$\int mv\rho \, dx = \int \Re(\psi^* \hat{p} \psi) \, dx. \tag{19}$$

Taking into consideration that the operator $\hat{p}$ has a real eigenvalue spectrum we get the well-known formula

$$\langle \hat{p} \rangle = \int \psi^* \hat{p} \psi \, dx. \tag{20}$$

It follows from Eqs. (4) an (13) that the mean value of the momentum operator is real

$$\langle \hat{p} \rangle = \int \frac{\partial s_1}{\partial x} \rho \, dx + i \int \frac{\partial s_2}{\partial x} \rho \, dx = \int \frac{\partial s_1}{\partial x} \rho \, dx. \tag{21}$$

For probability distributions that are close to zero everywhere except for a very narrow region along the classical trajectory $x_{cl} = x_{cl}(t)$ the probability density $\rho(x,t)$ can be replaced by the function $\delta(x - x_{cl})$. Denoting the corresponding limit of the function s_1 as $S = S(x_{cl})$ we get the formula known from classical mechanics [19,7]

$$p = \frac{\partial S}{\partial x}. \tag{22}$$

4. Heisenberg uncertainty relation

To derive the standard Heisenberg uncertainty relation we substitute Eqs. (15) and (16) into Eqs. (10) and (11). The resulting uncertainty relation has the form [3–5]

$$\langle x^2 \rangle I \geq 1, \tag{23}$$

where

$$I = \frac{4}{\hbar^2} \int \left(\frac{\partial s_2}{\partial x} \right)^2 e^{-2s_2/\hbar} \, dx. \tag{24}$$

Now we note that

$$I \leq I', \tag{25}$$

where

$$I' = \frac{4}{\hbar^2} \int \left[\left(\frac{\partial s_1}{\partial x} \right)^2 + \left(\frac{\partial s_2}{\partial x} \right)^2 \right] e^{-2s_2/\hbar} \, dx = 4 \int \left| \frac{\partial \psi}{\partial x} \right|^2 dx = \frac{4}{\hbar^2} \int |\hat{p}\psi|^2 dx \tag{26}$$

is the generalized Fisher information [3].

Physical importance of I' is given by the fact that it takes into account not only the form of the probability distribution given by ρ (or s_2) but also an analogous distribution given by j (or s_1 and s_2). Except for a numerical factor, the kinetic energy in quantum mechanics

$$T = \int |\hat{p}\psi|^2 \, dx/(2m) = \frac{\hbar^2}{8m} I' \tag{27}$$

equals the generalized Fisher information I'.

Evident uncertainty relation for I' following from Eqs. (23) and (25):

$$\langle x^2 \rangle I' \geq 1 \tag{28}$$

can be written also in a more familiar form with the momentum operator

$$\langle x^2 \rangle \int |\hat{p}\psi|^2 \, dx \geq \frac{\hbar^2}{4}. \tag{29}$$

This relation has to be valid independently of the choice of the origins a and b of the coordinate systems for measurement of the coordinate and momentum (see also Ref. [3])

$$\int (x-a)^2 |\psi|^2 \, dx \int |(\hat{p}-b)\psi|^2 \, dx \geq \frac{\hbar^2}{4}. \tag{30}$$

Calculating the minimum of the left-hand side of this relation with respect to a and b we get the well-known Heisenberg uncertainty relation [3]

$$\int (x-\langle x \rangle)^2 |\psi|^2 \, dx \int |(\hat{p}-\langle \hat{p} \rangle)\psi|^2 \, dx \geq \frac{\hbar^2}{4}. \tag{31}$$

In agreement with the above discussion, this uncertainty relation can be replaced by two stronger ones [4,5]

$$\langle (\Delta x)^2 \rangle \langle (\Delta p_1)^2 \rangle \geq \left\langle (x-\langle x \rangle)\left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle\right) \right\rangle^2 \tag{32}$$

and

$$\langle (\Delta x)^2 \rangle \langle (\Delta p_2)^2 \rangle \geq \hbar^2/4. \tag{33}$$

Here, the mean value of the function $F(x)$ is defined as

$$\langle F(x) \rangle = \int F(x) |\psi|^2 \, dx \tag{34}$$

and

$$\int |(\hat{p}-\langle \hat{p} \rangle)\psi|^2 \, dx = \langle (\Delta p_1)^2 \rangle + \langle (\Delta p_1)^2 \rangle, \tag{35}$$

$$\langle (\Delta p_1)^2 \rangle = \left\langle \left(\frac{\partial s_1}{\partial x}\right)^2 \right\rangle - \left\langle \frac{\partial s_1}{\partial x} \right\rangle^2, \tag{36}$$

$$\langle (\Delta p_2)^2 \rangle = \left\langle \left(\frac{\partial s_2}{\partial x}\right)^2 \right\rangle - \left\langle \frac{\partial s_2}{\partial x} \right\rangle^2 = \left\langle \left(\frac{\partial s_2}{\partial x}\right)^2 \right\rangle. \tag{37}$$

The first quantity $\langle (\Delta p_1)^2 \rangle$ depends on $(\partial s_1/\partial x)$ and ρ and can be different from zero for the nonzero probability density current j only. The second quantity $\langle (\Delta p_2)^2 \rangle$ appearing in the uncertainty relation (33) depends only on the envelop of the wave packet given by s_2 and is independent of j. Therefore, the separation of $\int |(\hat{p}-\langle \hat{p} \rangle)\psi|^2 \, dx$ into two parts given above has a good physical meaning. General discussion including the multidimensional case and the mixed states can be found in Refs. [4,5].

5. Commutation relation

Eqs. (6) and (16) yield

$$\int x \left(\frac{\partial \psi^*}{\partial x}\psi + \psi^* \frac{\partial \psi}{\partial x}\right) dx = -1. \tag{38}$$

By multiplying this equation by $-i\hbar$ we get

$$\int \left[-\left(-i\hbar \frac{\partial \psi}{\partial x}\right)^* x\psi + \psi^* x \left(-i\hbar \frac{\partial \psi}{\partial x}\right)\right] dx = i\hbar. \tag{39}$$

Assuming that $-i\hbar(\partial/\partial x)$ is the hermitian operator we obtain the equation

$$\int \psi^* \left[x, -i\hbar \frac{\partial}{\partial x}\right] \psi \, dx = i\hbar. \tag{40}$$

This result shows that the commutation relation between the coordinate x and $-i\hbar(\partial/\partial x)$ is closely related to Eqs. (6) and (16) and can be obtained even without the prior knowledge of the momentum operator $\hat{p}$. It is to be noted that the calculation given above is not a general proof of the commutation relation $[x, \hat{p}] = i\hbar$ that has to be valid for the inner product with arbitrary two quadratically integrable functions.

6. Equations of motion

To find equations of motion some additional principle must be applied. In physics, it is natural to require the relativistic invariance of equations of motion.

The first attempt to create a relativistically invariant generalization of the Fisher information I leads to the space–time information (see also Ref. [3])

$$J = \frac{1}{t_2 - t_1} \int_{t_1}^{t_2} \int \frac{1}{\rho} \left[\frac{1}{c^2} \left(\frac{\partial \rho}{\partial t}\right)^2 - \left(\frac{\partial \rho}{\partial x}\right)^2 \right] dx \, dt = const. \tag{41}$$

Here, we assume that the Fisher information J does not change its value *const.* if the Lorentz transformation is performed. The constant *const.* does not depend on the state of the measured particle, i.e., it is independent of ρ. The initial conditions at t_1 are given by $\rho(x, t_1)$. Since the initial conditions can be arbitrary including the case when $(\partial \rho/\partial x)^2$ has very small values for all x, we can conclude that $const. \geq 0$. The time integration is performed from t_1 when the initial conditions were given (first measurement or preparation of the particle in the state described by $\rho(x, t_1)$). At times $t \in (t_1, t_2)$ no measurement is performed. At t_2, the particle interacts with the measuring apparatus again (second measurement).

The corresponding equation of motion can be found by calculating the variation of Eq. (41) with respect to ρ and assuming that the variation of ρ can be arbitrary. It can be seen that the resulting equation for ρ is nonlinear and, therefore, it is very difficult to solve. The second problem is that the information J based on ρ only is the same for all the probability density currents j. For this reason, we will make the second attempt and use in analogy with Eq. (26) the relativistically invariant space–time information based on ψ (see also Ref. [3])

$$J' = \frac{4}{t_2 - t_1} \int_{t_1}^{t_2} \int \left(\frac{1}{c^2} \left|\frac{\partial \psi}{\partial t}\right|^2 - \left|\frac{\partial \psi}{\partial x}\right|^2 \right) dx \, dt = const. \tag{42}$$

This equation can be also written in the form

$$\int_{t_1}^{t_2} \int \left(\frac{1}{c^2} \left|\frac{\partial \psi}{\partial t}\right|^2 - \left|\frac{\partial \psi}{\partial x}\right|^2 - \frac{const.}{4} |\psi|^2 \right) dx \, dt = 0. \tag{43}$$

The variation of this equation yields

$$\int_{t_1}^{t_2} \int \left(\frac{1}{c^2} \frac{\partial \delta \psi^*}{\partial t} \frac{\partial \psi}{\partial t} - \frac{\partial \delta \psi^*}{\partial x} \frac{\partial \psi}{\partial x} - \frac{const.}{4} \delta \psi^* \psi + c.c. \right) dx \, dt = 0. \tag{44}$$

Performing integration by parts with respect to t in the first term and with respect to x in the second one and assuming that the variations of ψ equal zero at the borders of the integration region

$$\delta \psi(x, t_1) = \delta \psi(x, t_2) = 0, \quad \lim_{x \to \pm \infty} \delta \psi(x, t) = 0 \tag{45}$$

we get the equation

$$\int_{t_1}^{t_2} \int \delta \psi^* \left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{const.}{4} \right) \psi \, dx \, dt + c.c. = 0 \tag{46}$$

that has to be obeyed for arbitrary variations $\delta\psi$ and $\delta\psi^*$. It yields the equation of motion

$$\left(\frac{\partial^2}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\frac{const.}{4}\right)\psi=0 \tag{47}$$

and its complex conjugate.

Putting $const.=4m^2c^2/\hbar^2$ and using three spatial coordinates we obtain from the last equation the Klein–Gordon equation [20,21]

$$\left(\Delta-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\frac{m^2c^2}{\hbar^2}\right)\psi=0 \tag{48}$$

describing a free particle.

The corresponding non-relativistic time Schrödinger equation

$$i\hbar\frac{\partial\varphi}{\partial t}=-\frac{\hbar^2}{2m}\Delta\varphi \tag{49}$$

follows from the Klein–Gordon equation (48) if the well-known transformation [20,21]

$$\psi=e^{mc^2t/(i\hbar)}\varphi \tag{50}$$

is applied.

Similar discussion can be made also for the Dirac equation [3].

7. Potentials and antiparticles

Eq. (38) remains valid even if the operator $(\partial/\partial x)$ is replaced by the operator $(\partial/\partial x)+if(x,t)$, where $f(x,t)$ is a real function. It indicates that one can introduce additional functions or "potentials" into the theory that can describe external conditions in which the particle moves.

Similar replacement can be applied also to Eq. (43)

$$\int_{t_1}^{t_2}\int\left(\frac{1}{c^2}\left|\frac{\partial\psi}{\partial t}+if_t(x,t)\right|^2-\left|\frac{\partial\psi}{\partial x}+if_x(x,t)\right|^2-\frac{const.}{4}|\psi|^2\right)dx\,dt$$
$$=0, \tag{51}$$

where $f_t(x,t)$ and $f_x(x,t)$ are real functions.

Requiring now the invariance of the corresponding Fisher information J' with respect to the transformations $t\to-t$ and $x\to-x$ (the PT-invariance) we see that the functions f_t and f_x have to obey the conditions

$$f_x(x,t)=-f_x(-x,-t),\quad f_t(x,t)=-f_t(-x,-t). \tag{52}$$

Therefore, they must have the form

$$f_x(x,t)=qg_x(x,t),\quad f_t(x,t)=qg_t(x,t), \tag{53}$$

where $g_x(x,t)$ and $g_t(x,t)$ are real functions that are even in the both variables x and t, and q is a "charge" changing its sign during the transformation $t\to-t$ and $x\to-x$. As a result, the CPT-invariance is obtained.

The well-known prescriptions $\hat{\mathbf{p}}\to\hat{\mathbf{p}}-q\mathbf{A}(\mathbf{r},t)$ and $i\hbar(\partial/\partial t)\to i\hbar(\partial/\partial t)-qV(\mathbf{r},t)$, where $\mathbf{A}(\mathbf{r},t)$ and $V(\mathbf{r},t)$ are the vector and scalar electromagnetic potentials and q is the charge of the particle agree with the properties of the functions f_x and f_t given above.

Results of this discussion agree with the existence of particles and antiparticles with the charge q and $-q$ (see also Ref. [3]).

8. Operators

Now, we are interested in a mapping between events in experimental setups and mathematical objects representing the events. Events in experimental setups and their mathematical representation must obey the following conditions [6]:

(i) Parallel events do not depend on their order

$$a\vee b=b\vee a. \tag{54}$$

(ii) Serial events, except for special cases, do not commute

$$ab\neq ba. \tag{55}$$

(iii) Parallel and serial events obey the associative law

$$a\vee(b\vee c)=(a\vee b)\vee c, \tag{56}$$

$$a(bc)=(ab)c. \tag{57}$$

(iv) Finally, events obey the distributive laws

$$a(b\vee c)=(ab)\vee(ac), \tag{58}$$

$$(a\vee b)c=(ac)\vee(bc). \tag{59}$$

It has been shown in Ref. [6] that there exist always a mathematical representation $R(a)$ of the experimental events in which two parallel events a and b are represented by the sum $R(a)+R(b)$ and two serial events ab are represented by the product $R(b)R(a)$. Such representation exists independently of the concrete physical character of events.

Properties of linear hermitian operators used in quantum mechanics agree with these results.

9. Summary

We can conclude that the basic mathematical structure of quantum mechanics can be obtained in a few steps:

(i) Probabilistic description of the results of measurement of the coordinates by means of the probability density ρ. It leads to the uncertainty relations.
(ii) Description of motion by means of the probability density current j. Together with (i), it makes possible to introduce the complex wave function ψ, momentum operator $\hat{p}$, generalized space Fisher information (or kinetic energy) and commutation relation between x and $\hat{p}$.
(iii) Relativistic invariance of the space–time Fisher information. It leads to the relativistic Klein–Gordon equation and Dirac equation and to the non-relativistic Schrödinger equation.
(iv) The commutation relation between x and $\hat{p}$ makes possible to include external potentials. Their properties agree with the CPT-theorem and the existence of particles and antiparticles.
(v) Events in experimental setups can be always represented by a mathematical representation $R(a)$ in which parallel events a and b are represented by the sum $R(a)+R(b)$ and serial events ab are represented by the product $R(b)R(a)$. It agrees with the properties of operators used in quantum mechanics.

We have seen that the complex wave function ψ is a mathematically advantageous representation of the information carried by the probability density ρ and probability density current j. We note also that the relation $\rho=|\psi|^2$ between the probability density and probability amplitude is the most simple one leading to linear equations of motion. Another powers of $|\psi|$ or another functional relationship between ρ and $|\psi|$ lead to more complex nonlinear equations of motion (see Ref. [3]). From this point of view, the relation $\rho = |\psi|^2$ has unique mathematical properties.

Finally we note that the discussion given in this paper can easily be extended to three spatial dimensions.

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