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Quantum Mechanics, Probabilities and Mathematical Statistics

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Basic mathematical apparatus of quantum mechanics like the wave function, coordinate and momentum operator, corresponding commutation relation, kinetic energy, uncertainty relations, continuity equation and equations of motion is discussed from the point of view of probability theory and mathematical statistics. It is shown that the mathematical structure of quantum mechanics can be understood as generalization of classical mechanics in which the statistical character of results of measurement is taken into account and general properties of statistical theories are correctly respected.

Keywords: Quantum Mechanics, Probabilities, Mathematical Statistics.

RESEARCH ARTICLE

1. INTRODUCTION

Quantum mechanics and its meaning have been discussed in a large number of publications from many different points of view (see e.g., books[1,2]). It shows that quantum mechanics is, despite its numerous successful applications, difficult to understand.

In this paper, we discuss quantum mechanics from the point of view of probability theory and mathematical statistics that can, as we hope, contribute to its better understanding.

Similar discussion can be found for example in Refs. [3–6, 9–12].

2. STATISTICAL DESCRIPTION OF RESULTS OF MEASUREMENT

In this section, we discuss probably the most important difference between classical and quantum mechanics—statistical description of results of measurement in quantum mechanics.

For the sake of simplicity, we consider only one spatial coordinate x and time t.

We note that the measuring apparatus is not described in quantum mechanics on the microscopic level and the measured system interacts with the measuring apparatus. Therefore, in agreement with experimental experience, we assume that results of measurement of the coordinate x at time t can be described by the probability density $\rho(x,t)$ obeying the normalization condition

$$\int \rho \, \mathrm{d}x = 1 \tag{1}$$

where the integration is performed from minus infinity to plus infinity. We assume also that ρ has the property

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

Therefore, we limit ourselves to discussion of the so-called bound states obeying conditions (2).

Further we suppose that the mean value of the coordinate x resulting from repeated measurement is given by the integral

$$\langle x \rangle = \int x \rho \, \mathrm{d}x \tag{3}$$

In the limit

$$\rho(x,t) \to \delta(x - x_{cl}) \tag{4}$$

corresponding to transition to classical mechanics with the classical trajectory $x_{cl} = x_{cl}(t)$ the mean coordinate $\langle x \rangle$ equals x_{cl}.

Due to normalization condition (1) that is assumed to be valid at all times we suppose also validity of the continuity equation which has in one dimension the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0 \tag{5}$$

where $j(x,t)$ is the probability density current.

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3. WAVE FUNCTION

The wave function ψ can be introduced in the following simple way.

First, we introduce a real function $s_2 = s_2(x, t)$ by the equation

$$\rho = e^{-2s_2/\hbar} \tag{6}$$

or equivalently

$$s_2 = -\frac{\hbar}{2}\ln\rho \tag{7}$$

The constant $\hbar > 0$ could be an arbitrary real constant depending on the choice of units. However, to get formulas that agree with quantum mechanics, we will assume that $\hbar = h/(2\pi)$ denotes the reduced Planck constant. We note also that the transition $\rho(x, t) \to \delta(x - x_{cl})$ can be formally performed for $\hbar \to 0_+$.

In classical continuum mechanics in three dimensions, the current $j(r, t)$ can be written as $j = \rho v$, where v is the velocity. By analogy with this approach, we can write the probability density current j in one dimension in the form

$$j = \rho v \tag{8}$$

In classical mechanics, the velocity is given by the formula $v = p/m$, where $p = \partial S/\partial x$ is the momentum, m is the mass of the particle and S is the Hamilton principal action.

Since we are not in the limit case of classical mechanics, we replace the function S by a new real function $s_1 = s_1(x, t)$ and get (see also Ref. [12])

$$j = \rho\frac{p}{m} = \rho\frac{\partial s_1/\partial x}{m} \tag{9}$$

Now, we can introduce the complex function ψ

$$\psi = e^{(is_1 - s_2)/\hbar} \tag{10}$$

Using this function, the probability density and probability density current in one dimension can be written in the form known from quantum mechanics

$$\rho = |\psi|^2 \tag{11}$$

and

$$j = \frac{\hbar}{2mi}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right) \tag{12}$$

where the star denotes the complex conjugate.

The complex function ψ called the wave function in quantum mechanics is in this approach only a different way of representing the state of the particle described by two real functions ρ and j (or, equivalently, s_1 and s_2).

We note that our expression for the wave function (10) is similar to that of Bohm.[7,8] However, we do not assume the existence of hidden variables here and use the approach that is extension of standard mathematical statistics.

4. MOMENTUM OPERATOR

By analogy with Eq. (3), the mean momentum can be written in the form

$$\langle p\rangle = \int \frac{\partial s_1}{\partial x}\rho\,dx \tag{13}$$

It follows from Eq. (2) that the integral

$$\int \frac{\partial s_2}{\partial x}\rho\,dx = -\frac{\hbar}{2}\int\frac{\partial}{\partial x}e^{-2s_2/\hbar}dx = -\frac{\hbar}{2}\int\frac{\partial\rho}{\partial x}dx = -\frac{\hbar}{2}\rho|_{x=-\infty}^{\infty} = 0 \tag{14}$$

equals zero. Using this result it is easy to verify that Eq. (13) can be also written as

$$\langle\hat{p}\rangle = \int\psi^*\hat{p}\,\psi\,dx \tag{15}$$

where the momentum operator equals

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \tag{16}$$

We see that in case of the mean momentum Eqs. (13) and (15) yield the same result. However, it may not be true in more complicated cases as it will be seen in Section 7.

5. MEAN VALUE OF XP

In this section, we investigate the mean value of the product of the coordinate and momentum which is important in the uncertainty relations.

As it is known, the mean value of the product of the coordinate and momentum is in quantum mechanics given by the expression

$$\frac{\langle x\hat{p}\rangle + \langle\hat{p}x\rangle}{2} = \frac{1}{2}\int\psi^*\left[x\left(-i\hbar\frac{\partial}{\partial x}\right) + \left(-i\hbar\frac{\partial}{\partial x}\right)x\right]\psi\,dx \tag{17}$$

Using Eq. (10) we get

$$\frac{\langle x\hat{p}\rangle + \langle\hat{p}x\rangle}{2} = \frac{1}{2}\int e^{(-is_1-s_2)/\hbar}\left[2x\left(-i\hbar\frac{\partial}{\partial x}\right) - i\hbar\right]e^{(is_1-s_2)/\hbar}dx \tag{18}$$

Now we calculate the integral

$$\int e^{(-is_1-s_2)/\hbar}x\left(-i\hbar\frac{\partial}{\partial x}\right)e^{(is_1-s_2)/\hbar}dx = \int x\frac{\partial s_1}{\partial x}e^{-2s_2/\hbar}dx + i\int x\frac{\partial s_2}{\partial x}e^{-2s_2/\hbar}dx \tag{19}$$

By using integration by parts in the last integral and Eqs. (1) and (2) we obtain

$$\int x\frac{\partial s_2}{\partial x}e^{-2s_2/\hbar}dx = x\frac{-\hbar}{2}e^{-2s_2/\hbar}|_{x=-\infty}^{\infty} + \frac{\hbar}{2}\int e^{-2s_2/\hbar}dx = \frac{\hbar}{2} \tag{20}$$

The resulting formula

$$\frac{\langle x\hat{p}\rangle + \langle \hat{p}x\rangle}{2} = \int x\frac{\partial s_1}{\partial x}\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x = \int x\frac{\partial s_1}{\partial x}\rho\,\mathrm{d}x \tag{21}$$

agrees with the expresion

$$\langle xp\rangle = \int x\frac{\partial s_1}{\partial x}\rho\,\mathrm{d}x \tag{22}$$

analogous to Eqs. (3) and (13).

Summarizing results of the last two sections we see that contribution of the function $\partial s_2/\partial x$ to the mean values $\langle\hat{p}\rangle$ and $(\langle x\hat{p}\rangle + \langle\hat{p}x\rangle)/2$ equals zero and the momentum operator can be in these cases represented either by the function $p = \partial s_1/\partial x$ or by the operator $\hat{p} = -i\hbar(\partial/\partial x)$.

6. FISHER INFORMATION

The Fisher information is a very important quantity appearing in mathematical statistics (see e.g., Refs. [13, 14]). In our case, it can be introduced in the following simple way (see also Refs. [3–5, 9–12]).

We start with normalization condition (1) for the probability density ρ in which we perform integration by parts and use Eq. (14)

$$\left[(x-a)\rho\right]_{x=-\infty}^{\infty} - \int (x-a)\frac{\partial\rho}{\partial x}\mathrm{d}x = 1 \tag{23}$$

where a is an arbitrary real number. Taking into account Eq. (2) we get the starting point of the following discussion

$$\int (x-a)\frac{\partial\rho}{\partial x}\mathrm{d}x = -1 \tag{24}$$

Now we make use of the Schwarz inequality for the inner product $(u, v) = \int u^* v\,\mathrm{d}x$ of two complex functions u and v

$$(u, u)(v, v) \geq |(u, v)|^2 \tag{25}$$

Putting

$$u = (x-a)\sqrt{\rho}, \quad v = \frac{1}{\sqrt{\rho}}\frac{\partial\rho}{\partial x} \tag{26}$$

and using inequality (25) we get

$$\int (x-a)^2\rho\,\mathrm{d}x \int \frac{1}{\rho}\left(\frac{\partial\rho}{\partial x}\right)^2\mathrm{d}x \geq 1 \tag{27}$$

where the second integral is called the Fisher information

$$I_x = \int \frac{1}{\rho}\left(\frac{\partial\rho}{\partial x}\right)^2\mathrm{d}x \geq 0 \tag{28}$$

Inequality (27) is usually written in the form[13]

$$\int (x-a)^2\rho\,\mathrm{d}x\, I_x \geq 1 \tag{29}$$

This result is very general and does not depend on the concrete meaning of the variable x. Interpretation of the last inequality is similar to that of the uncertainty relations in quantum mechanics since for given I_x the integral $\int (x-a)^2\rho\,\mathrm{d}x$ cannot be smaller than $1/I_x$ and vice versa. The minimum of the integral $\int (x-a)^2\rho\,\mathrm{d}x$ is obtained for $a = \langle x\rangle$.

We note that inequality (29) in a more general form is known in mathematical statistics as the Rao-Cramér inequality.[14–17] Hence, any correctly formulated statistical theory has to lead to inequality (29) or an analogous one.

Using Eq. (6) for the probability density the Fisher information can be written in the equivalent form

$$I_x = \frac{4}{\hbar^2}\int \left(\frac{\partial s_2}{\partial x}\right)^2 \mathrm{e}^{-2s_2/\hbar}\mathrm{d}x \tag{30}$$

which will appear in the following discussion.

7. KINETIC ENERGY

Now we discuss the kinetic energy T in quantum mechanics and its relation to the Fisher information

$$T = \int \frac{|(\hat{p} - qA)\psi|^2}{2m}\mathrm{d}x \tag{31}$$

where q denotes the charge of the particle, m is its mass and A is the vector potential in one dimension.

Using Eq. (10) for the wave function and Eq. (16) for the momentum operator we get

$$(\hat{p} - qA)\psi = \left(\frac{\partial s_1}{\partial x} + i\frac{\partial s_2}{\partial x} - qA\right)\mathrm{e}^{(is_1 - s_2)/\hbar} \tag{32}$$

and

$$|(\hat{p} - qA)\psi|^2 = \left[\left(\frac{\partial s_1}{\partial x} - qA\right)^2 + \left(\frac{\partial s_2}{\partial x}\right)^2\right]\mathrm{e}^{-2s_2/\hbar} \tag{33}$$

Therefore, kinetic energy (31)

$$T = \int \frac{(\partial s_1/\partial x - qA)^2 + (\partial s_2/\partial x)^2}{2m}\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x \tag{34}$$

can be written as a sum of two terms

$$T = T_1 + T_2 \tag{35}$$

where

$$T_1 = \int \frac{(\partial s_1/\partial x - qA)^2}{2m}\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x \tag{36}$$

and

$$T_2 = \int \frac{(\partial s_2/\partial x)^2}{2m}\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x = \frac{\hbar^2 I_x}{8m} \tag{37}$$

We see that the second part of the kinetic energy T_2 depending on $\partial s_2/\partial x$ is proportional to the Fisher information I_x. It is worth noting that if the momentum would not be represented by the operator $\hat{p} = -i\hbar(\partial/\partial x)$ but by the function $p = \partial s_1/\partial x$, the term T_2 were not be obtained.

8. HEISENBERG UNCERTAINTY RELATIONS

For the sake of simplicity, we assume that the potential A equals zero.

The Heisenberg uncertainty relation[18] for the coordinate x and momentum p has the form

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle \geq \frac{\hbar^2}{4} \tag{38}$$

where

$$\langle(\Delta x)^2\rangle = \int (x-\langle x\rangle)^2|\psi|^2 \mathrm{d}x \tag{39}$$

and

$$\langle(\Delta p)^2\rangle = \int \left|\left(-i\hbar\frac{\partial}{\partial x} - \langle\hat{p}\rangle\right)\psi\right|^2 \mathrm{d}x \tag{40}$$

Using Eqs. (10) and (14) we get

$$\langle(\Delta p)^2\rangle = \langle(\Delta p_1)^2\rangle + \langle(\Delta p_2)^2\rangle \tag{41}$$

where

$$\langle(\Delta p_1)^2\rangle = \int \left(\frac{\partial s_1}{\partial x} - \left\langle\frac{\partial s_1}{\partial x}\right\rangle\right)^2 \mathrm{e}^{-2s_2/\hbar}\mathrm{d}x \tag{42}$$

and

$$\langle(\Delta p_2)^2\rangle = \int \left(\frac{\partial s_2}{\partial x}\right)^2 \mathrm{e}^{-2s_2/\hbar}\mathrm{d}x = \frac{\hbar^2}{4}I_x \tag{43}$$

We see that, analogously to the kinetic energy T, the mean square deviation of the momentum $\langle(\Delta p)^2\rangle$ can be split into two parts.

The first part $\langle(\Delta p_1)^2\rangle$ corresponds to the representation of the momentum by the function $p = \partial s_1/\partial x$ and the part of the kinetic energy T_1.

The second part $\langle(\Delta p_2)^2\rangle$ is proportional to the Fisher information I_x and corresponds to T_2. We note that for $\langle(\Delta p_1)^2\rangle = 0$, the Heisenberg uncertainty relation (38) has the form of inequality (29) for the Fisher information with $a = \langle x\rangle$ (see also Refs. [5, 19]). From this point of view, general structure of statistical theories is in quantum mechanics correctly respected.

9. TWO NEW UNCERTAINTY RELATIONS

We show in this section that the Heisenberg uncertainty relation can be replaced by two uncertainty relations for $\langle(\Delta p_1)^2\rangle$ and $\langle(\Delta p_2)^2\rangle$ (see also Refs. [20, 21]).

According to the well-known result of mathematical statistics, the product of variances of two quantities is greater than or equal to the square of their covariance.[17] In the following cases, it is equivalent to the Schwarz inequality (25) with a suitable choice of the functions u and v.

First, we put

$$u = \Delta x\sqrt{\rho} \tag{44}$$

and

$$v = \left(\frac{\partial s_1}{\partial x} - \left\langle\frac{\partial s_1}{\partial x}\right\rangle\right)\sqrt{\rho} \tag{45}$$

Then, the Schwarz inequality yields the first uncertainty relation

$$\langle(\Delta x)^2\rangle\langle(\Delta p_1)^2\rangle \geq \left[\int \Delta x\left(\frac{\partial s_1}{\partial x} - \left\langle\frac{\partial s_1}{\partial x}\right\rangle\right)\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x\right]^2 \tag{46}$$

As it follows from Section 5, the function $\partial s_1/\partial x$ in the last integral represents the momentum and this relation has the usual above mentioned meaning known from mathematical statistics. Depending on the functions s_1 and s_2, the square of the covariance of the coordinate and momentum at the right-hand side of this relation can have arbitrary values greater than or equal to zero.

The second uncertainty relation can be obtained in an analogous way for

$$u = \Delta x\sqrt{\rho} \tag{47}$$

and

$$v = \left(\frac{\partial s_2}{\partial x} - \left\langle\frac{\partial s_2}{\partial x}\right\rangle\right)\sqrt{\rho} \tag{48}$$

with the result

$$\langle(\Delta x)^2\rangle\langle(\Delta p_2)^2\rangle \geq \left[\int (x-\langle x\rangle)\left(\frac{\partial s_2}{\partial x} - \left\langle\frac{\partial s_2}{\partial x}\right\rangle\right)\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x\right]^2 \tag{49}$$

It follows from Eq. (14) that the right-hand side of this relation can be simplified

$$\langle(\Delta x)^2\rangle\langle(\Delta p_2)^2\rangle \geq \left(\int x\frac{\partial s_2}{\partial x}\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x\right)^2 \tag{50}$$

Then, Eq. (20) leads to the final form of the second uncertainty relation

$$\langle(\Delta x)^2\rangle\langle(\Delta p_2)^2\rangle \geq \frac{\hbar^2}{4} \tag{51}$$

This uncertainty relation follows from the Schwarz inequality in a similar way as the first one, however, the covariance (u, v) is in this case constant and equals $\hbar/2 > 0$ independently of the concrete form of the functions s_2 or ρ. We note also that relation (51) is for $\langle x\rangle = a$ equivalent to inequality (29) for the Fisher information. It confirms again that general structure of statistical theories is in quantum mechanics correctly respected.

Analogous uncertainty relations can be derived also in the multidimensional case[20, 21] and for the mixed states described by the density matrix.[21]

The sum of uncertainty relations (46) and (51) gives the relation

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle \geq \left[\int \Delta x\left(\frac{\partial s_1}{\partial x} - \left\langle\frac{\partial s_1}{\partial x}\right\rangle\right)\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x\right]^2 + \frac{\hbar^2}{4} \tag{52}$$

The Heisenberg uncertainty relation (38) can be obtained from this relation by neglecting the first term on its right-hand side. Therefore, uncertainty relations (46) and (51) are stronger than the corresponding Heisenberg uncertainty relation (38).

10. ROBERTSON–SCHRÖDINGER UNCERTAINTY RELATION

Relationship of uncertainty relations (46) and (51) to the Robertson–Schrödinger uncertainty relation[22–25] can be clarified as follows.

For the linear hermitian operators $\hat{A}$ and $\hat{B}$, the Robertson–Schrödinger uncertainty relation can be written in the form

$$\langle(\Delta\hat{A})^2\rangle\langle(\Delta\hat{B})^2\rangle \geq \frac{1}{4}\left(\langle\{\Delta\hat{A},\Delta\hat{B}\}\rangle^2+\left|\langle[\hat{A},\hat{B}]\rangle\right|^2\right) \quad (53)$$

where $\langle\hat{A}\rangle = \langle\psi|\hat{A}\psi\rangle$ is the mean value of the operator $\hat{A}$ in the state described by the wave function ψ, $\Delta\hat{A} = \hat{A}-\langle\hat{A}\rangle$, $\{\hat{A},\hat{B}\} = \hat{A}\hat{B}+\hat{B}\hat{A}$ denotes the anticommutator and $[\hat{A},\hat{B}] = \hat{A}\hat{B}-\hat{B}\hat{A}$ the commutator of the operators $\hat{A}$ and $\hat{B}$.

For the operators $\hat{x}=x$ and $\hat{p}=-i(\hbar\partial/\partial x)$ the straightforward calculation yields

$$\begin{aligned}\frac{1}{2}&\langle\{\Delta x,\Delta\hat{p}\}\rangle\\ &=\frac{1}{2}\int \mathrm{e}^{(-is_1-s_2)/\hbar}\left[\Delta x\left(-i\hbar\frac{\partial}{\partial x}-\langle\hat{p}\rangle\right)\right.\\ &\qquad\left.+\left(-i\hbar\frac{\partial}{\partial x}-\langle\hat{p}\rangle\right)\Delta x\right]\mathrm{e}^{(is_1-s_2)/\hbar}\mathrm{d}x\\ &=\int \Delta x\left(\frac{\partial s_1}{\partial x}-\left\langle\frac{\partial s_1}{\partial x}\right\rangle\right)\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x \end{aligned}\quad (54)$$

Further, taking into account the commutation relation $[x,\hat{p}]=i\hbar$, relation (53) leads to Eq. (52). Therefore, relations (46) and (51) are stronger than the Heisenberg and Robertson–Schrödinger relations (38) and (52) and yield more detailed information in terms of the mean square deviations $\langle(\Delta x)^2\rangle$, $\langle(\Delta p_1)^2\rangle$ and $\langle(\Delta p_2)^2\rangle$.

For the momentum represented by the function $p=\partial s_1/\partial x$, the mean value $\langle[\Delta x,\Delta p]\rangle$ equals zero and the Heisenberg and Robertson–Schrödinger uncertainty relations (38) and (52) do not contain the term $\hbar^2/4$. It shows again that this representation of the momentum is not except for cases discussed in Sections 4 and 5 correct.

11. GAUSSIAN WAVE PACKET

In this section, we discuss uncertainty relations (38), (46), (51) and (52) in case of the gaussian wave packet.

We assume that the wave function of a free particle is at time $t=0$ described by the gaussian wave packet

$$\psi(x,0)=\frac{1}{\sqrt{a\sqrt{\pi}}}\mathrm{e}^{-x^2/(2a^2)+ikx} \quad (55)$$

with the energy

$$E=\frac{\hbar^2}{4ma^2}+\frac{\hbar^2k^2}{2m} \quad (56)$$

where $a>0$ a k are real constants. By solving the time Schrödinger equation we get

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{a\sqrt{\pi}}}\frac{\sqrt{1-i\hbar t/ma^2}}{\sqrt{1+(\hbar t/ma^2)^2}}\\ &\times\exp\left\{-\frac{(x-(\hbar k/m)t)^2}{2a^2[1+(\hbar t/ma^2)^2]}\right.\\ &\left.+i\left[\frac{kx+(\hbar t x^2/2ma^4)-(\hbar k^2/2m)t}{1+(\hbar t/ma^2)^2}\right]\right\}\end{aligned} \quad (57)$$

The corresponding functions s_1 and s_2 and their derivatives equal

$$\begin{aligned}s_1(x,t) &= \hbar k\frac{x+((\hbar t x^2)/(2ma^4k))-(\hbar k/2m)t}{1+(\hbar t/ma^2)^2}\\ &-\hbar\arctan\frac{\hbar t}{ma^2}\end{aligned} \quad (58)$$

$$\begin{aligned}s_2(x,t) &= \frac{\hbar}{2}\left\{\frac{(x-(\hbar k/m)t)^2}{a^2[1+(\hbar t/ma^2)^2]}\right.\\ &\left.-\ln\frac{1}{a\sqrt{\pi}\sqrt{1+(\hbar t/ma^2)^2}}\right\}\end{aligned} \quad (59)$$

and

$$\frac{\partial s_1}{\partial x}=\hbar k\frac{1+((\hbar t x)/(ma^4k))}{1+(\hbar t/ma^2)^2} \quad (60)$$

$$\frac{\partial s_2}{\partial x}=\frac{\hbar(x-(\hbar k/m)t)}{a^2[1+(\hbar t/ma^2)^2]} \quad (61)$$

As it could be anticipated, the mean momentum and the mean coordinate equal

$$\langle\hat{p}\rangle=\left\langle\frac{\partial s_1}{\partial x}\right\rangle=\hbar k \quad (62)$$

and

$$\langle x\rangle=\frac{\hbar k}{m}t \quad (63)$$

The mean square deviations of the coordinate and momentum are given by the equations

$$\langle(\Delta x)^2\rangle=\frac{a^2}{2}\left[1+\left(\frac{\hbar t}{ma^2}\right)^2\right] \quad (64)$$

and

$$\langle(\Delta p_1)^2\rangle=\frac{\hbar^4t^2}{2m^2a^6[1+(\hbar t/ma^2)^2]} \quad (65)$$

$$\langle(\Delta p_2)^2\rangle=\frac{\hbar^2}{2a^2[1+(\hbar t/ma^2)^2]} \quad (66)$$

The left-hand side of relation (46) equals

$$\langle(\Delta x)^2\rangle\langle(\Delta p_1)^2\rangle=\frac{\hbar^4t^2}{4m^2a^4} \quad (67)$$

Calculating the right-hand side, we get the same result

$$\left\langle \Delta x\left(\frac{\partial s_1}{\partial x}-\left\langle\frac{\partial s_1}{\partial x}\right\rangle\right)\right\rangle^2=\frac{\hbar^4 t^2}{4m^2a^4} \tag{68}$$

Therefore, uncertainty relation (46) is fulfilled with the equality sign.

Calculating the left-hand side of uncertainty relation (51) we obtain

$$\langle(\Delta x)^2\rangle\langle(\Delta p_2)^2\rangle=\frac{\hbar^2}{4} \tag{69}$$

and see that uncertainty relation (51) is fulfilled with the equality sign, too.

The corresponding Robertson–Schrödinger uncertainty relation has the form

$$\langle(\Delta x)^2\langle(\Delta p)^2\rangle\rangle]=\frac{\hbar^4 t^2}{4m^2a^4}+\frac{\hbar^2}{4} \tag{70}$$

and is fulfilled with the equality sign for all $t\geq 0$. The Heisenberg uncertainty relation (38) for our wave packet can be obtained if the first term on the right-hand side of the last equation is neglected.

The equality sign in Schwarz inequality (25) is obtained if the functions u and v are collinear, i.e., for $u=\text{const}\,v$, where const is a complex number. However, since the functions s_1, s_2 and ρ are real, the corresponding functions u and v are also real. Therefore, *const* must be a real number or a real function of t. It follows from the conditions $u=\text{const}\,v$ for the functions s_1 and s_2 that these functions have to be quadratic functions of x of the form $p(t)x^2+q(t)x+r(t)$, where real coefficients $p(t)$, $q(t)$ and $r(t)$ can depend on time. Both functions s_1 and s_2 given by Eqs. (58) and (59) fulfill this condition.

It is worth to notice that the condition for the equality sign in relation (51) is independent of the form of the function s_1. Therefore, the equality sign in this relation can be achieved for much larger class of the wave functions than in case of the Heisenberg or Robertson–Schrödinger uncertainty relations. It is interesting not only from the theoretical point of view but also from the point of view of some applications.

12. VECTOR POTENTIAL

To introduce potentials, we make use of Eq. (24)

$$\int(x-a)\frac{\partial\rho}{\partial x}\,\mathrm{d}x=-1 \tag{71}$$

Using Eqs. (11) and (24) we get

$$\int(x-a)\left(\frac{\partial\psi^*}{\partial x}\psi+\psi^*\frac{\partial\psi}{\partial x}\right)\mathrm{d}x=-1 \tag{72}$$

Multiplying this equation by $-i\hbar$ and taking into account that $\hat{p}$ is the hermitian operator we can write this equation in the form

$$\int\psi^*[x-a,\hat{p}-f]\psi\,\mathrm{d}x=i\hbar \tag{73}$$

where $f=f(x,t)$ denotes a real function.

This result indicates that the momentum operator $\hat{p}$ can be replaced by a more general operator $\hat{p}-f$, where the function f can describe external conditions in which the system in question moves. It is in agreement with the fact that the commutation relation $[x,\hat{p}]=i\hbar$ can be replaced by a more general relation $[x,\hat{p}-f]=i\hbar$. For the electromagnetic field, the function f corresponds to the expression qA in the kinetic energy (31) (see also Refs. [3–5]).

13. TIME

Systems investigated in standard quantum mechanics have infinite life time and normalization condition (1) is valid at all times t from the preparation of the system in a given state ψ at time $t=0$ to the subsequent measurement at later time. Therefore, the probability to find the measured system anywhere in space equals one for all times $t\geq 0$ and it does not make sense to introduce the probability density in time analogous to the probability density in space with the properties (1) and (2). For this reason, time is taken as a parameter in quantum mechanics.

Rather different situation is obtained if we assume that the investigated system has a finite life time (like free neutrons and some other particles) and the integral $\int\rho(x,t)\,\mathrm{d}x$ decays in time (see also Refs. [3–5]). In such a case, we can assume that the normalization of $\rho=|\psi|^2$ can be performed not only over space but also over time

$$\int_{t=0}^{\infty}\int|\psi(x,t)|^2\mathrm{d}x\mathrm{d}t=1 \tag{74}$$

This condition expresses the fact that the particle existed at $t=0$ and some time later.

We note that this generalization includes standard quantum mechanics as a limit case.

By analogy with the coordinate x, it is possible to define the mean life time

$$\tau=\langle t\rangle=\int_{t=0}^{\infty}t\int|\psi(x,t)|^2\mathrm{d}x\mathrm{d}t \tag{75}$$

the mean square deviation

$$\langle(t-\langle t\rangle)^2\rangle=\int_{t=0}^{\infty}(t-\langle t\rangle)^2\int|\psi(x,t)|^2\mathrm{d}x\mathrm{d}t \tag{76}$$

and derive the corresponding time-energy uncertainty relation.[5]

14. SCALAR POTENTIAL

Similarly to Eq. (23), we perform integration by parts with respect to time in Eq. (74) and get

$$\left[t\int\rho\,\mathrm{d}x\right]_{t=0}^{\infty}-\int_{t=0}^{\infty}t\frac{\mathrm{d}}{\mathrm{d}t}\left[\int\rho\,\mathrm{d}x\right]\mathrm{d}t=1 \tag{77}$$

Assuming analogously to Eq. (2)

$$\lim_{t\to\infty} t^n \int \rho(x,t)\,\mathrm{d}x = 0, \quad n = 0, 1, 2 \tag{78}$$

and using Eq. (10) we obtain from Eq. (77) the result

$$\int_{t=0}^{\infty} t\left[\int\left(\frac{\partial\psi^*}{\partial t}\psi + \psi^*\frac{\partial\psi}{\partial t}\right)\mathrm{d}x\right]\mathrm{d}t = -1 \tag{79}$$

Multiplying this equation by $-i\hbar$ and taking into account that $i\hbar(\partial/\partial t)$ is the hermitian operator we get

$$\int_{t=0}^{\infty}\int\left[\left(i\hbar\frac{\partial\psi}{\partial t}\right)^*(t\psi) - (t\psi)^*\left(i\hbar\frac{\partial\psi}{\partial t}\right)\right]\mathrm{d}x\mathrm{d}t = i\hbar \tag{80}$$

or

$$\int_{t=0}^{\infty}\int \psi^*\left[i\hbar\frac{\partial}{\partial t} - g, t\right]\psi\,\mathrm{d}x\mathrm{d}t = i\hbar \tag{81}$$

where $g = g(x,t)$ is a real function.

This results indicates that for systems with a finite life time one can define the operator $i\hbar(\partial/\partial t)$ that has similar mathematical properties as the momentum operator $\hat{p}$. It is seen that the operator $i\hbar(\partial/\partial t)$ can be replaced by a more general operator $i\hbar(\partial/\partial t) - g$, where the function g has analogous properties as the function f. It is also in agreement with the fact that the commutation relation $[i\hbar(\partial/\partial t), t] = i\hbar$ can be replaced by a more general relation $[i\hbar(\partial/\partial t) - g, t] = i\hbar$. The function g corresponds to the expression qV known from quantum mechanics, where q is the charge of the particle and V is the scalar potential (see also Refs. [3–5]).

15. EQUATIONS OF MOTION

In physics, we have to take into account not only the probability density j given by the function s_2 but also the probability density current depending on the functions s_1 and s_2. For this reason, we introduce generalized spatial and time Fisher informations I_x'' and I_t'' analogous to Eq. (30) (see also Refs. [3–5])

$$\begin{aligned} I_x'' &= \frac{4}{\hbar^2}\int_{t=0}^{\infty}\int\left[\left(\frac{\partial s_1}{\partial x}\right)^2 + \left(\frac{\partial s_2}{\partial x}\right)^2\right]\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x\mathrm{d}t \\ &= \int_{t=0}^{\infty}\int\left|\frac{\partial\psi}{\partial x}\right|^2\mathrm{d}x\mathrm{d}t \geq 0 \end{aligned} \tag{82}$$

and

$$\begin{aligned} I_t'' &= \frac{4}{\hbar^2}\int_{t=0}^{\infty}\int\left[\left(\frac{\partial s_1}{\partial t}\right)^2 + \left(\frac{\partial s_2}{\partial t}\right)^2\right]\mathrm{e}^{-2s_2/\hbar}\mathrm{d}x\mathrm{d}t \\ &= \int_{t=0}^{\infty}\int\left|\frac{\partial\psi}{\partial t}\right|^2\mathrm{d}x\mathrm{d}t \geq 0 \end{aligned} \tag{83}$$

depending on the derivatives of the functions s_1 and s_2. Since there are no potentials in the last two equations, they correspond to a free particle.

To find equations of motion, we need some additional physical principle. To describe physical phenomena in a way independent of the choice of the concrete inertial system, we require that the combined space-time Fisher information equals a real constant K independent of the state of the investigated system

$$\frac{I_t''}{c^2} \pm I_x'' = K \tag{84}$$

where c is the speed of light and the sign in front of the spatial Fisher information I_x'' can be either + or −.

First we notice that the initial conditions for the wave function ψ at $t = 0$ can be from the mathematical point of view chosen arbitrarily and I_x'' can have arbitrary values greater than or equal to zero. In contrast to it, the wave function ψ at later times is given by the evolution consistent with Eq. (84).

Further, to determine the sign in Eq. (84), we consider a free particle which is in rest in the inertial system. It follows from Eq. (34) that it is obtained for very small values of $|\partial s_1/\partial x|$ and $|\partial s_2/\partial x|$. In such a case, the Fisher information I_x'' is close to zero and it follows from Eq. (84) that

$$K \geq 0 \tag{85}$$

Then, we consider a particle having large kinetic energy T and large Fisher information $I_x'' > K$. In such a case, it is impossible to obey Eq. (84) with the plus sign. Therefore, we can conclude that the sign in Eq. (84) must be negative

$$\frac{I_t''}{c^2} - I_x'' = K \tag{86}$$

It is seen that this combination of the Fisher informations is Lorentz invariant.

Using Eq. (74) the last equation can be written in the form

$$\int_{t=0}^{\infty}\int\left(\frac{1}{c^2}\left|\frac{\partial\psi}{\partial t}\right|^2 - \left|\frac{\partial\psi}{\partial x}\right|^2 - \frac{\hbar^2 K}{4}|\psi|^2\right)\mathrm{d}x\mathrm{d}t = 0 \tag{87}$$

This functional must be independent of ψ. Therefore, we get

$$\begin{aligned} \int_{t=0}^{\infty}\int\Bigg(&\frac{1}{c^2}\frac{\partial\delta\psi^*}{\partial t}\frac{\partial\psi}{\partial t} - \frac{\partial\delta\psi^*}{\partial x}\frac{\partial\psi}{\partial x} \\ &- \frac{\hbar^2 K}{4}\delta\psi^*\psi\Bigg)\mathrm{d}x\mathrm{d}t + c.c. = 0 \end{aligned} \tag{88}$$

where δ denotes the variation. Now we perform integration by parts with respect to t in the first term and with respect to x in the second one and assume that variations $\delta\psi$ and $\delta\psi^*$ equal zero at the borders of the integration region. Then we get

$$\int_{t=0}^{\infty}\int\delta\psi^*\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\hbar^2 K}{4}\right)\psi\,\mathrm{d}x\mathrm{d}t + c.c. = 0 \tag{89}$$

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

$$\left(\frac{\partial^2}{\partial x^2}-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\frac{\hbar^2 K}{4}\right)\psi=0 \tag{90}$$

Introducing the rest mass m_0 by the equation

$$K=\frac{4m_0^2c^2}{\hbar^4} \tag{91}$$

and generalizing Eq. (90) to three dimensions we obtain the well-known Klein-Gordon equation

$$\left(\Delta-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}-\frac{m_0^2c^2}{\hbar^2}\right)\psi=0 \tag{92}$$

We note that another derivation of the Klein-Gordon equation based on the principle of minimum of Fisher information was given in Ref. [12]. From the mathematical point of view, both approaches are similar. However, use of the operator $\partial/\partial t$ in Eq. (83), different signs of the time and space Fisher informations in Eq. (86) and the variation in Eq. (88) is in our case motivated physically.

As it is known, the Schrödinger equation for a free particle

$$i\hbar\frac{\partial\varphi}{\partial t}=-\frac{\hbar^2}{2m_0}\Delta\varphi \tag{93}$$

can be obtained from the Klein-Gordon equation (92) as the nonrelativistic approximation for the function φ given by the equation

$$\psi=e^{m_0c^2t/(i\hbar)}\varphi \tag{94}$$

The Dirac equation for a free particle can be also obtained in a similar way (see also Refs. [3–5, 9–11]).

The potentials can be included into the theory by the method described in Sections 12 and 14.

It worth to notice that the equations of motion discussed above are linear and the superposition principle is for them valid. This property can be traced back to the expression (28) for the Fisher informations I_x. By using the substitution $\rho=\exp(-2s_2/\hbar)$, I_x can be written in terms of the square of the function $\partial s_2/\partial x$ (see Eq. (30)). Similar approach is used in Eqs. (82) and (83) for I_x'' and I_t'', too. Then, using Eq. (86) and performing the variations and integration by parts in Eq. (87), the squares disappear, equations become linear and the second partial derivatives with respect to the coordinates and time are obtained.

We note also that the role of the operator $i\hbar(\partial/\partial t)$ is different from the role of the energy operator—hamiltonian. In agreement with discussion in this section, the operator $i\hbar(\partial/\partial t)$ is important for describing the time evolution of the wave function in agreement with the equations of motion.

Finally we note that quantization known from quantum mechanics is consequence of the boundary conditions applied to the wave function ψ. As it is known, only some solutions of the equations of motion obey these conditions and possible states of quantum systems can be quantized.

16. CONCLUSION

Concluding, results of this paper show that the basic mathematical structure of quantum mechanics can be understood as generalization of classical mechanics in which the statistical character of results of measurement is taken into account and the most important general properties of statistical theories known from mathematical statistics are correctly respected. It is not therefore surprising that quantum mechanics has been successfully applied to a very large spectrum of systems of microscopic and mesoscopic character.

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