Quantum mechanics as applied mathematical statistics

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ABSTRACT

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

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] and recent paper [3]). 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 that is different from the previous ones and that can, as we hope, contribute to its better understanding. Our aim is to compare (a) statistical extension of the Hamilton–Jacobi equation of classical mechanics in which the probability density $\rho(x,t)$ describing the statistical character of measurement of the coordinate x and momentum p at time t is introduced (Section 2) and (b) analogous approach to the Schrödinger equation in which the mean values of these quantities are calculated (Section 6). For the sake of simplicity, only the bound states having the property $\lim_{x \to \pm\infty} x^n \rho = 0$, $n = 0, 1, 2$ are investigated. By comparing results

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of (a) and (b) we are then able to find differences of both approaches and identify the terms that are present in quantum mechanics and that do not appear in approach (a).

To be consistent, we consider the same statistical ensemble in both cases (a) and (b). In contrast to standard statistical mechanics, where the mean values are calculated over different states of the system, we consider in case (a) the same statistical ensemble as in quantum mechanics (b). It means that the mean coordinate and momentum are measured in both cases on different members of the statistical ensemble of systems in a given state or in repeated measurement on one system in this state (Section 2).

In more detail, we show that results following from the Schrödinger equation are, in contrast to those following from the extension of the Hamilton–Jacobi theory (a), in agreement with general structure of statistical theories or, more exactly, with the Schwarz inequality. Therefore, quantum mechanics is from this point of view formulated correctly.

Basic mathematical apparatus of quantum mechanics like the wave function, probability density, probability density current, coordinate and momentum operators, their commutation relation, kinetic energy, uncertainty relations and continuity equation is also discussed.

It is assumed that the momentum can be represented in approach (a) in the form $p = \partial s_1/\partial x$, where s_1 a real function (Sections 2–4). This expression is generalization of the formula $p = \partial S/\partial x$ known from classical mechanics, where S denotes the Hamilton principal action and can be used for calculating the mean values $\langle \hat{p} \rangle$ and $\langle x\hat{p} + \hat{p}x \rangle/2$. However, in more complicated cases as in case of the square of the momentum, such representation of the momentum leads to results that are incorrect from the point of view of the Schwarz inequality. In contrast to it, representation of the momentum by means of the differential operator $\hat{p} = -i\hbar(\partial/\partial x)$ used in quantum mechanics (approach (b)) leads to formulae that are not in contradiction with this inequality.

In our statistical approach, the complex wave function $\psi = \exp[(is_1 - s_2)/\hbar]$ is only a different way of writing the statistical information carried by two real functions $s_1(x,t)$ and $s_2(x,t)$, where $\rho = \exp(-2s_2/\hbar)$ (Section 3). Its main advantage is simple formulation of the theory in terms of the operators acting on the wave function ψ.

Further it is shown that main differences of approaches (a) and (b) are closely related to the so-called Fisher information introduced to mathematical statistics in 1925, i.e. before the first Schrödinger's papers on quantum mechanics were published (Section 7). It appears that the kinetic energy in quantum mechanics equals the kinetic energy in approach (a) plus a term that is proportional to the Fisher information $I = \int_{-\infty}^{\infty} (\partial \rho/\partial x)^2/\rho \, dx$. This term is responsible for the non-zero kinetic energy of the bound states in quantum mechanics as is for example the ground state energy of the linear harmonic oscillator. It shows that this well-known quantum mechanical result is closely related to the statistical character of quantum mechanics and representation of the momentum by the operator $\hat{p} = -i\hbar(\partial/\partial x)$.

Another typical quantum result is the existence of the uncertainty relations. We show that the Heisenberg uncertainty relation for the coordinate x and momentum $\hat{p}$ is closely related to the Rao–Cramér inequality known from mathematical statistics that appears in any similarly formulated statistical theory. The Heisenberg and Robertson–Schrödinger uncertainty relations for the coordinate and momentum and two new uncertainty relations that are stronger than the original Heisenberg and Robertson–Schrödinger relations are from this point of view discussed (Sections 9–11).

The first uncertainty relation from the new ones has its classical analogy and can be understood as the well-known inequality according to which the product of variances of two quantities is greater than or equal to the square of their covariance. At the same time, the square of the covariance can have arbitrary values greater than or equal to zero.

The second uncertainty relation mentioned above is closely related to the Rao–Cramér inequality for the coordinate x and the Fisher information I. It has the same meaning as the above mentioned inequality between the variances and covariance, however, it appears that the square of the covariance is independent of the statistical state of the system described by the wave function ψ and equals $\hbar^2/4$. The second uncertainty relation has not its classical analogy and is related to the differential form of the momentum operator.

Results of Sections 9–11 are illustrated in case of the Gaussian wave packet (Section 12).

The continuity equation in quantum mechanics is usually derived from the Schrödinger equation. It is shown that this equation and the expression for the probability density current can be obtained in analogy with classical continuum mechanics if the probability density current is calculated from the

expression $\mathbf{j} = \rho\mathbf{v}$, where the velocity $\mathbf{v}$ equals $\mathbf{v} = \mathbf{p}/m$ and m is the mass (Section 13). Then, using the analogy of the expression for the momentum $\mathbf{p} = \nabla S$ known from the Hamilton–Jacobi theory one gets the continuity equation of quantum mechanics. It shows that the continuity equation in quantum mechanics is analogous to the continuity equation known from classical continuum mechanics.

2. Statistical description of results of measurement

In this section, we discuss an important step making possible to compare mathematical formalism of quantum and classical mechanics – statistical description of results of measurement. More detailed discussion of this approach can be found in [4–7].

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

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

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

where the integration is performed from minus infinity to plus infinity. For the sake of simplicity, 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 measurement is given by the integral

$$\langle x \rangle = \int x \rho \, dx. \tag{3}$$

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}.

To avoid confusion, we would like to point out that the mean value given by Eq. (3) is different from the mean value of the coordinate used in statistical mechanics. In standard statistical mechanics, the mean values are calculated over different states of the system that are possible in agreement with classical mechanics. In case of Eq. (3), the mean value $\langle x \rangle$ takes into account the fact that measurement of the coordinate x performed on different members of the statistical ensemble of systems in a given state (or in repeated measurement on one system in this state) leads in real experiments to different values of x that has to be averaged with the corresponding statistical weight ρ. Therefore, the statistical ensemble considered here is the same as that used in quantum mechanics (approach (b)). If necessary, averaging over different states could be included into the theory in a similar way as it is done in quantum statistics for mixed states by introducing the statistical weights of different states into Eq. (3).

In classical mechanics, the motion of a particle is described by the Hamilton–Jacobi equation [8,9]

$$\frac{(p - qA)^2}{2m} + V + \frac{\partial S}{\partial t} = 0, \tag{5}$$

where $S = S(x_{cl}, t)$ is the Hamilton principal action, x_{cl} denotes the classical coordinate of the particle,

$$p = \frac{\partial S}{\partial x_{cl}} \tag{6}$$

is the momentum, m and q are the mass and charge of the particle and $A = A(x_{cl}, t)$ and $V = V(x_{cl}, t)$ denote the vector and scalar potentials in one dimension, respectively.

Statistical generalization of the last equation analogous to Eq. (3) can be in approach (a) written in the form

$$\langle p \rangle = \int p\rho \, \mathrm{d}x = \int \frac{\partial s_1}{\partial x} \rho \, \mathrm{d}x, \tag{7}$$

where $s_1 = s_1(x,t)$ is a new real function corresponding to the Hamilton function S. It is assumed that the function s_1 leads for $\rho(x,t) \to \delta(x - x_{cl})$ and $s_1 \to S$ to the same momentum as Eq. (6)

$$\langle p \rangle = \frac{\partial s_1}{\partial x_{cl}} = \frac{\partial S}{\partial x_{cl}}. \tag{8}$$

It is to be noted that a similar comment as in case of Eq. (3) applies here. Different results of measurement of the momentum are given by the function $\partial s_1/\partial x$ and their statistical distribution is described by ρ.

It is assumed here that the function ρ characterizing the distribution of results of measurement x and p is the same in Eqs. (3) and (7).

3. Momentum operator

In this section, we introduce the wave function ψ and show that for calculating the mean momentum $\langle p \rangle$, the momentum can be equivalently represented either by the function $p = \partial s_1/\partial x$ used in the preceding section or by the momentum operator $\hat{p} = -i\hbar(\partial/\partial x)$.

We start from Eq. (7) and re-write it into the form

$$\langle p \rangle = \int \frac{\partial s_1}{\partial x} \rho \, \mathrm{d}x = \int \rho e^{-is_1/\hbar} \left(-i\hbar \frac{\partial}{\partial x} \right) e^{is_1/\hbar} \, \mathrm{d}x. \tag{9}$$

The constant $\hbar > 0$ could be an arbitrary real constant depending on the choice of units. However, to get formulae that agree with quantum mechanics, we will assume that $\hbar = h/(2\pi)$ denotes the reduced Planck constant.

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

$$\rho = e^{-2s_2/\hbar} \tag{10}$$

or equivalently

$$s_2 = -\frac{\hbar}{2} \ln \rho. \tag{11}$$

It follows from Eq. (2) that the integral

$$\int \frac{\partial s_2}{\partial x} \rho \, \mathrm{d}x = -\frac{\hbar}{2} \int \frac{\partial}{\partial x} e^{-2s_2/\hbar} \, \mathrm{d}x = -\frac{\hbar}{2} \int \frac{\partial \rho}{\partial x} \, \mathrm{d}x = -\frac{\hbar}{2} \rho \Big|_{x=-\infty}^{\infty} = 0 \tag{12}$$

equals zero. Therefore, we can write the mean momentum also in the form

$$\langle p \rangle = \int e^{(-is_1 - s_2)/\hbar} \left(-i\hbar \frac{\partial}{\partial x} \right) e^{(is_1 - s_2)/\hbar} \, \mathrm{d}x \tag{13}$$

or

$$\langle p \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x} \right) \psi \, \mathrm{d}x, \tag{14}$$

where the function ψ equals

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

and the star denotes the complex conjugate. The function ψ called the wave function in quantum mechanics is in our approach only a different way of representing the state of the particle described by the functions s_1 and s_2.

It is worth noting that our expression for the wave function (15) is similar to that of Bohm [10,11]. However, we do not assume the existence of hidden variables here.

From Eq. (14) we get the usual expression for the mean momentum in the form

$$\langle \hat{p} \rangle = \int \psi^* \hat{p} \psi \, dx, \tag{16}$$

where the momentum operator equals

$$\hat{p} = -i\hbar \frac{\partial}{\partial x}. \tag{17}$$

As shown in Eq. (12), the derivative $\partial s_2 / \partial x$ does not contribute to the mean momentum $\langle \hat{p} \rangle$ and the mean momentum can be calculated either from Eq. (7) or Eq. (16). Therefore, both representations of the momentum $p = \partial s_1 / \partial x$ and $\hat{p} = -i\hbar(\partial/\partial x)$ are in this case equivalent.

4. 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.

We investigate the quantum-mechanical mean value

$$\frac{\langle x\hat{p} + \hat{p}x \rangle}{2} = \frac{1}{2} \int \psi^* \left[x \left(-i\hbar \frac{\partial}{\partial x} \right) + \left(-i\hbar \frac{\partial}{\partial x} \right) x \right] \psi \, dx. \tag{18}$$

Using Eq. (15) for the wave function we get

$$\frac{\langle x\hat{p} + \hat{p}x \rangle}{2} = \frac{1}{2} \int e^{(-is_1 - s_2)/\hbar} \left[2x \left(-i\hbar \frac{\partial}{\partial x} \right) - i\hbar \right] e^{(is_1 - s_2)/\hbar} \, dx. \tag{19}$$

Now we calculate the integral

$$\int e^{(-is_1 - s_2)/\hbar} x \left(-i\hbar \frac{\partial}{\partial x} \right) e^{(is_1 - s_2)/\hbar} \, dx = \int x \frac{\partial s_1}{\partial x} e^{-2s_2/\hbar} \, dx + i \int x \frac{\partial s_2}{\partial x} e^{-2s_2/\hbar} \, dx. \tag{20}$$

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

$$\int x \frac{\partial s_2}{\partial x} e^{-2s_2/\hbar} \, dx = x \frac{-\hbar}{2} e^{-2s_2/\hbar} \bigg|_{x=-\infty}^{\infty} + \frac{\hbar}{2} \int e^{-2s_2/\hbar} \, dx = \frac{\hbar}{2}. \tag{21}$$

The resulting formula

$$\frac{\langle x\hat{p} + \hat{p}x \rangle}{2} = \int x \frac{\partial s_1}{\partial x} e^{-2s_2/\hbar} \, dx = \int x \frac{\partial s_1}{\partial x} \rho \, dx \tag{22}$$

agrees with generalization of the expression $x(\partial S / \partial x_{cl})$ from classical mechanics in the sense of approach (a)

$$\langle xp \rangle = \int x \frac{\partial s_1}{\partial x} \rho \, dx. \tag{23}$$

Here, the classical momentum $\partial S / \partial x_{cl}$ is replaced by $\partial s_1 / \partial x$ and the probability density ρ is taken into account.

Summarizing the 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 $\langle x\hat{p} + \hat{p}x \rangle / 2$ equals zero and the momentum operator can be in these cases represented by the function $p = \partial s_1 / \partial x$. Therefore, the quantum mechanical expressions for the mean coordinate $\langle x \rangle$, mean momentum $\langle \hat{p} \rangle$ and their product in the form $\langle x\hat{p} + \hat{p}x \rangle / 2$ give the same results as Eqs. (3), (7) and (23). However, in more complicated cases as for example in case of the square of the momentum the derivative $\partial s_2 / \partial x$ does play the important role and the two representations of the momentum $p = \partial s_1 / \partial x$ and $\hat{p} = -i\hbar(\partial/\partial x)$ lead to different results (see Section 6 and the following sections).

5. Commutation relation between coordinate and momentum

It has been shown in the preceding section that the mean value $\langle x\hat{p} + \hat{p}x \rangle/2$ can be calculated from Eq. (23) in which the coordinate x and momentum $p = \partial s_1/\partial x$ commute

$$\langle xp \rangle = \int x \frac{\partial s_1}{\partial x} \rho \, dx = \langle px \rangle. \tag{24}$$

The fact that the coordinate x and momentum $p = \partial s_1/\partial x$ commute agrees with our experience from macroworld. However, it is in contradiction with experimental evidences known from microworld according to which results of measurement of the coordinate and momentum depend on the order in which measurement is performed (for general discussion, see e.g. [12]). It shows that representation of the momentum by the function $p = \partial s_1/\partial x$ is not in microworld usable.

If we use the differential representation of the momentum (17), application of the commutator $[x, \hat{p}]$ to the wave function yields the commutation relation

$$[x, \hat{p}] = i\hbar \tag{25}$$

known from quantum mechanics.

6. Hamilton–Jacobi and Schrödinger equations

To compare approaches (a) and (b), we first replace the action S in the Hamilton–Jacobi equation (5) by the function s_1 as in Section 2, multiply the resulting equation by the probability density $\rho = \exp(-2s_2/\hbar)$ and integrate over x from minus infinity to plus infinity (see also [7])

$$\int \left[\frac{(\partial s_1/\partial x - qA)^2}{2m} + V + \frac{\partial s_1}{\partial t} \right] e^{-2s_2/\hbar} \, dx = 0. \tag{26}$$

Now we perform analogous steps with the time Schrödinger equation [13]

$$\left[\frac{(\hat{p} - qA)^2}{2m} + V \right] \psi = i\hbar \frac{\partial \psi}{\partial t}. \tag{27}$$

Multiplying the last equation from the left-hand side by ψ^* and integrating over x from minus infinity to plus infinity we can write the result in the form (see also [7])

$$\int \left[\frac{|(\hat{p} - qA)\psi|^2}{2m} + V|\psi|^2 - \psi^* i\hbar \frac{\partial \psi}{\partial t} \right] dx = 0. \tag{28}$$

Using Eq. (15) for the wave function and Eq. (17) for the momentum operator we get

$$(\hat{p} - qA)\psi = \left(\frac{\partial s_1}{\partial x} + i \frac{\partial s_2}{\partial x} - qA \right) e^{(is_1 - s_2)/\hbar} \tag{29}$$

and

$$|(\hat{p} - qA)\psi|^2 = \left[\left(\frac{\partial s_1}{\partial x} - qA \right)^2 + \left(\frac{\partial s_2}{\partial x} \right)^2 \right] e^{-2s_2/\hbar}. \tag{30}$$

Analogously, we obtain

$$\psi^* i\hbar \frac{\partial \psi}{\partial t} = -\left(\frac{\partial s_1}{\partial t} + i \frac{\partial s_2}{\partial t} \right) e^{-2s_2/\hbar}. \tag{31}$$

Therefore, Eq. (28) can be written as

$$\int \left[\frac{(\partial s_1/\partial x - qA)^2 + (\partial s_2/\partial x)^2}{2m} + V + \frac{\partial s_1}{\partial t} + i \frac{\partial s_2}{\partial t} \right] e^{-2s_2/\hbar} \, dx = 0. \tag{32}$$

Due to Eq. (1) the integral

$$\int \frac{\partial s_2}{\partial t} e^{-2s_2/\hbar} \, dx = -\frac{\hbar}{2} \frac{\partial}{\partial t} \int e^{-2s_2/\hbar} \, dx = 0 \tag{33}$$

equals zero and the resulting equation

$$\int \left[\frac{(\partial s_1/\partial x - qA)^2 + (\partial s_2/\partial x)^2}{2m} + V + \frac{\partial s_1}{\partial t} \right] e^{-2s_2/\hbar} \, dx = 0 \tag{34}$$

can be compared with Eq. (26).

We see that Eq. (34) following from the Schrödinger equation differs from Eq. (26) only by the term

$$\frac{1}{2m} \int \left(\frac{\partial s_2}{\partial x} \right)^2 e^{-2s_2/\hbar} \, dx \tag{35}$$

representing a part of the kinetic energy depending on the shape of the probability density ρ given by $\partial s_2/\partial x$. This term disappears either in the limit of classical mechanics when we can assume $\rho(x, t) \to \delta(x - x_{cl})$ and $\partial s_2/\partial x|_{x \to x_{cl}} \to 0$ [7] or if the function $(\partial s_2/\partial x)^2$ has very small values. It has purely quantum character and is related to the so-called Fisher information discussed in the following section.

7. Fisher information

The Fisher information is a very important quantity appearing in mathematical statistics (see e.g. [14,15]). In our case, it can be introduced in the following simple way (see also [4,6,16–19]).

We start with normalization condition (1) for the probability density ρ in which we perform integration by parts and use Eq. (12)

$$[(x - a)\rho]_{x=-\infty}^{\infty} - \int (x - a) \frac{\partial \rho}{\partial x} \, dx = 1, \tag{36}$$

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

$$\int (x - a) \frac{\partial \rho}{\partial x} \, dx = -1. \tag{37}$$

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

$$(u, u)(v, v) \geqslant |(u, v)|^2. \tag{38}$$

Putting

$$u = (x - a)\sqrt{\rho}, \quad v = \frac{1}{\sqrt{\rho}} \frac{\partial \rho}{\partial x} \tag{39}$$

and using inequality (38) we get

$$\int (x - a)^2 \rho \, dx \int \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 dx \geqslant 1, \tag{40}$$

where the second integral is called the Fisher information I

$$I = \int \frac{1}{\rho} \left(\frac{\partial \rho}{\partial x} \right)^2 dx. \tag{41}$$

Inequality (40) is usually written in the form [14]

$$\int (x-a)^2 \rho \, \mathrm{d}x I \geqslant 1. \tag{42}$$

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 the integral $\int (x-a)^2 \rho \, \mathrm{d}x$ cannot be smaller than $1/I$ 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 (42) in a more general form is known in mathematical statistics as the Rao–Cramér inequality [15,20–22]. Hence, any similarly formulated statistical theory has to lead to inequality (42) or an analogous one.

Using the expression $\rho = \exp(-2s_2/\hbar)$ for the probability density the Fisher information can be written in the equivalent form

$$I = \frac{4}{\hbar^2} \int \left(\frac{\partial s_2}{\partial x} \right)^2 \mathrm{e}^{-2s_2/\hbar} \, \mathrm{d}x \tag{43}$$

which will appear in the following discussion.

8. Kinetic energy

Now, we express the mean kinetic energy appearing in Eq. (34)

$$T = \int \frac{(\partial s_1/\partial x - qA)^2 + (\partial s_2/\partial x)^2}{2m} \mathrm{e}^{-2s_2/\hbar} \, \mathrm{d}x \tag{44}$$

as a sum of two terms

$$T = T_1 + T_2, \tag{45}$$

where

$$T_1 = \int \frac{(\partial s_1/\partial x - qA)^2}{2m} \mathrm{e}^{-2s_2/\hbar} \, \mathrm{d}x \tag{46}$$

and

$$T_2 = \frac{\hbar^2 I}{8m}. \tag{47}$$

The first part of the kinetic energy T_1 depending on $\partial s_1/\partial x$ is the same as the kinetic energy appearing in Eq. (26). The second part of the kinetic energy T_2 depending on $\partial s_2/\partial x$ is proportional to the Fisher information I and does not appear in Eq. (26).

We note also that, in contrast to classical mechanics, the kinetic energy T for the bound states obeying condition (2) cannot equal zero.

9. Heisenberg uncertainty relations

In this and the following two sections we discuss the uncertainty relations known from quantum mechanics and their relation to inequality (42).

For the sake of simplicity, we assume that the potential A equals zero. The Heisenberg uncertainty relation [23] for the coordinate x and momentum p has then the form

$$\langle (\Delta x)^2 \rangle \langle (\Delta p)^2 \rangle \geqslant \frac{\hbar^2}{4}, \tag{48}$$

where

$$\langle (\Delta x)^2 \rangle = \int (x - \langle x \rangle)^2 |\psi|^2 \, \mathrm{d}x \tag{49}$$

and

$$\langle (\Delta p)^2 \rangle = \int \left| \left(-i\hbar \frac{\partial}{\partial x} - \langle \hat{p} \rangle \right) \psi \right|^2 \mathrm{d}x. \tag{50}$$

Discussion of the mutual relation of the Heisenberg uncertainty relation (48) and inequality (42) for the Fisher information can be found for example in [6,24].

Using Eqs. (12), (15) and (43) we get

$$\langle (\Delta p)^2 \rangle = \langle (\Delta p_1)^2 \rangle + \langle (\Delta p_2)^2 \rangle, \tag{51}$$

where

$$\langle (\Delta p_1)^2 \rangle = \int \left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle \right)^2 \mathrm{e}^{-2s_2/\hbar} \, \mathrm{d}x \tag{52}$$

and

$$\langle (\Delta p_2)^2 \rangle = \int \left(\frac{\partial s_2}{\partial x} \right)^2 \mathrm{e}^{-2s_2/\hbar} \, \mathrm{d}x = \frac{\hbar^2 I}{4}. \tag{53}$$

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 $\langle (\Delta p_1)^2 \rangle$ can be interpreted within approach (a) in which the classical momentum $p = \partial S / \partial x_{cl}$ is replaced by $\partial s_1 / \partial x$ and the probability density $\rho = \exp(-2s_2/\hbar)$ is introduced.

The second part $\langle (\Delta p_2)^2 \rangle$ is proportional to the Fisher information I given by Eq. (43). We note also that for $\langle (\Delta p_1)^2 \rangle = 0$ the Heisenberg uncertainty relation (48) can be re-written in form of inequality (42) for the Fisher information with $a = \langle x \rangle$.

We see that the constant $\hbar^2/4$ at the right-hand side of the Heisenberg uncertainty relation (48) has the same origin as the right-hand side of inequality (42). Therefore, existence of the Heisenberg uncertainty relation (48) is closely related to the statistical description of results of measurement by means of the probability density ρ and the differential form of the momentum operator $\hat{p}$ (approach (b)). This point is discussed in the following section in more detail.

10. Two new uncertainty relations

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 [22]. For the following two cases it is equivalent to the Schwarz inequality (38) with a suitable choice of the functions u and v.

Now we show 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 [25–27]).

First, we take

$$u = \Delta x \sqrt{\rho} \tag{54}$$

and

$$v = \left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle \right) \sqrt{\rho}. \tag{55}$$

Then, the Schwarz inequality yields the first uncertainty relation

$$\langle (\Delta x)^2 \rangle \langle (\Delta p_1)^2 \rangle \geqslant \left[\int \Delta x \left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle \right) \mathrm{e}^{-2s_2/\hbar} \, \mathrm{d}x \right]^2. \tag{56}$$

As it follows from Section 4, the function $\partial s_1/\partial x$ in the last integral represents in this case the classical 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

$$u = \Delta x \sqrt{\rho} \tag{57}$$

and

$$v = \left(\frac{\partial s_2}{\partial x} - \left\langle \frac{\partial s_2}{\partial x} \right\rangle\right)\sqrt{\rho} \tag{58}$$

with the result

$$\langle(\Delta x)^2\rangle\langle(\Delta p_2)^2\rangle \geqslant \left[\int (x - \langle x\rangle)\left(\frac{\partial s_2}{\partial x} - \left\langle \frac{\partial s_2}{\partial x} \right\rangle\right)e^{-2s_2/\hbar}\,dx\right]^2. \tag{59}$$

The right-hand side of this relation can be due to Eq. (12) simplified

$$\langle(\Delta x)^2\rangle\langle(\Delta p_2)^2\rangle \geqslant \left(\int x \frac{\partial s_2}{\partial x} e^{-2s_2/\hbar}\,dx\right)^2. \tag{60}$$

Then, Eq. (21) leads to the final form of the second uncertainty relation

$$\langle(\Delta x)^2\rangle\langle(\Delta p_2)^2\rangle \geqslant \frac{\hbar^2}{4}. \tag{61}$$

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 function s_2. We note also that relation (61) is for $\langle x\rangle = a$ equivalent to relation (42) for the Fisher information.

We see that the Heisenberg uncertainty relation (48) can be replaced by two more detailed uncertainty relations (56) and (61). First uncertainty relation (56) can be understood as the standard statistical inequality between the coordinate x and momentum represented by the function $p = \partial s_1/\partial x$. Second uncertainty relation (61) can be understood as the standard statistical inequality, too. However, because of the specific form of the covariance (u, v) which equals $\hbar/2$ independently of s_2, the left-hand side of this relation must be greater than or equal to $\hbar^2/4$.

Similar uncertainty relations can be derived also in the multidimensional case [25,26] and for the mixed states described by the density matrix [26].

The sum of uncertainty relations (56) and (61) gives the relation

$$\langle(\Delta x)^2\rangle\langle(\Delta p)^2\rangle \geqslant \left[\int \Delta x\left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle\right)e^{-2s_2/\hbar}\,dx\right]^2 + \frac{\hbar^2}{4}. \tag{62}$$

The Heisenberg uncertainty relation (48) can be obtained from this relation by neglecting the first term on its right-hand side. Therefore, uncertainty relations (56) and (61) are stronger than the corresponding Heisenberg uncertainty relation (48).

11. Robertson–Schrödinger uncertainty relation

Relationship of uncertainty relations (56) and (61) to the Robertson–Schrödinger uncertainty relation [28–31] can be clarified as follows.

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

$$\langle(\Delta\widehat{A})^2\rangle\langle(\Delta\widehat{B})^2\rangle \geqslant \frac{1}{4}\left(\langle\{\Delta\widehat{A}, \Delta\widehat{B}\}\rangle^2 + |\langle[\widehat{A}, \widehat{B}]\rangle|^2\right), \tag{63}$$

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

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

$$
\begin{aligned}
\frac{1}{2} \langle \{\Delta x, \Delta \hat{p}\} \rangle &= \frac{1}{2} \int e^{(-is_1 - s_2)/\hbar} \left[\Delta x \left(-i\hbar \frac{\partial}{\partial x} - \langle \hat{p} \rangle \right) + \left(-i\hbar \frac{\partial}{\partial x} - \langle \hat{p} \rangle \right) \Delta x \right] e^{(is_1 - s_2)/\hbar} \, dx \\
&= \int \Delta x \left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle \right) e^{-2s_2/\hbar} \, dx.
\end{aligned}
\tag{64}
$$

Further, taking into account the commutation relation $[x, \hat{p}] = i\hbar$, relation (63) leads to Eq. (62). Therefore, relations (56) and (61) are stronger than the corresponding Heisenberg and Robertson–Schrödinger relations and yield more detailed information in terms of the mean square deviations $\langle (\Delta x)^2 \rangle$, $\langle (\Delta p_1)^2 \rangle$ and $\langle (\Delta p_2)^2 \rangle$. As mentioned in the preceding section, Heisenberg uncertainty relation (48) can be obtained from Robertson–Schrödinger relation (62) if the first term on the right-hand side of Eq. (62) is omitted.

We noted at the end of Section 4 that the momentum can be in some cases represented by the function $p = \partial s_1 / \partial x$. For this representation, the commutator $[x, p]$ equals zero and the term $\hbar^2/4$ in the uncertainty relations (48) and (62) is replaced by zero. Since the resulting relations are not in agreement with Eq. (42) following from the Schwarz inequality, we see again that this non-operator representation of the momentum is not in general case usable.

12. Gaussian wave packet

In this section, we discuss uncertainty relations (48), (56), (61) and (62) 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

$$
\psi(x, 0) = \frac{1}{\sqrt{a\sqrt{\pi}}} e^{-x^2/(2a^2) + ikx}
\tag{65}
$$

with the energy

$$
E = \frac{\hbar^2}{4ma^2} + \frac{\hbar^2 k^2}{2m},
\tag{66}
$$

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

$$
\psi(x, t) = \frac{1}{\sqrt{a\sqrt{\pi}}} \frac{\sqrt{1 - \frac{i\hbar t}{ma^2}}}{\sqrt{1 + \left(\frac{\hbar t}{ma^2} \right)^2}} \exp \left\{ -\frac{\left(x - \frac{\hbar k}{m} t \right)^2}{2a^2 \left[1 + \left(\frac{\hbar t}{ma^2} \right)^2 \right]} + i \left[\frac{kx + \frac{\hbar t x^2}{2ma^4} - \frac{\hbar k^2}{2m} t}{1 + \left(\frac{\hbar t}{ma^2} \right)^2} \right] \right\}.
\tag{67}
$$

The corresponding functions s_1 and s_2 and their derivatives equal

$$
s_1(x, t) = \hbar k \frac{x + \frac{\hbar t x^2}{2ma^4 k} - \frac{\hbar k}{2m} t}{1 + \left(\frac{\hbar t}{ma^2} \right)^2} - \hbar \arctan \frac{\hbar t}{ma^2},
\tag{68}
$$

$$
s_2(x, t) = \frac{\hbar}{2} \left\{ \frac{\left(x - \frac{\hbar k}{m} t \right)^2}{a^2 \left[1 + \left(\frac{\hbar t}{ma^2} \right)^2 \right]} - \ln \frac{1}{a\sqrt{\pi} \sqrt{1 + \left(\frac{\hbar t}{ma^2} \right)^2}} \right\}
\tag{69}
$$

and

$$\frac{\partial s_1}{\partial x} = \hbar k \frac{1 + \frac{\hbar t x}{m a^4 k}}{1 + \left(\frac{\hbar t}{m a^2}\right)^2},\tag{70}$$

$$\frac{\partial s_2}{\partial x} = \frac{\hbar \left(x - \frac{\hbar k}{m} t\right)}{a^2 \left[1 + \left(\frac{\hbar t}{m a^2}\right)^2\right]}.\tag{71}$$

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

$$\langle \hat{p} \rangle = \left\langle \frac{\partial s_1}{\partial x} \right\rangle = \hbar k\tag{72}$$

and

$$\langle x \rangle = \frac{\hbar k}{m} t.\tag{73}$$

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

$$\langle (\Delta x)^2 \rangle = \frac{a^2}{2} \left[1 + \left(\frac{\hbar t}{m a^2}\right)^2\right]\tag{74}$$

and

$$\langle (\Delta p_1)^2 \rangle = \frac{\hbar^4 t^2}{2 m^2 a^6 \left[1 + \left(\frac{\hbar t}{m a^2}\right)^2\right]},\tag{75}$$

$$\langle (\Delta p_2)^2 \rangle = \frac{\hbar^2}{2 a^2 \left[1 + \left(\frac{\hbar t}{m a^2}\right)^2\right]}.\tag{76}$$

The left-hand side of relation (56) equals

$$\langle (\Delta x)^2 \rangle \langle (\Delta p_1)^2 \rangle = \frac{\hbar^4 t^2}{4 m^2 a^4}.\tag{77}$$

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

$$\left\langle \Delta x \left(\frac{\partial s_1}{\partial x} - \left\langle \frac{\partial s_1}{\partial x} \right\rangle \right)\right\rangle^2 = \frac{\hbar^4 t^2}{4 m^2 a^4}.\tag{78}$$

Therefore, uncertainty relation (56) is fulfilled with the equality sign.

Calculating the left-hand side of uncertainty relation (61) we obtain

$$\langle (\Delta x)^2 \rangle \langle (\Delta p_2)^2 \rangle = \frac{\hbar^2}{4}\tag{79}$$

and see that uncertainty relation (61) is fulfilled with the equality sign, too.

The corresponding Robertson–Schrödinger uncertainty relation has the form

$$\langle (\Delta x)^2 \langle (\Delta p)^2 \rangle] = \frac{\hbar^4 t^2}{4 m^2 a^4} + \frac{\hbar^2}{4}\tag{80}$$

and is fulfilled with the equality sign for all $t \geqslant 0$. The Heisenberg uncertainty relation (48) 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 (38) is obtained if the functions u and v are collinear, i.e. for $u = const\, v$, 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 $u = const\, v$ for the functions s_1 and s_2 that these functions have to be

quadratic functions of x of the form $\alpha(t)x^2 + \beta(t)x + \gamma(t)$, where real coefficients $\alpha(t)$, $\beta(t)$ and $\gamma(t)$ can depend on time. Both functions s_1 and s_2 given by Eqs. (68) and (69) fulfill this condition.

It is worth to notice that the condition for the equality sign in relation (61) 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 theoretical but also from the experimental point of view.

13. Continuity equation

In contrast to standard mathematical statistics, probability density $\rho(x,t)$ in quantum mechanics depends on time. For particles with the infinite life time investigated in standard quantum mechanics normalization condition (1) is valid at all times from the initial measurement (or preparation of the system in the state given by the functions s_1 and s_2 or, equivalently, by the wave function ψ) till the following measurement at later time. For this reason, the continuity equation in three dimensions

$$\frac{\partial \rho}{\partial t} + \mathrm{div}\,\mathbf{j} = 0 \tag{81}$$

analogous to the continuity equation known from classical continuum mechanics must be valid in quantum mechanics, too. In a similar way as in continuum mechanics, we can write the probability density current in the form $\mathbf{j} = \rho\mathbf{v}$, where $\mathbf{v} = \mathbf{p}/m$ is the velocity and $\mathbf{p}$ is the momentum. It follows from Section 3 that the momentum $\mathbf{p}$ can be in three dimensions represented by the vector ∇s_1 with the result

$$\mathbf{j} = \rho\mathbf{v} = \rho\frac{\mathbf{p}}{m} = \rho\frac{\nabla s_1}{m}. \tag{82}$$

Using wave function (15) this formula can be written in the form known from quantum mechanics

$$\mathbf{j} = \frac{\hbar}{2mi}(\psi^*\nabla\psi - \psi\nabla\psi^*). \tag{83}$$

It is seen that in contrast to the kinetic energy or uncertainty relations, there are no purely quantum terms in the quantum continuity equation and that this equation has its analogue in classical continuum mechanics and in approach (a).

14. Conclusion

In this paper, two approaches (a) statistical extension of the Hamilton–Jacobi theory with the momentum $p = \partial s_1/\partial x$ and (b) analogous approach following from the time Schrödinger equation with the momentum operator $\hat{p} = -i\hbar(\partial/\partial x)$ have been compared. Only the bound states obeying the boundary condition (2) have been discussed.

The statistical ensemble used in approach (a) is different from that used in standard statistical mechanics. In contrast to statistical mechanics where the mean values are calculated over different states of the system, the mean values defined by Eqs. (3) and (7) take into account the fact that measurement of the coordinate and momentum on different members of the statistical ensemble of systems in a given state (or in repeated measurement on one system in this state) yields in real experiments different values of x and p. Therefore, the statistical ensemble considered in case (a) is the same as that used in quantum mechanics (b). The actually measured values of the coordinate and momentum are given by x and $\partial s_1/\partial x$ and the statistical weight of different results of measurement is described by the probability density $\rho(x,t)$.

The function corresponding to the principal Hamilton action S appearing in classical mechanics has been denoted in both cases (a) and (b) as $s_1(x,t)$. It has been assumed that in the limit $\rho(x,t) \to \delta(x - x_{cl})$ or $\hbar \to 0_+$ corresponding to transition to classical mechanics with the trajectory $x_{cl} = x_{cl}(t)$ the function s_1 leads to the same momentum as the formula from classical mechanics $p = \partial S/\partial x$. Then, we have introduced the second real function $s_2(x,t)$ by the relation $\rho = \exp(-2s_2/\hbar)$. Two real functions s_1 and s_2 give uniquely two important quantities used in the statistical description of

measurement – probability density ρ and probability density current **j**. Instead of two real functions s_1 and s_2 it is then possible to introduce the complex wave function $\psi = \exp[(is_1 - s_2)/\hbar]$ known from quantum mechanics.

In case of the mean values $\langle \hat{p} \rangle$ or $\langle x\hat{p} + \hat{p}x \rangle/2$ the momentum can be represented either by the function $p = \partial s_1/\partial x$ or the momentum operator $\hat{p} = -i\hbar(\partial/\partial x)$ acting on the wave function ψ. However, in more complicated cases as in case of the kinetic energy these two representations of the momentum lead to different results.

The difference of the kinetic energies in cases (b) and (a) equals $T_2 = \hbar^2 I/(8m)$, where $I = \int (\partial \rho/\partial x)^2/\rho \, dx = \int (\partial s_2/\partial x)^2 \rho \, dx$ is the Fisher information, important quantity appearing in mathematical statistics. The Fisher information appears also in the inequality $\int (x-a)^2 \rho \, dx I \geqslant 1$, Eq. (42), known from mathematical statistics.

Heisenberg and Robertson–Schrödinger uncertainty relations known from quantum mechanics follow from two stronger uncertainty relations (56) and (61).

First relation (56) can be understood as the inequality for the product of variances of the deviation of the coordinate x and momentum $p = \partial s_1/\partial x$ from their mean values which must be greater than or equal to the square of the covariance of these quantities. Therefore, relation (56) has the well-known statistical meaning and appears in both approaches (a) and (b).

Second relation (61) is equivalent to the above mentioned inequality (42) for the Fisher information. It can be also understood as the inequality between the variances and covariance of the deviation of the coordinate x and the function $\partial s_2/\partial x$ from their mean values. However, the covariance is constant and equals $\hbar/2$. Its square then yields the constant $\hbar^2/4$ appearing at the right-hand side of the Heisenberg uncertainty relation. Uncertainty relation (61) is not obtained in approach (a).

Heisenberg (48) and Robertson–Schrödinger (63) uncertainty relations and two new uncertainty relations (56) and (61) are analytically calculated for the Gaussian wave packet (Section 12). In this case, the Robertson–Schrödinger uncertainty relation and two new uncertainty relations are fulfilled with the equality sign for all times $t \geqslant 0$.

It follows from the Schwarz inequality that in any statistical theory with the same averaging as in (a) and (b) must exist an inequality analogous to Eq. (42). Since there is no such relation in approach (a), this approach is from this point of view incorrect. In contrast to it, mathematical structure of quantum mechanics with the momentum operator $\hat{p} = -i\hbar(\partial/\partial x)$ is from this point of view correct.

In contrast to the kinetic energy and uncertainty relations there are no typically quantum terms in the quantum continuity equation (Section 13). The continuity equation in quantum mechanics can be introduced in analogy with the continuity equation known from classical continuum mechanics.

Finally we note that quantization known from quantum mechanics is consequence of the statistical description of results of measurement, differential form of the momentum operator $\hat{p}$ and boundary conditions applied to the wave function ψ. As it is known, only some solutions of the Schrödinger equation obey these conditions and possible states of quantum systems can be quantized.

In summary, 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 in physics, chemistry, biology and other fields.

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