

Uncertainty Principle and Position Operator in Quantum Theory

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Abstract

The Heisenberg uncertainty principle is a consequence of the postulate that coordinate and momentum representations are related to each other by the Fourier transform. This postulate has been accepted from the beginning of quantum theory by analogy with classical electrodynamics. We argue that the postulate is based neither on strong theoretical arguments nor on experimental data. A position operator proposed in our recent publication resolves inconsistencies of standard approach and sheds a new light on important problems of quantum theory. We do not assume that the reader is an expert in the given field and the content of the paper can be understood by a wide audience of physicists.

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1 Introduction

The postulate that in quantum theory the coordinate and momentum representations are related to each other by the Fourier transform is described in every textbook on quantum mechanics. The Heisenberg uncertainty principle is a consequence of this postulate. However, in our opinion, even in textbooks the following issues are not clearly explained:

- 1) Are the representations equivalent or one of them is more fundamental?
- 2) In what situations do we need to use transformations from one representation to another?
- 3) Is the above postulate based on strong theoretical arguments and/or experimental data?

In Ref. [1] those problems have been discussed in detail with motivations, calculations and their comparison with experimental data. The goal of the present paper is to discuss the most fundamental problems related to issues 1)-3) on the level accepted in textbooks such that the material should be understandable by a wide audience of physicists.

In Sec. 2 we describe how those issues are treated in standard quantum theory. In particular, we argue that the definition of standard position operator is not physically consistent. A consistent construction of this operator is described in Sec. 3. The results shed a new light on important problems of quantum theory. They are briefly discussed in Sec. 4.

2 Uncertainty principle and position operator in standard theory

Standard quantum theory is based on the postulate that physical states are described by wave functions ψ which are elements of a Hilbert space H , and physical quantities are described by selfadjoint operators in this space. To formulate the Heisenberg uncertainty principle one needs to use the following notions. If (\dots, \dots) is the scalar product in H then the norm in H is defined as $\|\psi\| = (\psi, \psi)^{1/2}$. If $\|\psi\| = 1$ and A is an operator of a some physical quantity then its mean value and uncertainty in the state ψ are defined as $\bar{A} = (\psi, A\psi)$ and $\Delta A = \|(A - \bar{A})\psi\|$, respectively.

In terms of these notions the Heisenberg uncertainty principle states that if ΔX_j is the uncertainty of the j th component of the position operator \mathbf{X} and ΔP_k is the uncertainty of the k th component of the momentum operator \mathbf{P} ($j, k = 1, 2, 3$) then $\Delta X_j \Delta P_k \geq \hbar \delta_{jk}/2$ where δ_{jk} is the Kronecker symbol.

The coordinate representation is defined as a space of states $\psi(\mathbf{x})$ such that the operator \mathbf{X} in this space is the operator of multiplication by \mathbf{x} . Analogously, the momentum representation is defined as a space of states $\chi(\mathbf{p})$ such that the operator \mathbf{P} in this space is the operator of multiplication by \mathbf{p} . It is usually assumed that the scalar products in those representations are chosen as $(\psi_2, \psi_1) = \int \psi_2(\mathbf{x})^* \psi_1(\mathbf{x}) d^3\mathbf{x}$ and $(\chi_2, \chi_1) = \int \chi_2(\mathbf{p})^* \chi_1(\mathbf{p}) d^3\mathbf{p}$, respectively.

The uncertainty principle is a consequence of the postulate accepted from the beginning of quantum theory that the coordinate and momentum representations are related to each other by the Fourier transform. The historical reason was that in classical electrodynamics the coordinate and wave vector \mathbf{k} representations are related analogously and we postulate that $\mathbf{p} = \hbar\mathbf{k}$. Then, although the interpretations of classical fields on one hand and wave functions on the other are fully different, from mathematical point of view classical electrodynamics and quantum mechanics have much in common (and such a situation does not seem to be natural).

For example, in classical electrodynamics a wave packet moving even in empty space inevitably spreads out and this fact is well known. As pointed out by

Schrödinger (see pp. 41-44 in Ref. [2]), in standard quantum mechanics a packet does not spread out if a particle is moving in a harmonic oscillator potential in contrast to "a wave packet in classical optics, which is dissipated in the course of time". However, as a consequence of the similarity, a free quantum mechanical wave packet inevitably spreads out too. This effect is called wave packet spreading (WPS) and is described in textbooks and many papers (see e.g. Ref. [3] and references therein).

In particular, the WPS effect has been investigated by de Broglie, Darwin and Schrödinger. The fact that WPS is inevitable has been treated by several authors as unacceptable and as an indication that standard quantum theory should be modified. For example, de Broglie has proposed to describe a free particle not by the Schrödinger equation but by a wavelet which satisfies a nonlinear equation and does not spread out (a detailed description of de Broglie's wavelets can be found e.g. in Ref. [4]).

At the same time, it has not been explicitly shown that numerical results on WPS are incompatible with experimental data. For example, it follows from Darwin's result [5] that for macroscopic bodies the effect of WPS is extremely small. Probably it is also believed that in experiments on the Earth with atoms and elementary particles spreading does not have enough time to manifest itself. Probably for these reasons the majority of physicists do not treat WPS as a drawback of the theory.

However, a natural problem arises what happens to photons which can travel from distant objects to Earth even for billions of years. As shown in Ref. [1], a standard treatment of the WPS in directions perpendicular to the photon momentum leads to several striking paradoxes. Hence a problem arises whether the postulate can be substantiated.

As shown in textbooks on quantum mechanics (see e.g. Ref. [6]), the above postulate is equivalent to ones that the momentum operator in coordinate representation is $\mathbf{P} = -i\hbar\partial/\partial\mathbf{x}$ or the position operator in momentum representation is $\mathbf{X} = i\hbar\partial/\partial\mathbf{p}$. In either case the commutation relations between the position and momentum operators are

$$[X_j, X_k] = [P_j, P_k] = 0, \quad [X_j, P_k] = i\hbar\delta_{jk} \quad (j, k = 1, 2, 3) \quad (1)$$

and it is well-known that the uncertainty principle is a rigorous *mathematical* consequence of those relations (see e.g. Ref. [1]).

In Ref. [7] Heisenberg argues in favor of his principle by considering *Gedankenexperiment* with Heisenberg's microscope. Since that time the problem has been investigated in many publications. A discussion of the current status of the problem can be found e.g. in Ref. [8] and references therein. A general opinion based on those investigations is that Heisenberg's arguments are problematic but the uncertainty principle is valid, although several authors argue whether the above mathematical notion of uncertainty is relevant for describing a real process of measurement. However, a common assumption in those investigations is that one can

consider uncertainty relations for all the components of the position and momentum operators independently. Below we argue that this assumption is not based on solid physical arguments.

In view of the above discussion one might think that the position and momentum operators are on equal footing. However, this is not the case for several reasons. For example, as argued in Ref. [9], symmetry on quantum level should be defined not by the choice of the space-time background but by the choice of the symmetry algebra. In particular, Poincare symmetry is defined by the choice of the Poincare algebra as the symmetry algebra. Then each elementary particle is described by an irreducible representation (IR) of this algebra. This IR has a natural implementation in momentum space and the components of the momentum operator are three of ten linearly independent representation operators. Hence those operators are consistently defined. On the other hand, among the representation operators there is no position operator. In addition, the *results* of existing fundamental quantum theories describing interactions on quantum level (QED, electroweak theory and QCD) are formulated exclusively in terms of the S-matrix in momentum space without any mentioning of space-time. Hence *for investigating such stationary quantum problems as calculating energy levels, form-factors etc., the notion of the position operator is not needed.*

As an example, one of the arguments in favor of choosing standard position and momentum operators is that the nonrelativistic Schrödinger equation correctly describes the hydrogen energy levels, the Dirac equation correctly describes fine structure corrections to these levels etc. Historically these equations have been first written in coordinate space and in textbooks they are still discussed in this form. However, from the point of view of the present knowledge those equations should be treated as follows.

A fundamental theory describing electromagnetic interactions on quantum level is QED *the results of which are formulated exclusively in momentum space.* As follows from Feynman diagrams for the one-photon exchange, in the approximation $(v/c)^2$ the electron in the hydrogen atom can be described in the potential formalism where the potential acts on the wave function in momentum space. So for calculating energy levels one should solve the eigenvalue problem for the Hamiltonian with this potential. This is an integral equation which can be solved by different methods. One of the convenient methods is to apply the Fourier transform and get standard Schrödinger or Dirac equation. Hence the fact that the results for energy levels are in good agreement with experiment shows only that QED defines the potential correctly and *standard coordinate Schrödinger and Dirac equations are only convenient mathematical ways of solving the eigenvalue problem.* For this problem the physical meaning of the position operator is not important at all. One can consider other transformations of the original integral equation and define other position operators.

However, the choice of the position operator is important in nonstationary problems when evolution is described by the time dependent Schrödinger equation

(with the nonrelativistic or relativistic Hamiltonian). For any new theory there should exist a correspondence principle that at some conditions the new theory should reproduce results of the old well tested theory with a good accuracy. In particular, quantum theory should reproduce the motion of a particle along the classical trajectory defined by classical equations of motion.

Our conclusion on issues 1) and 2) in Sec. 1 is that the momentum representation is fundamental while the coordinate one and the position operator are needed only in semiclassical approximation and they should be *defined* from additional considerations. Hence one should start from momentum space and try to find arguments for constructing a physical position operator. Note that in textbooks (see e.g. Ref. [6]) the standard choices for the momentum and position operators are justified from the point of view that they give a correct description in semiclassical approximation. However, the requirement that an operator should have correct properties in semiclassical approximation does not define the operator unambiguously. Indeed, if an operator B disappears in semiclassical approximation then on semiclassical level the operators A and $A + B$ are equivalent.

By definition, a quantity corresponding to the operator A is semiclassical in state ψ if the uncertainty is much less than the mean value, i.e. $\Delta A \ll |\bar{A}|$. Therefore the quantity cannot be semiclassical if \bar{A} is rather small or $\bar{A} = 0$. In particular, as explained in textbooks on quantum mechanics (see e.g. Ref. [6]), semiclassical approximation cannot be valid in situations when the momentum is rather small.

Consider first a one-dimensional case. If the mean value of the x component of the momentum p_x is rather large, the definition of the coordinate operator $i\hbar\partial/\partial p_x$ can be justified but this definition does not have a physical meaning in situations when p_x is small.

Consider now the three-dimensional case. If all the components p_j ($j = 1, 2, 3$) are rather large then all the operators $i\hbar\partial/\partial p_j$ can have a physical meaning. A semiclassical wave function $\chi(\mathbf{p})$ in momentum space should describe a narrow distribution around the mean value \mathbf{p}_0 . Suppose now that coordinate axes are chosen such \mathbf{p}_0 is directed along the z axis. Then the mean values of the x and y components of the momentum operator equal zero and, in view of the above remarks the operators $i\hbar\partial/\partial p_j$ cannot be physical for $j = 1, 2$, i.e. in directions perpendicular to the particle momentum. The situation when a definition of an operator is physical or not depending on the choice of coordinate axes is not acceptable. Hence our conclusion is that standard definition of the position operator is not physical.

In view of the above remarks, a position operator should exist not only in the nonrelativistic case but in the relativistic case as well. A generalization of standard position operator to the relativistic case has been first proposed by Newton and Wigner [10]. Several authors proposed modifications of the Newton-Wigner position operator (see the discussion in Ref. [1]) but in semiclassical approximations all the modified operators are equivalent to the Newton-Wigner one. In the Newton-Wigner

construction the coordinate and momentum representations are also related to each other by the Fourier transform. Hence the Newton-Wigner position operator has the same foundational problems as standard one (see the discussion in Ref. [1]).

We conclude that standard position operator in directions perpendicular to the particle momentum is unphysical. As a consequence, the results on WPS in those directions are not trustworthy. As shown in Ref. [1], in the case of photons moving to Earth for a rather long period of time the results on WPS obtained with standard position operator lead to several striking paradoxes. Hence, at least in directions perpendicular to the particle momentum, standard position operator should be modified.

Our conclusion on issue 3) in Sec. 1 is that the postulate that the momentum and coordinate representations are related to each other by the Fourier transform is based neither on strong theoretical arguments nor on experimental data.

3 Consistent construction of position operator

Before discussing a consistent construction of the position operator, let us make the following remark. On elementary level students treat the mass m and the velocity \mathbf{v} as primary quantities such that the momentum is $m\mathbf{v}$ and the kinetic energy is $m\mathbf{v}^2/2$. However, from the point of view of Special Relativity, the primary quantities are the momentum \mathbf{p} and the total energy E and then the mass and velocity are defined as $m^2c^4 = E^2 - \mathbf{p}^2c^2$ and $\mathbf{v} = \mathbf{p}c^2/E$, respectively. This example has the following analogy. In standard quantum theory the primary operators are the position and momentum operators and the orbital angular momentum operator \mathbf{L} is defined as their cross product. However, if one proceeds from IRs then the operators \mathbf{P} and \mathbf{L} are on the same footing and they are consistently defined as representation operators of the Poincare algebra. At the same time, the definition of the position operator is a problem. Hence a question arises whether the position operator can be defined in terms of \mathbf{P} and \mathbf{L} .

One might seek the position operator such that on classical level the relation $\mathbf{x} \times \mathbf{p} = \mathbf{l}$ will take place where \mathbf{l} is the classical value of the angular momentum. Note that on quantum level this relation is not necessary. Indeed, the very fact that some elementary particles have a half-integer spin shows that the total angular momentum for those particles does not have the orbital nature but in semiclassical approximation the contribution of the spin operator to the total angular momentum is much less than the contribution of the orbital angular momentum. However, if the values of \mathbf{p} and \mathbf{l} are known and $\mathbf{p} \neq 0$ then the requirement that $\mathbf{x} \times \mathbf{p} = \mathbf{l}$ does not define \mathbf{x} uniquely. One can define parallel and perpendicular components of \mathbf{x} as $\mathbf{x} = x_{\parallel}\mathbf{p}/p + \mathbf{x}_{\perp}$ where $p = |\mathbf{p}|$. Then the relation $\mathbf{x} \times \mathbf{p} = \mathbf{l}$ defines uniquely only \mathbf{x}_{\perp} as $\mathbf{x}_{\perp} = (\mathbf{p} \times \mathbf{l})/p^2$.

On quantum level \mathbf{x}_{\perp} should be replaced by a selfadjoint operator \mathbf{X}_{\perp} . For this purpose one should know the form of the operator \mathbf{L} in momentum representation.

A well-known form of this operator in standard quantum mechanics is $\mathbf{L} = i\hbar(\partial/\partial\mathbf{p}) \times \mathbf{p}$. This expression is rather general because it is valid not only in nonrelativistic quantum mechanics but also in the cases of Poincare and de Sitter symmetries [11].

Taking into account that the operators \mathbf{P} and \mathbf{L} do not commute with each other and the operator \mathbf{X}_\perp should be Hermitian, a quantum generalization of the expression for \mathbf{x}_\perp is

$$\mathbf{X}_\perp = \frac{1}{2p^2}(\mathbf{P} \times \mathbf{L} - \mathbf{L} \times \mathbf{P}) \quad (2)$$

In nonrelativistic quantum mechanics the Hamiltonian of a free particle with the mass m is $p^2/2m$ and in relativistic quantum mechanics it is $(m^2c^4 + p^2c^2)^{1/2}$. Therefore an immediate consequence of the definition (2) follows: *Since the momentum and angular momentum operators commute with the Hamiltonian, the distribution of all the components of \mathbf{x}_\perp does not depend on time. In particular, there is no WPS in directions defined by \mathbf{X}_\perp .* On classical level the conservation of \mathbf{x}_\perp is obvious since it is defined by the conserved quantities \mathbf{p} and \mathbf{l} . It is also obvious that since a free particle is moving along a straight line, a vector from the origin perpendicular to this line does not change with time.

However, the relation $\mathbf{x} \times \mathbf{p} = \mathbf{l}$ does not make it possible to define the parallel component of the position operator and a problem arises what physical arguments should be used for that purpose.

We define \mathbf{G} as the operator of multiplication by the unit vector $\mathbf{n} = \mathbf{p}/p$. A direct calculation shows that if $\partial/\partial\mathbf{p}$ is written in terms of p and angular variables then

$$i\hbar \frac{\partial}{\partial\mathbf{p}} = \mathbf{G}X_\parallel + \mathbf{X}_\perp \quad (3)$$

where the operator X_\parallel acts only over the variable p :

$$X_\parallel = i\hbar \left(\frac{\partial}{\partial p} + \frac{1}{p} \right) \quad (4)$$

The correction $1/p$ is related to the fact that the operator X_\parallel is Hermitian since in variables (p, \mathbf{n}) the scalar product is given by

$$(\chi_2, \chi_1) = \int \chi_2(p, \mathbf{n})^* \chi_1(p, \mathbf{n}) p^2 dp d\omega \quad (5)$$

where $d\omega$ is the element of the solid angle.

While the components of standard position operator commute with each other, the operators X_\parallel and \mathbf{X}_\perp satisfy the following commutation relation:

$$[X_\parallel, \mathbf{X}_\perp] = -\frac{i\hbar}{p} \mathbf{X}_\perp, \quad [X_\perp_j, X_\perp_k] = -\frac{i\hbar}{p^2} \sum_{l=1}^3 e_{jkl} L_l \quad (j, k = 1, 2, 3) \quad (6)$$

where e_{jkl} is the absolutely antisymmetric tensor and $e_{123} = 1$. An immediate consequence of these relation follows: *Since the operator X_{\parallel} and different components of \mathbf{X}_{\perp} do not commute with each other, the corresponding quantities cannot be simultaneously measured and hence there is no wave function $\psi(x_{\parallel}, \mathbf{x}_{\perp})$ in coordinate representation.*

As follows from Eq. (4), $[p, X_{\parallel}] = -i\hbar$, i.e. in the longitudinal direction the commutation relation between the coordinate and momentum is the same as in standard theory. One can also calculate the commutators between the different components of \mathbf{X}_{\perp} and \mathbf{P} . Those commutators are not given by such simple expressions as in standard theory but it is easy to see that all of them are of the order of \hbar as it should be.

Equation (3) can be treated as an implementation of the relation $\mathbf{x} = x_{\parallel}\mathbf{p}/|\mathbf{p}| + \mathbf{x}_{\perp}$ on quantum level. As argued in Sec. 2, standard position operator in the direction j is not consistently defined if p_j is not sufficiently large. However since the operator X_{\parallel} contains $i\hbar\partial/\partial p$, it is defined consistently if only the magnitude of the momentum is sufficiently large.

In summary, we propose to define the position operator not by the set $(i\hbar\partial/\partial p_x, i\hbar\partial/\partial p_y, i\hbar\partial/\partial p_z)$ but by the operators X_{\parallel} and \mathbf{X}_{\perp} which are consistently defined if only the magnitude of the momentum is sufficiently large.

One might pose the following question. What is the reason to work with the parallel and perpendicular components of the position operator separately if, according to Eq. (3), their sum is the standard position operator? The explanation follows.

In quantum theory every physical quantity corresponds to a selfadjoint operator but the theory does not define explicitly how a quantity corresponding to a specific operator should be measured. There is no guaranty that for each selfadjoint operator there exists a physical quantity which can be measured in real experiments.

Suppose that there are three physical quantities corresponding to the self-adjoint operators A , B and C such that $A + B = C$. Then in each state the mean values of the operators are related as $\bar{A} + \bar{B} = \bar{C}$ but in situations when the operators A and B do not commute with each other there is no direct relation between the distributions of the physical quantities corresponding to the operators A , B and C . For example, in situations when the physical quantities corresponding to the operators A and B are semiclassical and can be measured with a good accuracy, there is no guaranty that the physical quantity corresponding to the operator C can be measured in real measurements. As an example, the physical meaning of the quantity corresponding to the operator $L_x + L_y$ is problematic. Another example is the situation with WPS in directions perpendicular to the particle momentum. Indeed, as noted above, the physical quantity corresponding to the operator \mathbf{X}_{\perp} does not experience WPS. However, standard position operator is a sum of noncommuting operators corresponding to well defined physical quantities and, as a consequence, there are situations when standard position operator defines a quantity which cannot be

measured in real experiments.

4 Conclusion

In Sec. 2 we discuss standard uncertainty principle which is a consequence of choosing standard position operator. The major theoretical drawback of this choice is that the consistency of standard position operator depends on the choice of coordinate axis. In particular, a standard choice inevitably predicts a considerable wave packet spreading (WPS) in directions perpendicular to the particle momentum and, as shown in Ref. [1], this leads to several striking paradoxes.

In Sec. 3 we consider a new definition of the position operator proposed in Ref. [1]. We treat this definition as consistent because, in contrast to standard position operator, the new one does not depend on the choice of coordinate axis and is expected to be physical if only the *magnitude* of the momentum is rather large.

As a consequence of our construction, WPS in directions perpendicular to the particle momentum is absent and the paradoxes discussed in Ref. [1] are resolved. Another consequence of the new choice of the position operator is that now uncertainty relations do not have such a simple form as in Eq. (1). However, the correspondence principle between quantum and classical theory remains valid because all the commutators between different components of the momentum and position operators are proportional to \hbar and therefore they disappear in classical limit.

Different components of the new position operator do not commute with each other and, as a consequence, there is no wave function in coordinate representation. A possibility that coordinates can be noncommutative has been first discussed by Snyder [12] and is implemented in several modern theories. In those theories the measure of noncommutativity is defined by a parameter l called the fundamental length (the role of which can be played e.g. by the Planck length or the Schwarzschild radius). In the formal limit $l \rightarrow 0$ the coordinates become standard ones related to momenta by a Fourier transform. As follows from the above discussion, this is unacceptable for several reasons. One of ideas of those theories is that with a nonzero l it might be possible to resolve difficulties of standard theory where $l = 0$. At the same time, in our approach there can be no notion of fundamental length since commutativity of coordinates takes place only in the formal limit $\hbar \rightarrow 0$.

As discussed in Ref. [1], the new choice of the position operator also sheds a new light on other problems of quantum theory.

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