Geometric structure of the arrival time operator

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Uniqueness of the construction of the quantum arrival time operator, proposed by me in 1974, follows from the uniqueness of the “quantization through Lie derivative” which applies to any observable linear in momenta. Arguments given by Wolfgang Pauli against the “quantum time operator” are shown to be equivalent to the non-completeness of the constant vector field on the real half-line $\mathbb{R}_+$.

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1. Introduction

Consider a configuration space $Q$ equipped with an Euclidean structure and parametrized by Cartesian coordinates $(q^j), j = 1, \ldots, \dim Q$. Every hyperplane $H \subset Q$ gives rise to an observable $t_H$ equal to the “time of arrival of the particle on $H$”. The observable is a function defined on the classical phase space $P := T^* Q$ (cotangent bundle over $Q$) parametrized by positions $q^i$ and by the conjugate momenta $\pi^i$:

$$P = \{(\pi^i, q_j)\}. \quad (1)$$

Its numerical value $t_H(\pi_i, q^j)$ tells us “how much time would take the particle to reach $H$, if it starts from the actual position $q$, with the actual momentum $\pi$, assuming the free motion of the particle”. We have, therefore:

$$t_H = -\frac{d}{v}, \quad (2)$$

where $d$ denotes the (oriented) distance of the actual position $q$ of the particle from $H$ and $v$ denotes the (oriented) orthogonal component of its velocity.

Without any loss of generality we can choose Cartesian coordinates in such a way that $H = \{x = 0\}$, where $x = q^1$, $p = \pi_1$ and then we have $d = x$ and $p = mv$, 

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with \( m \) being the mass of the particle. In terms of these coordinates we have:

\[
t_H = -\frac{x}{v} = -\frac{m x}{p}.
\]

(3)

Many authors have already noticed that the naive quantization rule, consisting in replacing classical position and momentum by their quantum counterparts, i.e. the following formula:

\[
\hat{t}_H = -\frac{m \hat{x}}{\hat{p}},
\]

(4)

is meaningless, even if supplemented with extra rules concerning the multiplication order (e.g. symmetric) of non-commuting operators.

In paper [1], a quantum mechanical “arrival time” operator \( \hat{\tau}_H \) was constructed in a mathematically correct way and the uncertainty relation between time and energy was proved (cf. also [2–4]; this construction was briefly sketched also in [5]). In this paper, the uniqueness of this approach is analyzed. For purposes of our analysis, we use mathematical tools belonging to the classical repertoire of “geometric quantization theory” (see e.g. my recent paper [6] for a brief introduction). In fact, the uniqueness of this construction is implied immediately by the geometric content of the wave function in quantum mechanics.

2. Lie Derivative of a Wave Function

A wave function \( \psi \) encodes probabilities through integrals:

\[
P_D = \int_D |\psi(q)|^2 d^n q,
\]

(5)

where \( P_D \) is a probability to find the particle within the set \( D \subset Q \) or, more generally, transition amplitudes between two quantum states \( \psi_1 \) and \( \psi_2 \):

\[
A(\psi_1, \psi_2) = \int_Q \overline{\psi_1}(q)\psi_2(q) d^n q.
\]

(6)

Description of quantum states by scalar functions \( \psi \) has an obvious drawback: it depends upon a choice of the measure \( d^n q \) on the configuration space. This choice is non-physical and the wave function transforms in a non-trivial way if we choose another measure. An obvious way to overcome this difficulty is to consider an invariant object:

\[
\Psi := \psi \sqrt{d^n q},
\]

(7)

which is no longer a scalar but a half-density.\(^a\) Change of the measure implies the corresponding change of the coefficient \( \psi \) in such a way that the right-hand side of

\(^a\)The value \( \Psi(q) \) of a half-form at a point \( q \in Q \) is a function which assigns a number \( \langle V; \Psi(q) \rangle \) to any infinitesimal volume — i.e. a multivector of a maximal rank — \( V \) in a \( \frac{1}{2} \)-homogeneous way:

\[
\langle \alpha V; \Psi(q) \rangle = \sqrt{|\alpha|} \langle V; \Psi(q) \rangle.
\]

More information about the mathematical structures used here may be found in [5] and the references therein.
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(7) remains invariant. Now, formula (6) takes the following form:

\[ A(\Psi_1, \Psi_2) = \int_Q \Upsilon_1 \Psi_2, \]  

(8)

where any dependence upon the non-physical choice of the measure has been manifestly eliminated. Complex half-forms, square-integrable, absolutely continuous with respect to Lebesgue, form a Hilbert space which will be called \( L^2(Q) \), with the scalar product given by the above formula.\(^b\)

Suppose now that \( \mathcal{G} \) is a diffeomorphism of the configuration space \( Q \) onto itself. The corresponding transport of half-forms, denoted by \( \mathcal{G}^* \), defines a unitary operator in the Hilbert space \( L^2(Q) \). In terms of coordinates, if

\[ \mathcal{G}(q^1, \ldots, q^n) = (f^1(q), \ldots, f^n(q)), \]  

(9)

then

\[ (\mathcal{G}^* \Psi)(q) = \psi(f(q))\sqrt{|J|}\sqrt{d^n q}, \]  

(10)

where

\[ J := \det \left( \frac{\partial f^i}{\partial q^j} \right), \]  

(11)

denotes the Jacobian of the mapping (9).

Suppose now that we have a one-parameter group of diffeomorphisms of \( Q \). Such a group is always generated by a vector field on \( Q \). Denote this generator by \( X = \sum_i X^i \frac{\partial}{\partial q^i} \). The elements of the group will, consequently, be denoted by

\[ \mathcal{G}_X^t : Q \to Q. \]

The lift of \( \mathcal{G}_X^t \) to the cotangent bundle defines a group of canonical transformations of the corresponding phase space \( \mathcal{P} = T^*Q = \{(\pi_i, q^i)\} \). It is generated by the following observable, linear in momenta:

\[ \mathcal{X}(q, \pi) = X^i(q)\pi_i. \]

(12)

On the other hand, we have also the group \( (\mathcal{G}_X^t)^* \), \( t \in \mathbb{R}^1 \), of unitary operators in \( L^2(Q) \). We show in the Appendix that the group is continuous in the weak topology of operators. Hence, by virtue of the Stone’s theorem (see e.g. [7–9]) there is a self-adjoint operator \( \hat{X} \) such that the group is of the form:

\[ (\mathcal{G}_X^t)^* = \exp \left( \frac{\hat{X}t}{\hbar} \right). \]  

(13)

Operator \( \hat{X} \) in \( L^2(Q) \) is called a generator of the unitary group. It is self-adjoint \textit{a priori} and can be considered as the quantum counterpart of the classical observable \( \mathcal{X} \) given by (12). But the infinitesimal version of the transport \( (\mathcal{G}_X^t)^* \) is the

\(^b\)Elements of this Hilbert space cannot be identified with physical states of the system. They represent physical states only \textit{up to a generalized Galilei transformation}. Indeed, change of a reference frame implies multiplication of a wave function by a non-local phase factor which is uniquely determined by geometry of the phase space, cf. [6]. This structure, however, will not be used in this paper.
Lie derivative. This means that, differentiating (13) with respect to the variable $t$, we obtain:

$$\frac{1}{\hbar} \hat{X} \Psi = \frac{d}{dt} \bigg|_{t=0} (G^t_X)^* \Psi = \mathcal{L}_X \Psi,$$

or, equivalently:

$$\hat{X} = \frac{\hbar}{i} \mathcal{L}_X.$$

Above formula gives us an unambiguous quantization rule for any observable $X$ which is: (1) linear in momenta and such that (2) the corresponding vector field $X$ on $Q$ is complete, i.e. generates a global group diffeomorphisms. The rule becomes dubious if we begin our construction not with a group of diffeomorphisms $G^t_X$, but with a generic observable (12) which is linear in momenta. The outcome of the above procedure is not obvious because, for a generic vector field $X$, the right-hand side of (15) does not need to be self-adjoint. In fact, it always defines a symmetric operator and the following formula holds:

$$\hbar \frac{i}{t} \mathcal{L}_X = \frac{1}{2} (\hat{X} \hat{\pi}_i + \hat{\pi}_i \hat{X}^i),$$

where $\hat{X}^i$ denotes the operator of multiplication by the function $X^i(q)$ and $\hat{\pi}_i$ is the momentum operator. One could naively conclude that the quantization of (12) consists merely in symmetrization:

$$(X^i \pi_i)^* = \frac{1}{2} (\hat{X}^i \hat{\pi}_i + \hat{\pi}_i \hat{X}^i).$$

Such a conclusion is, however, highly misleading. Indeed, in a generic case the right-hand side of the above formula does not define a self-adjoint operator, unless the field $X$ is complete like in the example above, i.e. unless $X$ defines a global group of diffeomorphisms. A generic vector field $X$ defines only the so-called local group. The corresponding operator given by formula (15) (or, equivalently, by (16)) can either: (1) be essentially self-adjoint (i.e. can have a unique self-adjoint extension), or (2) possess many non-equivalent self-adjoint extensions, or, finally (3) have no self-adjoint extension. This trivial observation would probably not even be worthwhile to mention. Unfortunately, many theoreticians consider the symmetricity of the operator (16) as a relevant property, whereas its relation (15) with the Lie derivative is not even noticed. This is very misleading because the topological properties of the field $X$ (and not any algebraic properties of (16)) are decisive for the self-adjointness of the corresponding quantum observable.

**Example 1.** Let $Q = \mathbb{R}^1$ and $X(x) = x^2 \frac{\partial}{\partial x}$. Solving equation $\dot{x} = x^2$ with appropriate initial condition we obtain:

$$G^t_X(x) = \frac{x}{1 - tx}.$$

The formula is valid for $t < \frac{1}{x}$ if $x > 0$ and for $t > \frac{1}{x}$ if $x < 0$. Hence, $G^t_X(x)$ is not global. However, formula (17) defines a global group of measurable transformations.
of \( Q \). Indeed, it is defined for \( x \neq \frac{1}{t} \) only, i.e. almost everywhere, which is sufficient for a measurable mapping. Consequently, the corresponding transport operators \((G^t_X)^*\) form a group of unitary operators in \( L^2(Q) \). Its generator is a unique self-adjoint extension of the symmetric operator defined by formula (15). We conclude that in this case the quantization via Lie derivative works perfectly, even if the field \( X \) was not complete.

**Example 2.** Let \( Q = \mathbb{R}_+ \) (the positive half-line) and \( X(x) = \frac{\partial}{\partial x} \) is a constant vector field. The corresponding momentum operator “\( \frac{\hbar}{i} \frac{\partial}{\partial x} \)” is a typical example of a symmetric operator which has no self-adjoint extension. Hence, the “quantization procedure” (15) fails in this case.

### 3. Arrival Time Operator as a Lie Derivative

The arrival time (3) is linear with respect to the position \( x \). But “\( -x \)” is the momentum canonically conjugate to the variable \( p \), because \((x, p) \rightarrow (p, -x)\) is a canonical transformation. Hence, in momentum representation, this observable corresponds to the vector field

\[
X = \frac{m}{p} \frac{\partial}{\partial p},
\]

defined on real line \( \mathbb{R}^1 \), parametrized by the momentum variable \( p \). We are going to analyze the properties of the group \( G^t_X \), generated by (18) in order to see whether or not quantization procedure (15) can be used in this case. Technically, the easiest way to perform such an analysis consists in finding a new variable \( s \) which trivializes the field, i.e. such that \( X = \frac{\partial}{\partial s} \). For this purpose, we solve equation

\[
\frac{m}{p} \frac{\partial}{\partial p} = \frac{\partial}{\partial s} = \frac{dp}{ds} \frac{\partial}{\partial p},
\]

which implies:

\[
\frac{p}{m} = \frac{ds}{dp}
\]

and

\[
s = \frac{p^2}{2m}.
\]

The new parameter would be equal to energy \( E = \frac{p^2}{2m} \). However, the above parametrization is not one-to-one and does not cover the entire configuration space. If we use it for \( p > 0 \), then we cannot use it for \( p < 0 \). Hence, \( X = \frac{\partial}{\partial s} \) cannot hold globally. To overcome this difficulty we chose another, globally defined variable:

\[
s = \text{sgn}(p) \cdot E = \begin{cases} 
\frac{p^2}{2m} & \text{for } p > 0, \\
-\frac{p^2}{2m} & \text{for } p < 0,
\end{cases}
\]
equal to the energy for “right movers” and to minus energy for “left movers”. In this parametrization, we have:

\[ X = \text{sgn}(s) \frac{\partial}{\partial s} = \begin{cases} 
\frac{\partial}{\partial s} & \text{for } p > 0, \\
-\frac{\partial}{\partial s} & \text{for } p < 0.
\end{cases} \quad (23) \]

In classical papers like [11–13], the above equation is written as

\[ X = \frac{\partial}{\partial E}, \quad (24) \]

which, in principle, is true by virtue of (22). However, \( E \) is not a global parameter over the momentum space and, therefore, the above formula is ambiguous. It has led in the past to serious misunderstandings. On the other hand, the parameter \( s \) is global and provides a new, perfectly legitimate representation of quantum states.

The wave half-density acquires the following form in this representation:

\[ \Psi = \psi(p) \sqrt{dp} = \psi(\text{sgn}(s) \sqrt{2m|s|}) \cdot \sqrt{\frac{m}{2m|s|}} \cdot \sqrt{ds} = \phi(s) \sqrt{ds} \quad (25) \]

and, whence, the new “physical” wave function equals:

\[ \phi(s) = \psi(\text{sgn}(s) \sqrt{2m|s|}) \cdot \sqrt{\frac{m}{2m|s|}}. \quad (26) \]

According to the naive quantization rule (15), the quantum version of the observable (3) should act on \( \phi \) as the differential operator \( X \) given by formula (23) (multiplied by the factor \( \hbar \)). But this is a typical example of an operator which has no self-adjoint extension. In fact, we have here two disjoint copies of the vector field described in Example 2 of Sec. 2: one copy for the positive half-axis and another for the negative one. This observation simplifies, in fact, all the classical arguments against the possibility to measure time in quantum mechanics, given by Pauli (see footnote in [10, p. 60]) and Allcock (see [11–13]).

On the first glance, one could improve this operator by “smoothing” the field (23) in a neighborhood of the point \( s = 0 \). Unfortunately, such a procedure is highly non-stable: the self-adjoint operator obtained this way depends heavily upon the smoothing (cut-off) procedure and no limit exists when we remove it.

The construction proposed in [1] consists in choosing, instead of \( t_H = -\frac{x}{v} \), a new observable:

\[ \tau_H = \text{sgn}(p) \cdot t_H = -\frac{x}{|v|} = -\frac{m\epsilon}{|p|}, \quad (27) \]

equal to the arrival time \( t_H \) for “right movers” and to \(-t_H\) for “left movers”. This combination of “time” and “minus time” can be perfectly measured in quantum
mechanics. Indeed, the sign of the lower line of (23) is changed which implies the perfect self-adjointness of the following operator:

$$\hat{\tau}^H = \hbar \frac{i}{\partial s} \left( = \text{sgn}(p) \frac{\hbar}{i} \frac{\partial}{\partial E} \right).$$

The discussion above proves the uniqueness of the procedure.

Appendix A. Continuity of the Group of Unitary Transformations Generated by a Complete Vector Field

Assuming that the field $X$ is continuous we have, due to (9):

$$G^t_X(q^1, \ldots, q^n) = (f^1(q, t), \ldots, f^n(q, t)), \quad \text{(A.1)}$$

where $(f^1(q, 0), \ldots, f^n(q, 0)) = (q^1, \ldots, q^n)$ and

$$\left. \frac{d}{dt} f^i(q, t) \right|_{t=0} = X^i(q).$$

Then, in analogy with (10), we have:

$$(G^t_X)^*\Psi(q) = \psi(f(q, t)) \sqrt{|J(q, t)|} \sqrt{\text{d}^n q}, \quad \text{(A.2)}$$

where

$$J(q, t) := \det \left( \frac{\partial f^i(q, t)}{\partial q^j} \right), \quad \text{(A.3)}$$

denotes the Jacobian of the mapping (A.1). If $\Phi = \phi \sqrt{\text{d}^n q} \in L^2(Q)$ is another element of the Hilbert space $L^2(Q)$ then, according to (8), the corresponding scalar product is given by:

$$\langle \Phi | (G^t_X)^*\Psi \rangle = \int_Q \overline{\phi(q)} \cdot \psi(f(q, t)) \sqrt{|J(q, t)|} \sqrt{\text{d}^n q}.$$  

We want to prove the continuous dependence of the above quantity upon the parameter $t$. But, because $(G^t_X)^*$ is unitary, it is sufficient to prove it for $\Psi \in D$, where $D \subset L^2(Q)$ is any dense set. We choose, therefore, the subspace of continuous functions with compact support: $D = C_0(Q) \subset L^2(Q)$. In this case, the function $Q \times \mathbb{R} \ni (q, t) \mapsto \psi(f(q, t)) \sqrt{|J(q, t)|}$ is continuous. Moreover, it has a common bound over any compact interval $t \in [a, b] \subset \mathbb{R}$. Hence

$$t \rightarrow \langle \Phi | (G^t_X)^*\Psi \rangle$$

is continuous due to the Lebesgue’s dominated convergence theorem.

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