Time and energy operators in the canonical quantization of special relativity

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Abstract

Based on Lorentz invariance and Born reciprocity invariance, the canonical quantization of special relativity is shown to provide a unified origin for (i) the complex vector space formulation of quantum mechanics; (ii) the momentum and space commutation relations and the corresponding representations; (iii) the Dirac Hamiltonian in the formulation of relativistic quantum mechanics; (iv) the existence of a self adjoint time operator that circumvents Pauli’s objection.

Keywords: relativistic quantum mechanics, time operator, energy operator

1. Introduction

Quantum mechanics (QM) fails to treat time and space coordinates on the almost equal footing accorded by special relativity (SR), as it does with momentum and energy. In QM time appears as a parameter, not as a dynamical variable. It is a c-number, following Dirac’s designation [1]. This is the Problem of Time (PoT) in QM, which results in the extensive discussion of the existence and meaning of a time operator [2, 3], and of a time–energy uncertainty relation [4, 5] in view of Pauli’s objection [6].

The procedure usually termed ‘canonical quantization’ arises from applying to the Hamiltonian formulation of classical physics the rule of substituting dynamical variables by self adjoint operators acting on normalized vectors representing the physical system. In addition to considering the existence of Lorentz invariants, the Born reciprocity principle is brought into play [7]. This proposed principle arises from noting that the Hamiltonian formulation of classical mechanics is invariant under the transformations $x_i \rightarrow p_i, p_i \rightarrow -x_i$ and from the equivalence of the configuration and momentum representations in QM. Although
Born acknowledges being unsuccessful in his intended applications, the reciprocity principle is currently receiving renewed interest. In the present paper it is shown that it complements the required Lorentz invariance in the canonical quantization of SR to provide a unified origin for: (i) the complex vector space formulation of QM; (ii) the momentum and position operators’ commutation relations and their corresponding representations; (iii) the Hamiltonian in Dirac’s formulation of relativistic quantum mechanics; (iv) the existence of a self-adjoint time operator that circumvents Pauli’s objection.

2. Lorentz and reciprocity invariants in the canonical quantization of special relativity

In SR the invariants under Lorentz transformations for a free particle are the scalar products of the four vectors in a Minkowski space with metric \( \eta_{\mu \nu} = \text{diag}(1, -1, -1, -1) \), namely

\[
p_{\mu} p^{\mu} = \eta^{\mu \nu} p_{\mu} p_{\nu} = p_{0}^2 - \mathbf{p}^2 = (m_{0}c)^2 \quad \text{where } c \text{ is the constant light velocity and } m_{0} (\text{the rest mass} \text{ and } s_{0} (\text{to be interpreted}) \text{ are internal properties of the physical system (Einstein’s summation convention is assumed). To be included in addition are the constant products:}
\]

\[
O^{\pm} = n_{p} p^{\mu} \pm p^{\mu} n_{\mu}
\]

where the symmetrization is introduced as these dynamical variables will be transformed to operators where order matters.

(i) The Dirac free particle Hamiltonian

From the momentum invariant, the first relation in equation (1), one obtains upon quantization the QM constraint

\[
[\hat{p}_{\mu}, \hat{p}^{\mu} - (m_{0}c)^2] |\Psi\rangle = 0.
\]

This can be factorized as

\[
[\rho^{\mu}, \hat{p}_{\mu} + m_{0}c] [\rho^{\mu} \hat{p}_{\mu} - m_{0}c] |\Psi\rangle = 0,
\]

provided that, to cancel the cross terms, the momentum operators satisfy the commutation relation \( [\hat{p}_{\mu}, \hat{p}_{\nu}] = 0 \) and the coefficients \( \rho^{\mu} \) the anticommutation relation \( \{\rho^{\mu}, \rho^{\nu}\} = 2 \eta^{\mu \nu} I_{4} \), where \( I_{4} \) is the \( 4 \times 4 \) identity matrix. Thus the coefficients \( \rho^{\mu} \) obey a Clifford algebra and are represented by matrices.

Then the constraint is satisfied with the linear equation:

\[
[\rho^{\mu}, \hat{p}_{\mu} - m_{0}c] |\Psi\rangle = 0.
\]

Multiplying by \( c \rho^{0} \) and defining \( \rho^{0} := \beta, \rho^0 \rho^i = \alpha^i \) one obtains

\[
\rho^{0} \beta |\Psi\rangle = \{c\alpha^{\mu} \hat{p}_{\mu} + \beta m_{0}c^2\} |\Psi\rangle
\]

which exhibits the Dirac Hamiltonian \( H_{D} = c\alpha^{\mu} \hat{p}_{\mu} + \beta m_{0}c^2 \). One recognizes here the procedure followed by Dirac to obtain a first order linear equation in energy and momentum that agrees with the second order one resulting from the energy momentum relation in equation (1) [1, 11–13].

(ii) The free particle time operator

Born considered the phase space reciprocity invariant \( x_{\mu} v^{\mu} + p_{\mu} p^{\mu} \) as the base to deduce the elementary particle masses. It was too early.
In exactly the same way, from the second relation in equation (1), the displacement invariant yields upon quantization the QM constraint

\[ [\hat{x}_\mu, \hat{x}^\nu - s_0^2] |\Psi\rangle = 0. \]  

(7)

This can be factorized as

\[ [\rho^{\mu} \hat{x}_\mu + s_0][\rho^{\nu} \hat{x}_\nu - s_0] |\Psi\rangle = 0 \]

(8)

provided now \([\hat{x}_\mu, \hat{x}_\nu] = 0\) and again \(\{\rho^{\mu} \rho^{\nu} + \rho^{\nu} \rho^{\mu}\} = 2\eta^{\mu\nu} \mathbf{1}_4\). The constraint is then satisfied with the linear equation:

\[ [\rho^{\nu} \hat{x}_\nu - s_0] |\Psi\rangle = 0 \]

(9)

or, denoting \(s_0 = c\tau_0\) where \(\tau_0\) would be an internal time property of the system:

\[ (\hat{x}_0 / c) |\Psi\rangle = \{\alpha \hat{r} / c + \beta \tau_0\} |\Psi\rangle. \]

(10)

Here \(T = \alpha \hat{r} / c + \beta \tau_0\) is the time operator introduced earlier by analogy to the Dirac Hamiltonian [15].

(iii) The Born reciprocity invariant

The invariants

\[ \hat{O}^\pm = \{\hat{x}^{\mu} \hat{p}_\mu \pm \hat{p}^{\mu} \hat{x}_\mu\} = \{\hat{x}_0 \hat{p}_0 - \hat{r} \hat{\rho} \pm \{\hat{p}_0 \hat{x}_0 - \hat{p} \hat{r}\} = \{\hat{x}_0 \hat{p}_0 \pm \hat{p}_0 \hat{x}_0\} - \{\hat{r} \hat{\rho} \pm \hat{\rho} \hat{r}\} \]

(11)

give the constraint

\[ \{\hat{x}_0 \hat{p}_0 \pm \hat{p}_0 \hat{x}_0\} - \{\hat{r} \hat{\rho} \pm \hat{\rho} \hat{r}\} |\Psi\rangle = 0 \]

(12)

or equivalently

\[ \{\hat{x}_0 \hat{p}_0 \pm \hat{p}_0 \hat{x}_0\} |\Psi\rangle = \{\hat{r} \hat{\rho} \pm \hat{\rho} \hat{r}\} |\Psi\rangle. \]

(13)

The operator \(O^+\) is self adjoint and represents a real invariant. On the other hand \(O^-\) is a pure imaginary invariant as \((O^-)^* = - O^-\), but is the one to satisfy reciprocity invariance. An obvious choice for \(O^-\) to satisfy equations (12) and (13) is

\[ \{\hat{x}_0 \hat{p}_0 - \hat{p}_0 \hat{x}_0\} = \{\hat{r} \hat{\rho} - \hat{\rho} \hat{r}\} = i\hbar \]

(14)

where \(\hbar\) is the reduced Planck constant.

Thus reciprocity invariance complements Lorentz invariance to yield the commutation relations of the operators \(\hat{x}_\mu\) and \(\hat{p}_\mu\), namely

\[ [\hat{x}_\mu, \hat{x}_\nu] = 0, \quad [\hat{p}_\mu, \hat{p}_\nu] = 0, \quad [\hat{x}_\mu, \hat{p}_\nu] = i\hbar \varepsilon_{\mu\nu} \]

(15)

as an alternative to the postulate of transforming Poisson brackets to quantum commutators. In appendix A it is shown that these commutation relations are sufficient to derive: (a) the continuity from \(-\infty\) to \(+\infty\) of the spectra of \(\hat{x}_\mu\) and \(\hat{p}_\mu\); (b) the representations of \(\hat{x}_\mu\) and \(\hat{p}_\mu\) in the corresponding orthogonal eigenvector basis; (c) the Fourier transformation between the configuration and momentum representation of the system vector; (d) the Heisenberg uncertainty relations, including Bohr’s interpretation of the time–energy uncertainty relation (appendix B). Such a unified relationship is unfortunately not present in QM textbooks, where some of these elements are usually introduced as independent anzats.
3. Configuration and momentum representations

Considering equation (6), in the configuration representation where \( \hat{p}_x \rightarrow -i\hbar \frac{\partial}{\partial x_0} \), this equation reads

\[
i\hbar c \frac{\partial}{\partial x_0} \Psi(x, x_0) = \left\{ -i\hbar c \alpha^i \frac{\partial}{\partial x_i} + \beta m_0 c^2 \right\} \Psi(x, x_0).
\]

Substituting from SR \( x_0 = ct \), the result is Dirac’s relativistic equation as usually formulated, namely

\[
i\hbar \frac{\partial}{\partial t} \Psi(x, t) = \left\{ -i\hbar c \alpha^i \frac{\partial}{\partial x_i} + \beta m_0 c^2 \right\} \Psi(x, t).
\]

On the other hand, in the momentum representation where \( \hat{p}_x \rightarrow m \beta \), equation (10) yields

\[
i\hbar \frac{\partial}{\partial p_0} \Phi(p, p_0) = \left\{ (i\hbar/c) \alpha^i \frac{\partial}{\partial p_i} + \beta \right\} \Phi(p, p_0).
\]

Substituting \( \epsilon p_0 = e \), one obtains for the time operator the equation:

\[
i\hbar \frac{\partial}{\partial e} \Phi(p, e) = \left\{ (i\hbar/c) \alpha^i \frac{\partial}{\partial p_i} + \beta \right\} \Phi(p, e).
\]

4. The energy and time spectra, and Pauli’s objection

As is well known, the energy spectrum of the Dirac Hamiltonian has both positive and negative real values, namely \( \epsilon(p) = \pm \sqrt{cp^2 + m_0 c^2} \), separated by a \( 2m_0 c^2 \) gap. In the same way, the spectrum of the time operator contains positive and negative real values separated by a gap \( 2\tau_0 \), as \( \tau(r) = \pm \sqrt{(r/c)^2 + \tau_0} \).

Now, the actual interpretation of the effect of the Dirac Hamiltonian \( \hat{H}_D \) and the time operator \( \hat{T} \) is seen from the fact that they are self adjoint. By Stone–von Newmann’s theorem [17], they are generators of unitary transformations of the state vectors. It can then be shown that for infinitesimal changes [16]:

a) \( U_T = \exp[i\beta e T / \hbar] \approx \exp[i\beta \epsilon(p) / \hbar] \exp[i\beta \epsilon(0) / \hbar] \) generates continuous displacements in momentum \( \phi = (\alpha/c)\beta \epsilon = c\alpha(\beta \epsilon/c^2) \) and changes in the phase \( b = \beta \epsilon / \hbar \). A \( 2\pi \) finite phase change for positive energy waves (\( \beta = 1 \)) is obtained from setting

\[
\tau_0 = h/m_0 c^2 = T_B \quad \Delta e = m_0 e^2 = h/T_B.
\]

Then \( \tau_0 \) is seen to be the de Broglie period \( T_B \), in agreement with de Broglie’s daring assumptions [18, 19]. It is an intrinsic time property associated with the rest mass [20].

b) \( U_{H_0} = \exp[i\beta t / \hbar] \approx \exp[i\beta t c\alpha \cdot p / \hbar] \exp[i\beta t \beta m_0 c^2] \) generates displacements in space \( \delta \mathbf{r} = c\alpha \beta \delta t \) and changes in phase \( \delta \phi = \beta m_0 c^2 \delta t / \hbar \). For \( \beta = 1 \), a \( 2\pi \) finite change of phase requires a time lapse:

\[
\Delta t = 2\pi h / m_0 c^2 = h / m_0 c^2 = T_B.
\]
For wave packets the expectation value $\langle c \alpha \rangle$ is the group velocity $v_{gp}$ and the space displacement in a time lapse $\Delta t$ generated by $H_D$ corresponds to the classical $v_{gp} \Delta t$. On the other hand $T$ acts on the continuous momentum space, generating a change of momentum $\Delta p = m v_{gp} = m_0 \gamma v_{gp}$, where $\gamma = \left[ 1 - (v/c)^2 \right]^{-1}$ is the Lorentz factor, and consequently an energy change from $E(p)$ to $E(p + m v_{gp})$ in both branches of the relativistic energy spectrum. This circumvents Pauli’s correct objection that a commutation relation $[T, H] = i \hbar$ where $T$ acts on the energy spectrum, necessarily implies a continuum energy spectrum from $-\infty$ to $+\infty$, contradicting the fact that the energy expectation value is expected to be positive and that there also may be discrete eigenvalues [6].

To be remarked on finally is that, from equation (20), the energy gap $2m c^2$ and the time gap $2\hbar/m_0c^2$ are complementary of each other. The mass dependence of the Zitterbewegung period (twice the de Broglie period) has been correctly exhibited in the experimental simulation of the Dirac equation with trapped ions [21, 22].

5. Conclusion

It has been shown that the canonical quantization of SR that preserves the Lorentz and reciprocity invariants, is at the origin of the (usually postulated or inferred separately) commutation relations of the configuration and momentum dynamical operators, as well as of the Dirac relativistic Hamiltonian together with a self adjoint relativistic ‘time operator’. Furthermore, it brings about the derived properties—infinitesimal continuous space and momentum spectra, ensuing representations, and the uncertainty relation as shown in appendix A and B, that unfortunately in most quantum mechanics (QM) textbooks are introduced as independent anzats.

Also to be stressed is the reciprocity invariance which introduces an imaginary constant, opening the formulation to complex functions which are necessary to allow for ‘a non-negative probability function that is constant in time when integrated over the whole space’ [6], the basis for a probabilistic interpretation of QM.

The problem of time is very much present in the canonical quantization of general relativity, with many facets: indetermination of the spacetime foliation (‘many fingered time’), disappearance of time (‘frozen formalism’), and so on [24–27]. However, one condition to be satisfied is local concordance with special relativity, i.e. any acceptable theory of quantum gravity must allow to recover the classical spacetime in the appropriate limit [28]. It follows that an avenue to be explored is whether this bottom up completion of Dirac’s relativistic quantum mechanics with a time operator as derived above helps to resolve some of the issues noted [22, 23].

Appendix A. The lore of $[\hat{x}, \hat{p}] = i \hbar$

To represent observables the operators $\hat{x}_\mu$ and $\hat{p}_\mu$ are self adjoint ($\hat{x}_\mu = \hat{x}_\mu^\dagger$, $\hat{p}_\mu = \hat{p}_\mu^\dagger$), which insures real eigenvalues. Then, for each component $\hat{x}_\mu$ and $\hat{p}_\mu$, it follows:

1. Spectrum [13]

Consider the eigenvalue equation:

$$\hat{x} |x\rangle = x |x\rangle.$$  \hspace{1cm} (A.1)

By Stone–von Neumann’s theorem the operator $U(\alpha) = \exp(-i \alpha \hat{p}/\hbar)$ with $a$ real is unitary [17]. Then it can be shown that
\[ \hat{x} \{ U(\alpha)|x\} = (x + \alpha)\{ U(\alpha)|x\}. \]  
(A.2)

Therefore \( \{ U(\alpha)|x\} = C(x + \alpha) \). As \( \alpha \) is arbitrary, it follows that the eigenvalues of \( \hat{x} \) are continuous from \( -\infty \) to \( +\infty \), and that the eigenvectors satisfy

\[ \langle x'|x \rangle = \delta(x' - x) \quad \int dx \langle x|\hat{x}|x \rangle = I \]  
(A.3)

where \( \delta(x' - x) \) is the Dirac delta function and \( I \) is the identity operator.

In the same way one can prove that the eigenvalues in \( \hat{p} \mid p \rangle \rangle = p \mid p \rangle \rangle \) span a continuum from \( -\infty \) to \( +\infty \) and that the eigenvectors satisfy

\[ \langle p'|p \rangle = \delta(p' - p) \quad \int dp \langle p|p \rangle = I. \]  
(A.4)

(2) Representations

From equation (A.3):

\[ \langle x'|\hat{x}|x \rangle = x\delta(x' - x) \]

and

\[ \langle x'|[\hat{x}, \hat{p}]|x \rangle = i\hbar\delta(x' - x) = \langle x'| \hat{x}\hat{p} - \hat{p}\hat{x}|x \rangle = x'\langle x'| \hat{p}|x \rangle - x\langle x'| \hat{p}|x \rangle = (x' - x)\langle x'| \hat{p}|x \rangle. \]

It follows

\[ \langle x'| \hat{p}|x \rangle \rightarrow \frac{i\hbar\delta(x' - x)}{(x' - x)} \rightarrow_{x' \rightarrow x} i\hbar \frac{d}{dx'} \delta(x' - x). \]  
(A.5)

Introducing the vectors:

\[ |\Theta \rangle = \hat{x}|\Psi \rangle \quad |\Phi \rangle = \hat{p}|\Psi \rangle \]

their representations in configuration space are

\[ \Theta(x) = \langle x| \hat{x}|\Psi \rangle = x\langle x|\Psi \rangle = x\Psi(x) \]  
(A.6)

and using equation (A.5):

\[ \Psi(x) = \langle x|\hat{\Phi} \rangle = \langle x|\hat{p}|\Psi \rangle = \frac{i\hbar}{\pi} \int \frac{dx'}{(x' - x)} \delta(x' - x) \Psi(x'). \]  
(A.7)

i.e. the representation in configuration space of the vector \( |\Phi \rangle = \hat{p}|\Psi \rangle \) is obtained by taking the derivative of the representation of the vector \( |\Psi \rangle \), while the representation in configuration space of the vector \( |\Theta \rangle = \hat{x}|\Psi \rangle \) is obtained multiplying by \( x \) the representation of \( |\Psi \rangle \).

To conclude, in configuration space one has

\[ \hat{x} \rightarrow x \quad \hat{p} \rightarrow -i\hbar \frac{d}{dx}. \]  
(A.8)

In the same way in momentum space:

\[ \hat{x} \rightarrow i\hbar \frac{d}{dp} \quad \hat{p} \rightarrow p. \]  
(A.9)

(3) Transformation between representations
Consider
\[ \langle x | \hat{x}, \hat{p} | p \rangle = i \hbar \langle x | p \rangle. \]

Developing
\[ \langle x | \hat{x}, \hat{p} | p \rangle = \langle x | \hat{x} \hat{p} | p \rangle - \langle x | \hat{p} \hat{x} | p \rangle \]
\[ = x p \langle x | p \rangle - \int dx' \langle x | \hat{p} | x' \rangle \langle x' | \hat{x} | p \rangle \]
\[ = x p \langle x | p \rangle - i \hbar \int dx' \left[ \frac{d}{dx} \delta(x' - x) \right] x' \langle x' | p \rangle \]
\[ = x p \langle x | p \rangle + i \hbar [x | p \rangle + i \hbar \frac{d}{dx} \langle x | p \rangle] \]

one obtains
\[ x p \langle x | p \rangle + i \hbar [x | p \rangle + i \hbar \frac{d}{dx} \langle x | p \rangle] = i \hbar \langle x | p \rangle. \]

Thus
\[ i \hbar \frac{d}{dx} \langle x | p \rangle = -p \langle x | p \rangle \quad \text{(A.10)} \]

which is satisfied if
\[ \langle x | p \rangle = C e^{i p x / \hbar} \quad \langle p | x \rangle = C^* e^{-i p x / \hbar}. \quad \text{(A.11)} \]

Finally
\[ \Phi(p) = \langle p | \Psi \rangle = \int dx \langle p | x \rangle \langle x | \Psi \rangle = C^* \int dx \ e^{-i p x / \hbar} \Psi(x) \quad \text{(A.12)} \]

and
\[ \Psi(x) = \langle x | \Psi \rangle = \int dp \langle x | p \rangle \langle p | \Psi \rangle = C \int dx \ e^{i p x / \hbar} \Phi(p) \quad \text{(A.13)} \]

i.e. the representations of the state vector in the configuration and momentum spaces are *Fourier transforms* of each other. To preserve normalization one requires \( C = C^* = 1 / \sqrt{2 \pi \hbar} \).

(4) Uncertainty relation

Consider the state vectors
\[ | \Phi \rangle = (\hat{x} - \langle x \rangle) | \Psi \rangle \quad \text{and} \quad | \Xi \rangle = (\hat{p} - \langle p \rangle) | \Psi \rangle. \quad \text{(A.14)} \]

Then
\[ \langle \Phi | \Phi \rangle = \langle \Psi | \hat{x}^2 | \Psi \rangle - \langle \Psi | \hat{x} | \Psi \rangle^2 = (\Delta x)^2 \quad \langle \Xi | \Xi \rangle = \langle \Psi | \hat{p}^2 | \Psi \rangle - \langle \Psi | \hat{p} | \Psi \rangle^2 = (\Delta p)^2. \quad \text{(A.15)} \]

By a Schwarz inequality one has
\[ \langle \Phi | \Phi \rangle \langle \Xi | \Xi \rangle \geq \langle \Phi | \Xi \rangle^2 \]
\[ = \left| \langle \Psi | \frac{1}{2} [\hat{x}, \hat{p}] + \frac{1}{2} \{\hat{x}, \hat{p}\} - \langle x \rangle \langle p \rangle | \Psi \rangle \right|^2 \]
\[ \geq \left| \langle \Psi | \frac{1}{2} [\hat{x}, \hat{p}] | \Psi \rangle \right|^2 = (h/2)^2. \]

Finally
\[ (\Delta x)_\Psi (\Delta p)_\Psi \geq h/2. \quad \text{(A.16)} \]
Appendix B. The time–energy uncertainty relation

The Dirac Hamiltonian and the time operator satisfy the commutation relation

\[ [T, \mathcal{H}_D] = i\hbar \{ I + 2\beta K \} + 2\beta \{ \gamma_0 \mathcal{H}_D - m_0 c^2 T \} \quad (B.1) \]

where \( K = \beta (2sI/h^2 + 1) \) is a constant of motion \[11\]. In the usual manner an uncertainty relation follows, namely

\[ (\Delta T)(\Delta \mathcal{H}_D) \geq \left( \frac{\hbar}{2} \right) \left| 1 + 2 \frac{\beta K}{\hbar} \right| \quad \geq \left( \frac{\hbar}{2} \right) \left| 3 + 4sI/h^2 \right|. \quad (B.2) \]

Consider

\[ (\Delta T)^2 = \langle T^2 \rangle - \langle T \rangle^2 = \langle r^2/c^2 + \tau_0^2 \rangle - \langle \alpha r/c + \beta \tau_0 \rangle^2 = \]

\[ = \left( 1/c^2 \right) (\Delta r)^2 - \left[ (r/c) + \beta \tau_0 \right]^2 \geq \left( 1/c^2 \right) (\Delta r)^2. \quad (B.3) \]

In the same way:

\[ 1/c^2 (\Delta \mathcal{H}_D)^2 \geq (\Delta p)^2. \quad (B.4) \]

It follows finally

\[ (\Delta T)^2 (\Delta \mathcal{H}_D)^2 \geq (\Delta r)^2 (\Delta p)^2. \quad (B.5) \]

This corresponds to Bohr’s interpretation that the uncertainty in the time of passage at a certain point is given by the width of the wave packet, which is complementary to the momentum uncertainty, and thus to the energy uncertainty \[29\].

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