Canonical Quantization of the Classical Hamiltonian for a Relativistic Spin-0 Particle

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When quantizing the classical Hamiltonian $H(q, p, t) = \left[ m^2 c^4 + (p - eA(t, q))^2 \right]^{1/2} + eV(t, q)$, commutators of the form $[f(a), g(b)]$, where $[a, b]$ is not a c-number, have to be evaluated. The concept of continuously symmetrized products enables us to derive a number of statements, such as a continuity equation for the density operator $\rho(q(t) - x) = n(t, x)$, in a formally concise way. We can also show, then, that the dependence of the Hamiltonian on higher powers of the kinetic momentum destroys the relativistic invariance of the theory, even if we admit a more general coupling of the external potentials than above.

I. Introduction

A series of publications have treated bound systems with relativistic kinematics by the eigenvalue equation

$$\sqrt{m^2 c^4 - h^2 c^2 V^2} \psi(x) + U(x) \psi(x) = E \psi(x),$$

$$\int (dx) |\psi(x)|^2 = 1$$

(1)

with $U(x)$ being the Coulomb potential [1, 2], or a different potential, modelling, for instance, bound quarks in a confining potential [3–5]. We find it necessary to emphasize that the underlying Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(t, x) = c J(m c)^2 + \left( -i \hbar V - \frac{e}{c} A(t, x) \right)^2 \psi(t, x) + eV(t, x) \psi(t, x),$$

(2)

which has also been discussed in a recent paper by Trübenbacher [2] and by ourselves [6], does not have a relativistically invariant meaning. This has been shown, as early as 1963, by Sucher [7] for scalar fields $\psi(t, x)$, transforming locally under boosts [8]. However, Sucher left open the question [9] whether the same would be true for a non-local transformation behaviour of $\psi$.

As we shall show in this paper, the same holds, indeed, for an amplitude $\psi(t, \cdot) \in L^2(R^3, d^3x)$ which must transform non-locally under boosts in order to leave its norm invariant. In other words, this means that the canonical quantization of the classical Hamilton function

$$H(t, q, p) = c \sqrt{(m c)^2 + \left( p - eA(t, q) \right)^2} + eV(t, q)$$

(3)

with the aid of the commutation relations

$$[q_j, p_k] = i\hbar \delta_{jk}, \quad [q_j, q_k] = 0 = [p_j, p_k],$$

$$j, k = 1, 2, 3,$$

(4)

does not lead to a covariant dynamics.

The same is true, even, if we allow for a generalized coupling of the external fields to the dynamical variables of the particle, i.e., for a Hamiltonian

$$H_r = c \sqrt{(m c)^2 + (p - e/c A)^2} + eV_r$$

(5)

with potential operators of the form

$$A_r^\mu(q, p) := \int (dx) K(q, p, x) A_\mu(t, x), \quad A_r^0 \equiv V_r, \quad \mu = 0, 1, 2, 3.$$ 

(6)

Here, $A_r^\mu$ denotes the classical fields and $K(q, p, x)$ is a coupling function which obeys

$$\int (dx) K(q, p, x) = 1.$$ 

(7)

Definition (6) is the most general way [10] of introducing the classical external potentials as operators on the particle's state space. In position space, it describes a non-local coupling between the amplitude $\psi(t, x)$
and the fields $A_i^a(t,x)$. The standard form (3) is included in (5) and (6) if the special choice $K(q,p,x) = \delta(q-x)$ is made.

II. Symmetrization

We start from the Hamiltonian (3) and shall consistently work in the Heisenberg picture. Since the momentum $p$ and the vector potential $A$ are hermitean operators, the kinetic energy

$$H - e V = c \sqrt{(mc)^2 + (p - \frac{e}{c} A)^2}$$

(8)

is hermitean and positive, where the square root is understood to be defined with the aid of the spectral representation associated with the operator $(p - \frac{e}{c} A)^2$ [11]. For simplicity, we write

$$\pi_0 = H - e V, \quad \pi = p - \frac{e}{c} A$$

(9)

for the kinetic energy and the kinetic momentum, respectively.

For a classical particle, there is no problem with the velocity

$$v = \frac{\partial H}{\partial p} = \frac{c\pi}{\sqrt{(mc)^2 + \pi^2}}.$$  

(10)

In contrast, the quantum analog

$$v = \frac{1}{i\hbar} [q, c \sqrt{(mc)^2 + \pi^2}] = \frac{c\pi}{\sqrt{(mc)^2 + \pi^2}}.$$  

(11)

involves a function of the vector operator $\pi$ whose components may not commute with each other. In general terms, one must symmetrize the product of $c\pi$ and $[(mc)^2 + \pi^2]^{-1/2}$. The latter contains arbitrary powers of $\pi^2$ and, therefore, the required symmetrization procedure is somewhat sophisticated.

As an illustration we first consider a weakly relativistic particle in a magnetic field. The Hamiltonian

$$H^{(\text{wrt})} = \frac{\pi^2}{2m} - \frac{(\pi^2)^2}{2m^3 c^2} + \frac{(\pi^2)^3}{16m^5 c^4}, \quad \pi = \sum_{i=1}^{3} \pi_i^a,$$

implies the velocity

$$v^{(\text{wrt})} = \frac{1}{i\hbar} [q, H^{(\text{wrt})}] = \frac{\pi}{m} - \frac{1}{2m^3 c^2} \pi \cdot \pi^2 + \frac{3}{8m^5 c^4} \pi \cdot (\pi^2)^2,$$

(12)

where

$$\pi \cdot \pi^2 = \frac{1}{2} (\pi^2)^2 + \frac{1}{2} \pi^2$$

(13)

denotes the ordinarily symmetrized product of the operators $\pi$ and $\pi^2$, and

$$\pi \cdot (\pi^2)^2 = \frac{1}{3} (\pi (\pi^2)^2 + \pi^2 \pi^2 + (\pi^2)^2 \pi) \neq \pi \cdot (\pi^2)^2$$

(14)

exemplifies a refined symmetrization of $\pi$ and $(\pi^2)^2$.

II a. Continuously Symmetrized Products

In order to find an expression for the commutator $[q, \sqrt{(mc)^2 + \pi^2}]$ we first note that for two operators $a$ and $b$ the identity

$$[a, b^n] = \sum_{k=0}^{n-1} b^k [a, b] b^{n-k-1}, \quad n = 1, 2, 3, \ldots$$  

(15)

holds.

For arbitrary functions $f(b)$ of an operator $b$, (15) suggests to evaluate $[a, f(b)]$ through an expansion of $f$ into a power series. In general, however, such an expansion may not converge for all eigenvalues $b'$ of the operator $b$. If this is the situation, then the power series cannot be used as a stand-in for the operator function $f(b)$.

For hermitean operators $b$, to which we shall restrict the discussion from here on, we can utilize a Fourier decomposition [more about this at the end of this section]

$$f(b) = \int_{-\infty}^{\infty} d\beta e^{i\beta b} \tilde{f}(\beta)$$  

(16)

in conjunction with the identity

$$[a, e^{i\beta b}] = \frac{1}{i} \int_0^\infty dx e^{ixb} [a, i\beta b] e^{i(1-x)b},$$  

(17)

to evaluate the commutator $[a, f(b)]$ [12]. This results in the definition

$$[a, f(b)] = [a, b] \cdot f'(b),$$  

(18)

which introduces the concept of a continuously symmetrized product (CSP) of an operator $A$ with an operator function $F(B)$,

$$A \cdot F(B) = \int_{-\infty}^{\infty} d\beta \tilde{F}(\beta) \int_0^\infty dx e^{ix\beta b} A e^{i(1-x)\beta b},$$  

(19)

where $F(B)$ and $\tilde{F}(\beta)$ are related to each other as in (16). This continuous symmetrization is markedly different from the straight symmetrization illustrated by (13). In particular observe that the functional dependence of the operator $F(B)$ on $B$ enters the definition...
of the CSP explicitly. When the trace of an operator product is computed, it does not matter which symmetrization, if any, is used,

$$\text{tr} \{ A \cdot F(B) \} = \text{tr} \{ A \cdot F(B) \} = \text{tr} \{ A \cdot F(B) \}. \quad (20)$$

The CSP is linear, and illustrating examples are

$$A..e^B = \int_0^1 dx e^{x} A e^{(1-x)B},$$

$$A..B^n = \frac{1}{n+1} \sum_{k=0}^n B^k A B^{n-k},$$

$$A..B = \frac{1}{2} (A B + B A) = A.B,$$

$$A..1 = A,$$

including (14). The concept of CSP enables us to handle not only commutators efficiently but also variations of functions of operators according to

$$\frac{d}{d \beta} f(b(e)) = b'( e) \cdot f'(b) \quad (21)$$

Equations (18), (21) and (22) express a generalized chain rule for variations of operators. Note that (18) reduces to the familiar form

$$[q, f(p)] = q [p,b] \cdot f'(b) = i h \left[ q, b \cdot f'(b) \right]$$

if $$a = q$$ (position) and $$b = p$$ (momentum).

Before proceeding, let us extend the concept of CSP so that it applies to functions of a vector operator $$B = (B_1, B_2, B_3)$$ as well. This is achieved by

$$A..F(B) = \int (d\beta) \hat{F}(\beta) \int_0^1 dx e^{i x \cdot \beta - B} A e^{i(1-x)\beta - B}, \quad (23)$$

which is applicable if the components of $$B$$ commute with one another. The functions $$F(B)$$ and $$\hat{F}(\beta)$$ are here related by

$$f(b) = \int (d\beta) \hat{F}(\beta) e^{i \cdot \beta - B}. \quad (24)$$

As statements corresponding to (18), (21) and (22) we have

$$[a, f(b)] = \sum_{k=1}^3 [a, b_k] \cdot (\hat{c}_k f)(b), \quad (25)$$

$$\frac{d}{d \varepsilon} f(b(\varepsilon)) = \sum_{k=1}^3 \frac{db_k(\varepsilon)}{d \varepsilon} \cdot (\hat{c}_k f)(b), \quad (26)$$

$$\delta_b f(b) = \sum_{k=1}^3 \delta b_k \cdot (\hat{c}_k f)(b). \quad (27)$$

A comment concerning the Fourier integrals (16) and (24) is in order. The function $$\hat{f}(\beta)$$ in (16), say, is not uniquely determined by the operator function $$f(b)$$, unless all real numbers are eigenvalues of $$b$$. Consider, for example, a number operator $$N$$ with eigenvalues 0, 1, 2, 3... and

$$f(N) = (-1)^N. \quad (28)$$

In view of $$[\pi = 3.14...$$ there

$$f(N) = e^{i \pi N} = \cos(\pi N) = \frac{8}{\pi^2} \sum_{k=0}^{\infty} \cos \left[ \frac{(2k+1)\pi N}{2(k+1)^2} \right]$$

there are the options

$$\hat{f}(\beta) = \begin{cases} \delta(\beta - \pi), & \text{or} \quad \frac{1}{2} \delta(\beta - \pi) + \frac{1}{2} \delta(\beta + \pi), \text{ or} \quad \delta(\beta - (2k+1)\pi) + \delta(\beta + (2k+1)\pi), \end{cases} \quad (30)$$

which are quite different functions of $$\beta$$. Either one of them can be used in (16).

II b. Velocity and Currents

For notational simplicity and physical transparency we set $$h = 1$$, $$c = 1$$ for the further discussion.

The relations (18), (21), (22) and (25), (26), (27), respectively, allow us to handle the Hamiltonian (3) or (5) in a compact way. The operator function $$w(\pi^2)$$ corresponding to

$$w(x) := \begin{cases} \sqrt{m^2 + x}, & x \geq 0 \\ 0, & x < 0 \end{cases} \quad (31)$$

is the kinetic energy of the particle including its rest energy. From (25) we obtain the velocity

$$\frac{dq}{dt} = \frac{1}{i} [q, w(\pi^2)] = \frac{1}{i} [q, \pi^2] \cdot w'(\pi^2) = \pi \cdot w^{-1}(\pi^2). \quad (32)$$

This specifies -- with the aid of the CSP (19) -- the quantum analog of (10) that was left in limbo at (11).

The Lorentz-force equation reads

$$\frac{d\pi}{dt} = \frac{1}{i} [\pi, w(\pi^2) + e V] = e \left[ E + \frac{1}{2} (\pi \times B - B \times \pi) \cdot w^{-1}(\pi^2) \right], \quad (33)$$

where

$$E = E(t, q(t)) = - \left( V V + \frac{\partial A}{\partial t} \right)(t, q(t)),$$

$$B = (V \times A)(t, q(t))$$
are the operators of the external electric and magnetic fields. The two integro-differential equations (32) and (33) determine explicitly the time evolution of the dynamical observables \( q(t) \) and \( \pi(t) \).

As a further application we consider the time derivative of the particle density operator \( n(t,x) = \delta(q(t) - x) \) whose expectation value is the spatial probability density [13]. One way of evaluating the time derivative is

\[
\frac{d}{dt} \delta(q(t) - x) = \frac{1}{i} [\delta(q(t) - x), w(\pi^2)]
\]

\[
= \frac{1}{i} [\delta(q(t) - x), \pi^2] .. w'(\pi^2)
\]

\[
= - \sum_{k=1}^{3} \frac{\partial}{\partial x_k} (\pi_k, \delta(q(t) - x) .. w^{-1}(\pi^2)),
\]

which makes use of (18). Alternatively, we can expand the \( \delta \)-function in the first line to obtain

\[
\frac{d}{dt} \delta(q(t) - x) = \sum_{k=1}^{3} \frac{1}{i} [q_k(t), w(\pi^2)] .. (\dot{\delta}_k)(q(t) - x)
\]

\[
= - \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left( \frac{dq_k}{dt} .. \delta(q(t) - x) \right),
\]

which is an application of (26).

Consequently, we have obtained two candidates for the current density \( s(t,x) \) that supplements the density \( n(t,x) \) such that the continuity equation

\[
\frac{\partial}{\partial t} n + \frac{\partial}{\partial x} \cdot s = 0
\]

holds. The choice is between

\[
s(t,x) = (\pi, n(t,x)) .. w^{-1}(\pi^2) = (\pi .. n(t,x)) .. w^{-1}(\pi^2)
\]

and

\[
s(t,x) = \frac{dq}{dt} .. n(t,x) = (\pi .. w^{-1}(\pi^2)) .. n(t,x)
\]

where the CSP refers to the functional dependence of \( n \) on the position operator \( q \). The difference of the two \( s - s \) is, of course, sourceless.

Not surprisingly, the continuity equation alone does not uniquely identify the current density. A unique current is eventually found when the coupling of the particle to an external electromagnetic field is taken into account.

The change \( \delta E \) of the energy in response to variations of the external potentials \( V \) and \( A \) identifies the electric charge and current densities \( q \) and \( j \) according to

\[
\delta E = \int (dx) \{ q(t,x) \delta V(t,x) - j(t,x) \cdot \delta A(t,x) \},
\]

Upon expressing \( E, q, j \) as expectation values of \( H, n, e \), respectively, this tells us that (37) is the right choice for \( s \). The essential ingredient in this reasoning is the variation

\[
\delta_s H = -(\pi, e \delta A) .. w^{-1}(\pi^2),
\]

which employs (27).

So far, everything runs like in standard quantum theory, except for the appearance of continuously symmetrized products. However, as we shall see in the next section, it is exactly this symmetrization process which destroys the relativistic invariance of the theory, due to higher powers of \( \pi^2 \) in the kinetic energy.

III. (Non-)Invariance

The procedure that produced \( q \) and \( j \) can be carried through in any frame of reference. A necessary condition for relativistic invariance is, therefore, that the expressions obtained for the charge and current densities transform, as the potentials do, like the components of a four-vector field. Unfortunately, this is not the case, as we now proceed to show. As a matter of fact, the densities \( n(t,x) \) and \( s(t,x) \) as in (37) or (38) do not even transform covariantly in the field-free situation. Let us look at these circumstances first.

For \( V = 0, A = 0 \) the operators

\[
p, H = \sqrt{m^2 + p^2}, \quad L = q \times p, \quad N = q \cdot H - p \cdot t
\]

obey the Lie Algebra rules of the orthochronous Poincaré group [14], given that \([q_j, p_k] = i\delta_{jk}\). Therefore, under an infinitesimal boost to a frame moving at the velocity \( v = ve_1 \), the density transforms as follows:

\[
n'(t,x) = n(t,x) = \frac{1}{i} [n(t,x), vN_1]
\]

\[
= vq_1 \frac{\partial n}{\partial t}(t,x) + v \frac{\partial}{\partial x_1} n(t,x)
\]

\[
= -v \frac{dq_1}{dt} .. n(t,x)
\]

\[
+ v \left( x_1 \frac{\partial}{\partial t} + t \frac{\partial}{\partial x_1} \right) n(t,x),
\]

where we have used the fact that \((q_1 - x_1) \delta(q_1 - x_1) = 0\).
From the right hand side of (42) we learn that the current density must have the form
\[ \mathbf{J}(t,\mathbf{x}) = \frac{d\mathbf{q}}{dt} \cdot \delta (\mathbf{q}(t) - \mathbf{x}). \] (43)
On the other hand, we found
\[ \mathbf{J}(t,\mathbf{x}) = \frac{d\mathbf{q}}{dt} \cdot \delta (\mathbf{q}(t) - \mathbf{x}) \]
up to a divergenceless contribution. This implies that
\[ \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left( \frac{d\mathbf{q}}{dt} \cdot \delta (\mathbf{q}-\mathbf{x}) \right) = 3 \sum_{k=1}^{3} \frac{\partial}{\partial x_k} \left( \frac{d\mathbf{q}}{dt} \cdot \delta (\mathbf{q}-\mathbf{x}) \right) \] (44)
must hold. Here it suffices to evaluate \( q \)-matrix elements on both sides to see that this condition is not obeyed for \( dq/dt = \mathbf{p}/m^2 + \mathbf{p}^2 \). So the continuous symmetrization destroys the covariance of the formalism, unless the velocity \( dq/dt \) is linear in the momentum \( \mathbf{p} \), as in Dirac's theory for spin 1/2.

A different way of showing that the theory is not covariant, with no appeal to densities at all, is the following. When external fields are present, we require (i) that the kinetic energy \( \pi_0 \), together with the kinetic momentum \( \pi \), constitute a four vector \( \pi \). Additionally (ii), \( \pi_0 \) and \( \pi \) have to fulfill the energy-momentum relation \( \pi_0 = \sqrt{\mathbf{p}^2 + \mathbf{p}^2} \) in every frame of reference. Suppose that point (i) holds. Then, in a boosted system \( S' \) moving with velocity \( \mathbf{u} \) relative to the original system \( S \), the new operators must have the form
\[ \pi'_0 (\tau)= \frac{1}{\sqrt{1 - \mathbf{u}^2}} (\pi (\tau) - \mathbf{u} \cdot \pi (\tau)) \propto \pi_0 (\tau) - \mathbf{u} \cdot \pi (\tau), \]
\[ \pi' (\tau) = \frac{1}{\sqrt{1 - \mathbf{u}^2}} (\pi (\tau) - \mathbf{u} \pi_0 (\tau)) \propto \pi (\tau) - \mathbf{u} \pi_0 (\tau), \] (45) (46)
where the last equalities only hold for infinitesimally small \( \mathbf{u} \), and \( \tau \) denotes the proper time of the particle. Note that in the Heisenberg picture we transform the operators, whereas the states remain fixed. If, on the other hand, point (ii) is true, then one finds that the kinetic energy has to transform in the following way:
\[ \pi'_0 (\tau) - \pi_0 (\tau) = \sqrt{\mathbf{p}^2 + \pi' (\tau)^2} - \sqrt{\mathbf{p}^2 + \pi (\tau)^2} \]
\[ = \sqrt{\mathbf{p}^2 + (\pi - \mathbf{u} \pi_0)^2} - \sqrt{\mathbf{p}^2 + \pi^2} \]
\[ = \mathbf{u} \left( \frac{\partial}{\partial \mathbf{u}} \sqrt{\mathbf{p}^2 + (\pi - \mathbf{u} \pi_0)^2} \right)_{\mathbf{u} = 0} \]
\[ = - \sum_{k=1}^{3} u_k (\pi_k \cdot \mathbf{w} (\pi^2)) \cdot w^{-1} (\pi^2), \] (47)
where we have argued for infinitesimally small \( \mathbf{u} \). In order to be in accordance with (45), the last term in (47) must be equal to \(- \mathbf{u} \cdot \pi \), which would imply
\[ (\pi \cdot \mathbf{w} (\pi^2)) \cdot w^{-1} (\pi^2) = \pi \cdot (\mathbf{w} (\pi^2) \cdot w^{-1} (\pi^2)) \equiv \pi. \] (48)
As \( [\pi, \pi^2] \neq 0 \), this will in general (that is: for \( \mathbf{F} \times \mathbf{A} \neq 0 \)) not be the situation.

Note, that in the classical case (48) is trivially satisfied, as all operators commute. For the free particle, where \( \pi = \mathbf{p} \) and \( \mathbf{w} (\pi^2) = \sqrt{\mathbf{p}^2 + \mathbf{p}^2} \), condition (48) is obeyed as well (\( [\mathbf{p}, \mathbf{p}^2] = 0 \)), as it must be, for the invariance of the free relativistic Schrödinger equation is well known since the analysis of Wigner in 1939 [15].

We close with a comment on non-local coupling. If, in a relativistic quantum theory for a single particle, we stick to the principle that the classical energy-momentum relation \( \pi_0 = \sqrt{\mathbf{p}^2 + \pi^2} \) must hold for the corresponding operators, too, the only freedom we still have is to define the potential operators in a more general way.

An example is provided by introducing the classical potentials \( \mathcal{A}_\alpha (t,\mathbf{x}) \) as operators on the state space of the particle by means of definition (6), which introduces a general coupling function \( K (\mathbf{q}, \mathbf{p}, x) \) relating the classical position \( \mathbf{x} \), as a variable of the classical Maxwell fields \( \mathcal{A}_\alpha (t,\mathbf{x}) \), to the dynamical variables \( \mathbf{q}, \mathbf{p} \) of the quantum particle [16].

However, as condition (48) does not refer explicitly to the definition of the potential operators, it will again only by satisfied as long as \( [\pi, \pi^2] = 0 \), which again is inconsistent with the presence of magnetic fields [17].

IV. Summary

The concept of continuously symmetrized operator products enables us to handle the non-local square root, as Hamiltonian of a relativistic spinless particle, formally in a straightforward manner. The operators for the velocity, the Lorentz-force, the current density etc., acquire, apart from the symmetrization involved, the same form as in classical theory. However, concerning the transformation property of these operators under boosts, it is exactly the occurrence of the CSP, due to the dependence of the square root on higher powers of the kinetic momenta, which destroys the relativistic invariance of the theory. The same is true if we allow for a generalized non-local coupling of the potentials, at least as long as we demand that the energy-momentum relation has to be obeyed by the operators in the quantized theory, too.
[8] That is $\psi'(t',x') = \psi(t,x)$, where the primed quantities refer to the boosted frame of reference. A possible invariant normalization, in this case, is given by $\int dt(dx) |\psi(t,x)|^2 = 1$.
[9] See [7], footnote 7.
[12] Incidentally, Eq. (15) is reproduced when powers of $\beta$ are identified in (17).
[13] With $|t, x\rangle \langle t, x|$ being the projector onto an eigenstate of the position operator $q(t)$, the absolute square $|\psi(t,x)|^2 = \langle t, x | \psi(t,x) | \psi(t,x) \rangle$ is the natural form for the probability density of finding the particle at a certain point in space, rather than the expression given by Trübenbacher [2].
[16] Of course, there are further restrictions on the possible form of $K$, such as to assure the correct non-relativistic limit, for instance.
[17] Apart from condition (7), in the non-relativistic limit we require $K(q,p,x) \to \delta(q-x)$ so that $[\pi_i, \pi_j] \to -e\{[p_i, A_j] - [p_j, A_i]\} \propto \epsilon_{ijk} (V \times A)_k$. 