Relativistic invariance in direct derivation of a 4×4 diagonal matrix Schrödinger equation from relativistic total energy

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In this paper an algebraic method is presented to derive a non-Hermitian Schrödinger equation from total relativistic energy. Here, $E = V + c\sqrt{m^2c^2 + \left(\mathbf{p} - \frac{q}{c}\mathbf{A}\right)^2}$ with $E \rightarrow i\hbar\frac{\partial}{\partial t}$ and $\mathbf{p} \rightarrow -i\hbar\nabla$. In the derivation no use is made of Dirac's method of four vectors and the root operator isn't squared either. Instead, use is made of the algebra of operators. Proof is delivered that it is possible to derive Lorentz invariant forms in this way.

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I. INTRODUCTION

In many textbooks, treatises or lecture notes, e.g. [1, Chapter 2 page 40], [2, Chapter 6] or [3], one can find that Dirac's road to relativistic quantum mechanics is the way to quantize the total relativistic energy. In some, [4, Chapter 2, section 2.4], Kramer's work on the relativistic quantum mechanics or Weyls's equation is mentioned. However, Dirac's method is more general and is best known.

The main difficulty with the quantization of the energy expression below is that a direct more or less straightforward Schrödinger equation appears to be impossible because of the square root term in the total energy

$$E = V + c\sqrt{m^2c^2 + \left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2} \tag{1}$$

In this equation, V is the potential energy, m the mass of the quantum, $\mathbf{p}$ the momentum, e the unit of charge, c the velocity of light in vacuum and $\mathbf{A}$ the electromagnetic field vector. In the following section we present a method with operator algebra to tackle the operator form in the square root term of (1).

II. OPERATOR ALGEBRA

Let us rewrite equation (1) and write, $H_V = (E - V)/c$. Introduce a vector of operators, $\mathbf{p_A} = \mathbf{p} - \frac{e}{c}\mathbf{A}$. We suppose $\mathbf{A} \neq \mathbf{0}$. Nothing serious did happen here, so we have the equivalent.

$$H_V = \left(m^2c^2 + \mathbf{p_A}^2\right)^{1/2} \tag{2}$$

The quantized version of the operator then is

$$H_V = \frac{1}{c}\left(i\hbar\frac{\partial}{\partial t} - V\right)$$

Let us subsequently observe that because of $\mathbf{p} \to -i\hbar\nabla$ the operator $\mathbf{p_A}^2 = \left(-i\hbar\nabla - \frac{q}{c}\mathbf{A}\right)^2$ will contain a real, $\Re_e(\mathbf{p_A}^2)$ and an imaginary, $\Im_m(\mathbf{p_A}^2)$ part. Given this format it follows that

$$m^2c^2 + \mathbf{p_A}^2 = m^2c^2 + \Re_e(\mathbf{p_A}^2) + i\Im_m(\mathbf{p_A}^2) \tag{3}$$

If we then introduce two real operator 4-vector functions H_1 and H_2, the operator in (3) can be equal to $(H_1 + iH_2)^2$. So we look at

$$m^2c^2 + \mathbf{p_A}^2 = (H_1 + iH_2)^2 \tag{4}$$

Similar to $\mathbf{p_A}^2 = \mathbf{p_A} \cdot \mathbf{p_A}$, we have, $(H_1 + iH_2)^2 = (H_1 + iH_2) \cdot (H_1 + iH_2)$. Combining (3) with (4) the following two equations can be obtained

$$\begin{aligned} \beta &= m^2c^2 + \Re_e(\mathbf{p_A}^2) = H_1^2 - H_2^2 \\ \gamma &= \Im_m(\mathbf{p_A}^2) = H_1 \cdot H_2 + H_2 \cdot H_1 \end{aligned} \tag{5}$$

The H_1 and H_2 operators are spanned by $\{\hat{e}_\mu\}_{\mu=1}^4$ and for $\kappa = 1,2,3,4$, we have $(\hat{e}_\mu)_\kappa = \delta_{\mu,\kappa}$. This defines the four unit base vectors. The $\delta_{\mu,\nu}$, is the Kronecker delta, $\mu,\nu = 1,2,3,4$. The $\cdot$ product of basis vectors $\{\hat{e}_\mu\}_{\mu=1}^4$ therefore shows, $\hat{e}_\mu \cdot \hat{e}_\nu = \delta_{\mu,\nu}$.

III. DEFINITION OF THE H_1 AND H_2 OPERATOR

Let us define the operators that are used in (5). We have

$$\begin{aligned} H_1 &= \hat{e}_4\sigma mc + \frac{e}{c}\sum_{k=1}^{3}\hat{e}_k A_k(x,t) \\ H_2 &= \hbar\sum_{k=1}^{3}\hat{e}_k\frac{\partial}{\partial x_k} \end{aligned} \tag{6}$$

We will demonstrate that for $\sigma \in \{-1,1\}$, H_1 and H_2 can be employed in (5). Because the $\{\hat{e}_\mu\}_{\mu=1}^4$ are orthonormal it is found that, noting $\sigma^2 = 1$,

$$\begin{aligned} H_1^2 &= m^2c^2 + \left(\frac{e}{c}\right)^2 \left|\left|\mathbf{A}\right|\right|^2, \\ H_2^2 &= \hbar^2 \nabla^2, \\ H_1H_2 + H_2H_1 &= \frac{e\hbar}{c}\sum_{k=1}^{3}\left(\frac{\partial}{\partial x_k}A_k + A_k\frac{\partial}{\partial x_k}\right) \end{aligned} \tag{7}$$

Then, the operators in the previous equation match the definitions of β and γ in (5).

A. Four-vector root terms

Subsequently it must be noted that (5) has a "=" on the scalar level. Hence, we cannot flat out take the square root on both sides of (5) and have $H_1 + iH_2$, a 1×4 form, on the right hand and H_V, defined in (2) a 1×1 form on the left hand. However, let us define a 1×4 form $\mathcal{E}_V$ as

$$\mathcal{E}_V = \sum_{\mu=1}^{4} \hat{e}_\mu H_{V,\mu} \tag{8}$$

Let us suppose that the Hamiltonian operator breaks down as $H_{V,\mu} = c_\mu H_V$ and that $\sum_{\mu=1}^4 c_\mu^2 = 1$. Because the wave function equations contain complex entries, we are allowed to use complex valued c_μ. Hence, it is possible to select for instance

$$\begin{aligned} c_1 = c_2 = c_3 &= 1 \\ c_4 &= i\sqrt{2} \end{aligned} \tag{9}$$

In this way we may derive in a Euclidean metric operator 4-space, that, $||\mathcal{E}_V||^2 = H_V^2$.

B. Quantization equation

The result (9) can now be employed where the inner product of left and right hand side result in a Schrödinger equation. Let us define $\psi = \sum_{\nu=1}^4 \hat{e}_\nu \psi_\nu(\mathbf{x},t)$, and

$$\mathcal{E}_V \hat{e}_\nu \psi_\nu = (H_1 + iH_2)\hat{e}_\nu\psi_\nu \tag{10}$$

with $\nu = 1,2,3,4$. If, e.g. $\nu = 4$, looking at (8) and (9), then on the left hand of (10) we will find

$$\frac{i\sqrt{2}}{c}\left(i\hbar\frac{\partial}{\partial t} - V(\mathbf{x},t)\right)\psi_4.$$

On the right hand side, looking at (9) and the definitions in (6) we see

$$\sigma m c \psi_4$$

Hence, a Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi_4(\mathbf{x},t) = -\frac{i\sigma}{\sqrt{2}}mc^2\psi_4(\mathbf{x},t) + V(\mathbf{x},t)\psi_4(\mathbf{x},t) \tag{11}$$

is found. If $\nu = k = 1,2,3$, then it is found from (9) and the operator definitions in (6), that

$$i\hbar\frac{\partial}{\partial t}\psi_k(\mathbf{x},t) = i\hbar c\frac{\partial}{\partial x_k}\psi_k(\mathbf{x},t) + \{V(\mathbf{x},t) + eA_k(\mathbf{x},t)\}\,\psi_k(\mathbf{x},t). \tag{12}$$

C. Lorentz invariance

In order to demonstrate the principle possibility of Lorentz invariance, let us simplify the set of equations. So, $\psi_2 = \psi_3 \equiv 0$. Subsequently, let us zoom in on (x,t), with $x = x_1$, coordinate transformation. Of course, the Lorentz transformations for an observer with constant velocity v along the x-axis, related to the (x,t) system, are,

$$\begin{aligned} x' &= \gamma(x - vt) \\ t' &= \gamma\left(t - \frac{vx}{c^2}\right) \end{aligned} \tag{13}$$

with $\gamma = 1/\sqrt{1-(v/c)^2}$. The inverse transformation is equal to

$$\begin{aligned} x &= \gamma(x' + vt') \\ t &= \gamma\left(t' + \frac{vx'}{c^2}\right) \end{aligned} \tag{14}$$

For ease of argument, let us take in equations (11) and (12), $V = V_0 \equiv$ constant in (x,t).

We start the Lorentz transformation exercise by looking at the transformation rule of $\psi_4(x,t)$. Suppose

$$\psi_4(x,t) = \psi_4^0 \exp\left[\lambda_0(x + ct)\right] \tag{15}$$

Here, ψ_4^0 is a constant in (x,t). The constant λ_0 in this equation is defined by

$$\lambda_0 = \frac{V_0}{i\hbar c} - \frac{\sigma mc}{\hbar\sqrt{2}}$$

From the definitions one can derive that equation (11) for constant $V = V_0$ applies. Moreover, it is found for ψ_4 that

$$i\hbar\frac{\partial}{\partial t}\psi_4(x,t) = i\hbar c\frac{\partial}{\partial x}\psi_4(x,t) \tag{16}$$

Lorentz transformations of $\frac{\partial}{\partial t}$ and $\frac{\partial}{\partial x}$ are

$$\begin{aligned} \frac{\partial}{\partial x} &= \gamma\frac{\partial}{\partial x'} - \gamma\frac{v}{c^2}\frac{\partial}{\partial t'} \\ \frac{\partial}{\partial t} &= -\gamma v\frac{\partial}{\partial x'} + \gamma\frac{\partial}{\partial t'} \end{aligned} \tag{17}$$

This implies that equation (11) is Lorentz invariant and entails the transformation

$$\psi_4'(x',t') = \gamma\left(1 + \frac{v}{c}\right)\psi_4\left[x(x',t'), t(x',t')\right] \tag{18}$$

Here equation (14) is observed on the rhs. Hence, if $\lambda_0' = \gamma\left(1 + \frac{v}{c}\right)\lambda_0$, then

$$\psi_4'(x',t') = (\psi_4^0)'\exp\left[\lambda_0'(x' + ct')\right] \tag{19}$$

To continue with equation (12) the consistency with the transformation of λ_0 gives that $V_0' = \gamma\left(1 + \frac{v}{c}\right)V_0$. Making use of (14) in $A_1'(x',t') = \gamma\left(1 + \frac{v}{c}\right)A_1\left[x(x',t'), t(x',t')\right]$, together with $m' = \gamma\left(1 + \frac{v}{c}\right)m$ and (17) leads to the fact that the $k = 1$ equation of (12) is Lorentz invariant as well.

Hence, given $\psi_2 = \psi_3 \equiv 0$ and only (x,t) dependence, Lorentz invariance is demonstrated for our operator algebraic quantization of relativistic total energy.

IV. 4×4 SCHRÖDINGER EQUATION AND $\mathcal{P}, \mathcal{T}$ SYMMETRY.

From the equations (11) and (12) a 4×4 Schrödinger equation can be derived. Suppose, the 4×4 diagonal matrix H_0 is defined by

$$H_0(\mathbf{x},\sigma) = \mathrm{diag}\left(i\hbar c\frac{\partial}{\partial x_1}, i\hbar c\frac{\partial}{\partial x_2}, i\hbar c\frac{\partial}{\partial x_3}, -\frac{i\sigma}{\sqrt{2}}mc^2\right) \tag{20}$$

In addition, we define the 4×4 diagonal matrix $U = U(\mathbf{x}, t)$ as follows

$$U = \mathrm{diag}\left(V + eA_1, V + eA_2, V + eA_3, V\right) \tag{21}$$

From equations (11) and (12) and making use of (20) and (21), then, the 4×4 Schrödinger equation can be written down as

$$i\hbar \frac{\partial}{\partial t}\psi(\mathbf{x}, t) = H_0(\mathbf{x}, \sigma)\psi(\mathbf{x}, t) + U(\mathbf{x}, t)\psi(\mathbf{x}, t) \tag{22}$$

and the symmetry conditions of the non-hermitian $H(\mathbf{x}, t, \sigma) = H_0(\mathbf{x}, \sigma) + U(\mathbf{x}, t)$ can be studied. Concerning non Hermitian Hamiltonians and possible physical states, the following can be noted. In the first place there is the possibility to weak measure non Hermitian operators [5]. Secondly, there is the notion that Parity & Time symmetry would also be a condition for the physicalness of a non-Hermitian Hamiltonian. In that case we don't insist to have $H^\dagger(\mathbf{x}, t, \sigma) = H(\mathbf{x}, t, \sigma)$ but we want to see $H^{\mathcal{TP}}(\mathbf{x}, t, \sigma) = H(\mathbf{x}, t, \sigma)$. Here $\mathcal{P}$ is the parity operator $\mathcal{P}\mathbf{x} = -\mathbf{x}\mathcal{P}$. The operator $\mathcal{T}$ is the time reversal operator, with, $\mathcal{T}\mathbf{x} = \mathbf{x}\mathcal{T}$ and $\mathcal{T}i = -i\mathcal{T}$, [6].

A. Parity and Time reversal

Looking at the definition of the 4×4 diagonal H_0 it is easy to acknowledge that indeed $H_0^{\mathcal{TP}} = H_0$. So if it is assumed that $U^{\mathcal{TP}} = U$, then the Hamiltonian is $\mathcal{TP}$ symmetric. Hence, physical states can be associated to the 4×4 Schrödinger equation. This equation was directly derived from the relativistic total energy without using Clifford algebra or squaring the root term. If the non Hermitian Hamiltonian is unrelated to real physical phenomena then we can refer to [2, Page 148]. Non-Hermitian operators can be added to the description of physical relevant equations. In case of a totally unphysical Hemiltonian in (22) it would be an interesting mathematical exercise to find out if adding the obtained 4×4 Schrödinger equation to a Dirac description, would leave the physical phenomenon unchanged.

V. CONCLUSION & DISCUSSION

In the present paper a 4×4 Schrödinger equation was directly derived from the total relativistic energy equation. The latter is also the starting point for Dirac's treatment of relativistic quantum mechanics. We showed that there is a $\mathcal{TP}$ symmery in the 4×4 Hamiltonian diagonal matrix. Hence, the possibility exists that physical states can be associated to the obtained Schrödinger equation. It was demonstrated that Lorentz invariant equations can be derived from the algebraic operator method.

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