A 4×4 diagonal matrix Schrödinger equation from relativistic total energy with a 2×2 Lorentz invariant solution.

Han Geurdes[1] and Koji Nagata[2]

[1] *Geurdes datascience, 2593 NN, 164, Den Haag, Netherlands*
E-mail: han.geurdes@gmail.com
[2] *Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, Korea*
E-mail: ko_mi_na@yahoo.co.jp
(Dated: October 13, 2017)

In this paper an algebraic method is presented to derive a non-Hermitian Schrödinger equation from $E = V + c\sqrt{m^2c^2 + \left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2}$ 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. In this paper use is made of the algebra of operators to derive a matrix Schrödinger equation. It is demonstrated that the obtained equation is Lorentz invariant.

PACS numbers: 03.65Aa, 03.65-w, 03.67.Lx(Quantum computer)

I. INTRODUCTION

In many textbooks, treatises or lecture notes, e.g. [1, Chapter 2 page 40], [3, Chapter 6] or [4], one can read that Dirac's road to relativistic quantum mechanics is the way to quantize the total relativistic energy. In quantum field theory the Dirac spinor is the key object of research [2]. In some textbooks, for instance, [5, Chapter 2, section 2.4], Kramer's work on the relativistic quantum mechanics or Weyls's equation is mentioned as a curiosity. Weyl's work e.g. refers to neutrinos.

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

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

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 firstly 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 $\mathbf{A} \neq \mathbf{0}$. This results into the equivalent.

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

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

$$m^2c^2 + \mathbf{p_A}^2 = m^2c^2 + \mathfrak{R}_e(\mathbf{p_A}^2) + i\mathfrak{I}_m(\mathbf{p_A}^2) \tag{3}$$

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

$$\begin{aligned} \beta &= m^2c^2 + \mathfrak{R}_e(\mathbf{p_A}^2) = H_1^2 - H_2^2 \\ \gamma &= \mathfrak{I}_m(\mathbf{p_A}^2) = H_1 \cdot H_2 + H_2 \cdot H_1 \end{aligned} \tag{5}$$

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 (4) has a "=" on the scalar level. Hence, we cannot flat out take the square root on both sides of (4) 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

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

If, $H_{V,\mu} = c_\mu H_V$ then the following can be observed. In the first place we have from (2), (4) and (5) that

$$H_V^2 = (H_1 + iH_2)^2 \tag{9}$$

Secondly,

$$\mathcal{E}_V^2 = \mathcal{E}_V \cdot \mathcal{E}_V = \sum_{\mu=1}^{4}\{H_{V,\mu}\}^2 = H_V^2 \sum_{\mu=1}^{4} c_\mu^2.$$

Suppose we have, $\sum_{\mu=1}^4 c_\mu^2 = 1$. Then, we can have

$$\mathcal{E}_V = H_1 + iH_2 \tag{10}$$

as a solution of (9). In (8)-(10) $E \to i\hbar\frac{\partial}{\partial t}$. Hence, $H_{V,\mu} = \frac{c_\mu}{c}\left(i\hbar\frac{\partial}{\partial t} - V(\mathbf{x}, t)\right)$ for $\mu = 1, 2, 3, 4$. Bearing in mind that we work in the complex wave functions, we may take, $c_1 = 1, c_2 = c_3 = i$ and $c_4 = \sqrt{2}$ and note that $\sum_{\mu=1}^4 c_\mu^2 = 1 - 1 - 1 + 2 = 1$.

B. Quantisation equation

The result (10) 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

$$\mathcal{E}_V\hat{e}_\nu\psi_\nu = (H_1 + iH_2)\hat{e}_\nu\psi_\nu \tag{11}$$

with $\nu = 1, 2, 3, 4$. If, e.g. $\nu = 4$, looking at (8) and (10), then on the left hand of (11) we will find,

$$\frac{c_4}{c}\left(i\hbar\frac{\partial}{\partial t} - V(\mathbf{x}, t)\right)\psi_4.$$

On the right hand side, looking at (10) and the definitions in (6) we see, $\sigma \in \{-1, 1\}$,

$$\sigma mc\psi_4$$

Hence, a Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi_4(\mathbf{x}, t) = \sigma b_4\, mc^2\psi_4(\mathbf{x}, t) + V(\mathbf{x}, t)\psi_4(\mathbf{x}, t) \tag{12}$$

is found. If $\nu = k = 1, 2, 3$, then it is found from (10) and the operator definitions in (6) that

$$i\hbar\frac{\partial}{\partial t}\psi_k(\mathbf{x}, t) = b_k i\hbar c\frac{\partial}{\partial x_k}\psi_k(\mathbf{x}, t) + \{V(\mathbf{x}, t) + b_k eA_k(\mathbf{x}, t)\}\,\psi_k(\mathbf{x}, t). \tag{13}$$

Here $b_\mu = 1/c_\mu$, for, $\mu = 1, 2, 3, 4$.

C. 2×2 Lorentz invariance

Suppose we take, $c_1 = 1, c_2 = c_3 = i$ and $c_4 = \sqrt{2}$ together with the collapse $\psi_2 = \psi_3 \equiv 0$. In the Lorentz transformation we look at $\psi_4 = \psi_4(\mathbf{x}, t)$ and $\psi_1 = \psi_1(\mathbf{x}, t)$ and take for brevity, $x = x_1$. There is no transformation along x_2 and x_3. The resulting equations then can be written as,

$$
\begin{aligned}
i\hbar \frac{\partial}{\partial t}\psi_4(\mathbf{x}, t) &= \frac{\sigma}{2}\, mc^2 \psi_4(\mathbf{x}, t) + V(\mathbf{x}, t)\psi_4(\mathbf{x}, t) \\
i\hbar \frac{\partial}{\partial t}\psi_1(\mathbf{x}, t) &= i\hbar c \frac{\partial}{\partial x}\psi_1(\mathbf{x}, t) + \{V(\mathbf{x}, t) + eA_1(\mathbf{x}, t)\}\, \psi_1(\mathbf{x}, t)
\end{aligned} \tag{14}
$$

The (theoretical) phenomenon we are looking at has, hence, only one important spatial direction. The Lorentz transformations for an observer with constant velocity v along the x-axis, related to the (x, t) system, are,

$$
\begin{aligned}
x' &= \gamma(x - vt) \\
t' &= \gamma\left(t - \frac{vx}{c^2}\right)
\end{aligned} \tag{15}
$$

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

$$
\begin{aligned}
x &= \gamma(x' + vt') \\
t &= \gamma\left(t' + \frac{vx'}{c^2}\right)
\end{aligned} \tag{16}
$$

For ease of argument, let us take in equations (12), (13) and (14), $V = V_0 \equiv$ constant in (x, t), suppressing for convenience, the x_2 and x_3. We start the Lorentz transformation exercise by looking at the transformation rule of $\psi_4(x, t)$. Suppose

$$
\psi_4(x, t) = \psi_4^0 \exp\left[\lambda_0(x - ct)\right] \tag{17}
$$

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

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

From the definitions one can derive that the Shrödinger equation for, ψ_4, (12) for constant $V = V_0$ applies. Moreover, it is found for ψ_4 that

$$
i\hbar \frac{\partial}{\partial t}\psi_4(x, t) = -i\hbar c \frac{\partial}{\partial x}\psi_4(x, t) \tag{18}
$$

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

$$
\begin{aligned}
\frac{\partial}{\partial x} &= \gamma \frac{\partial}{\partial x'} - \gamma \frac{v}{c^2}\frac{\partial}{\partial t'} \\
\frac{\partial}{\partial t} &= -\gamma v \frac{\partial}{\partial x'} + \gamma \frac{\partial}{\partial t'}
\end{aligned} \tag{19}
$$

This implies that equation (12), with $V = V_0$ constant in (x, t), is Lorentz invariant and entails the transformation

$$
\psi_4'(x', t') = \gamma\left(1 - \frac{v}{c}\right)\psi_4\left[x(x', t'), t(x', t')\right] \tag{20}
$$

Here equation (16) is observed on the rhs. Hence, if $\lambda_0' = \gamma\left(1 - \frac{v}{c}\right)\lambda_0$, then

$$
\psi_4'(x', t') = (\psi_4^0)' \exp\left[\lambda_0'(x' - ct')\right] \tag{21}
$$

Looking at (17), $(\psi_4^0)' = \psi_4^0\gamma\left(1 - \frac{v}{c}\right)$. Looking at the definition of λ_0 we also find $V_0' = V_0\gamma\left(1 - \frac{v}{c}\right)$. The latter has to be in accordance with the Lorentz transformation of ψ_1. Let us take a closer look at this transformation. From (19) we find

$$
i\hbar\left(\gamma \frac{\partial}{\partial t'} - v\gamma \frac{\partial}{\partial x'}\right)\psi_1 = i\hbar c\left(\gamma \frac{\partial}{\partial x'} - \gamma \frac{v}{c^2}\frac{\partial}{\partial t'}\right)\psi_1 + \{V_0 + eA_1\}\,\psi_1 \tag{22}
$$

This leads us to Lorentz transformed

$$i\hbar\frac{\partial}{\partial t'}\psi_1' = i\hbar c\frac{\partial}{\partial x'}\psi_1' + \{V_0' + eA_1'\}\,\psi_1' \tag{23}$$

with $\psi_1' = \psi_1\gamma\left(1+\frac{v}{c}\right)$ and $A_1' = A_1\gamma\left(1-\frac{v}{c}\right)$ such that, together with $V_0' = V_0\gamma\left(1-\frac{v}{c}\right)$, we have

$$\{V_0' + eA_1'\}\,\psi_1' = \{V_0 + eA_1\}\,\psi_1$$

because $\gamma\left(1-\frac{v}{c}\right)\gamma\left(1+\frac{v}{c}\right) = 1$.

D. 2×2 Parity & Time

The 2×2 form which transforms with the Lorentz transformations is

$$i\hbar\frac{\partial}{\partial t}\,\underline{\psi}(x,t) = H\,\underline{\psi}(x,t) \tag{24}$$

Here, $\underline{\psi}(x,t) = (\psi_1(x,t), \psi_2(x,t))$ and $H = H_0 + U$, with,

$$\begin{aligned} U &= \mathrm{diag}\,(eA_1 + V_0, V_0) \\ H_0 &= \mathrm{diag}\left(i\hbar c\frac{\partial}{\partial x}, \frac{\sigma}{\sqrt{2}}mc^2\right) \end{aligned} \tag{25}$$

Employing the operators $\mathcal{P}$ and $\mathcal{T}$ (25) and noting, $\mathcal{P}^2 = \mathcal{T}^2 = 1$, [8, Equation (7), Page 3], it is easy to acknowledge,

$$H_0^{\mathcal{TP}} = \mathcal{PT}H_0\mathcal{TP} = \mathcal{PT}\mathrm{diag}\left(i\hbar c\frac{\partial}{\partial x}, \frac{\sigma}{\sqrt{2}}mc^2\right)\mathcal{TP} = H_0.$$

IV. CONCLUSION & DISCUSSION

In the present paper a 4×4 Schrödinger equation was directly derived from the total relativistic energy equation. The present authors already have established a 4×4, but not Lorentz invariant, equation [7]. The found equations are different from Dirac's quantization of the total relativistic energy. In our derivation, no use was made of Clifford algebra. We also did not square the root term of the total energy. Instead, use was made of operator algebra in a $\mathbb{R}^4$ Euclidean space. It is noted that the total relativistic energy is also the starting point for Dirac's treatment of relativistic quantum mechanics.

The obtained 2×2 set of equations represents a non-Hermitian system. The advanced operator algebra is opening a door to study different, possibly also Lorentz invariant, alternatives of quantization of relativistic total energy.

Looking at the definition of the 2×2 diagonal H_0 in equation (25) 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. Given the 2×2 Lorentz invariance, possibly physical states can be associated to the 2×2 Schrödinger equation. Note also [6].

In the case that there is no physical state associated to our set of equations, one can do mathematical experiments to see if the outcome of computations with Lagrangians of real physical states change under the addition of the found equations. We also refer to [3, Page 148]. The "adding terms to the Lagrangian" method resembles somewhat the speculative and "beyond standard model" addition of e.g. the axion equation to the Lagrangian. In the latter case the axion was introduced to solve the strong CP problem, see e.g. [9, Chapter 10].

---

[1] R. Clarkson and D. McKeon, *Quantum field theory*, lecture notes 2003.
[2] R.F. Streater and A.S. Wightman, *PCT, spin statistics and all that*, Walter Benjamin, NY, 1963.
[3] J. Ziman, *Elements of advanced quantum theory*, Camb Univ. Press, NY, 1969.
[4] T. Das, *Relativistic quatum mechanics of electrons*, Harper & Row, NY, 1973.
[5] H. Pilkunh, *Relativistic quantum mechanics*, Springer, N.Y. 2005.
[6] A.K. Pati, U. Singh, U. Sinha, *Measuring non-hermitian operators via weak values*, arXiv: quant-ph/1406.3007.
[7] H. Geurdes and K Nagata, *Relativistic invariance in direct derivation of a 4×4 diagonal matrix Schrödinger equation from relativistic total energy*, submitted High Eneergy Density Physics, 2017.
[8] C.M. Bender, *Making sense of non-Hermitian Hamiltonians*, arXiv: hep-th/0703096v1.
[9] E.W. Kolb and M.S. Turner, *The Early Universe*, Addison-Wesley, Redwood city, 1989.