

# Changes of representation and general boundary conditions for Dirac operators in 1+1 dimensions

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We introduce a family of four Dirac operators in 1+1 dimensions:  $\hat{h}_A = -i\hbar c \hat{\Gamma}_A \partial/\partial x$  ( $A = 1, 2, 3, 4$ ) for  $x \in \Omega = [a, b]$ . Here,  $\{\hat{\Gamma}_A\}$  is a complete set of  $2 \times 2$  matrices:  $\hat{\Gamma}_1 = \hat{1}$ ,  $\hat{\Gamma}_2 = \hat{\alpha}$ ,  $\hat{\Gamma}_3 = \hat{\beta}$ , and  $\hat{\Gamma}_4 = i\hat{\beta}\hat{\alpha}$ , where  $\hat{\alpha}$  and  $\hat{\beta}$  are the usual Dirac matrices. We show that the hermiticity of each of the operators  $\hat{h}_A$  implies that  $C_A(x=b) = C_A(x=a)$ , where the real-valued quantities  $C_A = c\psi^\dagger \hat{\Gamma}_A \psi$ , the bilinear densities, are precisely the components of a Clifford number  $\hat{C}$  in the basis of the matrices  $\hat{\Gamma}_A$ ; moreover,  $\hat{C}/2c\rho$  is a density matrix ( $\rho$  is the probability density). Because we know the most general family of self-adjoint boundary conditions for  $\hat{h}_2$  in the Weyl representation (and also for  $\hat{h}_1$ ), we can obtain similar families for  $\hat{h}_3$  and  $\hat{h}_4$  in the Weyl representation using only the aforementioned family for  $\hat{h}_2$  and changes of representation among the Dirac matrices. Using these results, we also determine families of general boundary conditions for all these operators in the standard representation. We also find and discuss connections between boundary conditions for the free (self-adjoint) Dirac Hamiltonian in the standard representation and boundary conditions for the free Dirac Hamiltonian in the Foldy-Wouthuysen representation.

**Keywords:** Dirac operators; bilinear densities; changes of representation; boundary conditions; Foldy-Wouthuysen representation

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## 1. Introduction

First, let us introduce the following four Hermitian matrix-valued (differential) Dirac operators:

$$\hat{h}_A = -i\hbar c \hat{\Gamma}_A \frac{\partial}{\partial x}, \quad (A = 1, 2, 3, 4), \quad (1)$$

where  $x \in \Omega = [a, b]$ . (In this article, we will retain the constants  $\hbar$  and  $c$  to avoid confusion.) We assume that each  $\hat{h}_A$  acts on two-component column vectors (or Dirac wave functions in 1+1 dimensions)  $\psi = \psi(t, x) = [\psi_1(t, x) \ \psi_2(t, x)]^\top$  (where the symbol  $\top$  represents the transpose of a matrix), which belong to the Hilbert space  $\mathcal{H} = \mathcal{L}^2(\Omega) \oplus \mathcal{L}^2(\Omega)$  (note that  $\hat{h}_A \psi$  also belongs to  $\mathcal{H}$ ). The scalar product of such vectors is denoted by  $\langle \psi, \xi \rangle = \int_\Omega dx \psi^\dagger \xi$  (where the symbol  $\dagger$  denotes the adjoint of a matrix). Each self-adjoint ( $\Rightarrow$  Hermitian) operator  $\hat{h}_A$  has a proper domain  $D(\hat{h}_A) \subset \mathcal{H}$ , *i.e.*, the set of functions on which  $\hat{h}_A$  can act, which includes a general boundary condition (the latter will be introduced later in this article). Note: in this paper we use the term Hermitian to refer to differential operators that are called symmetric (or formally self-adjoint) in the mathematical jargon. The  $2 \times 2$  (Hermitian) matrices  $\hat{\Gamma}_A = \hat{\Gamma}_A^\dagger$  are given by

$$\hat{\Gamma}_1 = \hat{1}, \quad \hat{\Gamma}_2 = \hat{\alpha}, \quad \hat{\Gamma}_3 = \hat{\beta}, \quad \hat{\Gamma}_4 = i\hat{\beta}\hat{\alpha}. \quad (2)$$

As is usually the case, the Dirac matrices  $\hat{\alpha} = \hat{\alpha}^\dagger$  and  $\hat{\beta} = \hat{\beta}^\dagger$  satisfy the following relations [1]:

$$\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha} = 0, \quad \hat{\alpha}^2 = \hat{\beta}^2 = \hat{1}. \quad (3)$$

As a consequence, the matrices  $\hat{\Gamma}_A$  also have the following properties: (i)  $\hat{\Gamma}_A^2 = \hat{1}$ ; (ii)  $\hat{\Gamma}_B \hat{\Gamma}_A \hat{\Gamma}_B = -\hat{\Gamma}_A$  for  $A \neq B$

and  $A, B = 2, 3, 4$ ; therefore, (iii)  $\text{tr}(\hat{\Gamma}_A) = 0$  (where  $\text{tr}$  denotes the trace of a matrix); and (iv) they are all linearly independent, and therefore, any  $2 \times 2$  matrix can be expanded in terms of the  $\hat{\Gamma}_A$ . In other words, we can write an arbitrary  $2 \times 2$  matrix, say  $\hat{C}$ , as

$$\hat{C} = \sum_{A=1}^4 C_A \hat{\Gamma}_A, \quad (4)$$

where  $C_A = \text{tr}(\hat{\Gamma}_A \hat{C})/2$  (for a good discussion of such matrix properties, see, for example, Ref. [2], p. 132). Naturally, the algebra generated by the  $\hat{\Gamma}_A$  is a Clifford algebra.

Let us now introduce the following four real-valued quantities:

$$C_A = c\psi^\dagger \hat{\Gamma}_A \psi. \quad (5)$$

These functions are usually known as bilinear densities, but they are also called bilinear covariants because they possess definite transformation properties under (proper orthochronous) Lorentz transformations and space inversion (in 1+1 dimensions). Specifically, the time component of a Lorentz 2-vector is  $C_1 = c\rho$ , where  $\rho = \rho(t, x) = \psi^\dagger \psi$  is the probability density. The spatial component of a 2-vector is  $C_2 = j$ , where  $j = j(t, x) = c\psi^\dagger \hat{\alpha} \psi$  is the probability current density. Furthermore, the scalar is  $C_3 \equiv cs = c\psi^\dagger \hat{\beta} \psi$ , and the pseudo-scalar is  $C_4 \equiv cw = c\psi^\dagger i\hat{\beta}\hat{\alpha} \psi$  [3]. In this article, we do not assign specific names to the densities  $s$  and  $w$ . Notice that if the quantities  $C_A$  given in Eq. (5) are precisely the coefficients of  $\hat{C}$  in the expansion (4), then the matrix  $\hat{C}$  can be written as  $\hat{C} = 2c\psi\psi^\dagger$ . In effect,  $C_A = \text{tr}(\hat{\Gamma}_A 2c\psi\psi^\dagger)/2 = \text{tr}(c\hat{\Gamma}_A \psi\psi^\dagger) = \text{tr}(c\psi^\dagger \hat{\Gamma}_A \psi) =$

$c\psi^\dagger \hat{\Gamma}_A \psi$ . Moreover, the following properties of  $\hat{C}$  can be verified: (i)  $(\hat{C}/2c\varrho)^\dagger = \hat{C}/2c\varrho$ , (ii)  $(\hat{C}/2c\varrho)^2 = \hat{C}/2c\varrho$ , and (iii)  $\text{tr}(\hat{C}/2c\varrho)^2 = 1$ . Hence,  $\hat{C}/2c\varrho$  is a density matrix and also a projector; therefore, it can represent the quantum state of the system, as well [4]. It is worth noting that property (ii) implies that  $(c\varrho)^2 = (cs)^2 + j^2 + (cw)^2$ , *i.e.*, only three of the bilinear densities are independent [3].

As is well known, if we have two sets of two Dirac matrices,  $\{\hat{\alpha}, \hat{\beta}\}$  and  $\{\tilde{\alpha}, \tilde{\beta}\}$ , that satisfy the algebraic relations given in Eq. (3), then there exists a (constant) non-singular matrix  $\hat{S}$  (defined to within a multiplicative constant) such that

$$\tilde{\alpha} = \hat{S}\hat{\alpha}\hat{S}^{-1}, \quad \tilde{\beta} = \hat{S}\hat{\beta}\hat{S}^{-1} \tag{6}$$

(and therefore also  $\tilde{\Gamma}_A = \hat{S}\hat{\Gamma}_A\hat{S}^{-1}$ ). Indeed,  $\hat{S}$  must be a unitary matrix to preserve the hermiticity of the Dirac matrices. Thus, distinct sets of Dirac matrices that satisfy (6) are referred to as sets of Dirac matrices in distinct (but trivially related) representations. In this paper, we use three of these representations, which are usually referred to as (i) the standard (or Dirac-Pauli) representation (SR),  $\{\hat{\alpha}, \hat{\beta}\} = \{\hat{\sigma}_x, \hat{\sigma}_z\}$ ; (ii) the Weyl (or spinor, or chiral) representation (WR),  $\{\tilde{\alpha}, \tilde{\beta}\} = \{\hat{\sigma}_z, \hat{\sigma}_x\}$ ; and (iii) the supersymmetric representation (SSR),  $\{\tilde{\alpha}, \tilde{\beta}\} = \{\hat{\sigma}_x, \hat{\sigma}_y\}$ . As we will see below, in 1+1 dimensions the last could also be considered to be a Majorana representation [5]. Notice that by using only the three Pauli matrices, we can construct only six distinct representations. The SR and the WR are related through the (unitary) matrix

$$\hat{S} = \frac{1}{\sqrt{2}}(\hat{\sigma}_x + \hat{\sigma}_z). \tag{7}$$

Similarly, the SR and the SSR are related via the (unitary) matrix

$$\hat{S} = \frac{1}{\sqrt{2}}(\hat{1} + \hat{\sigma}_y\hat{\sigma}_z). \tag{8}$$

Likewise, suppose that we have the following two (equivalent) relativistic wave equations, each in its own representation:

$$\hat{H}\psi = i\hbar\frac{\partial\psi}{\partial t}, \quad \tilde{H}\tilde{\psi} = i\hbar\frac{\partial\tilde{\psi}}{\partial t}, \tag{9}$$

where, for example,

$$\begin{aligned} \hat{H} &= -i\hbar c\hat{\alpha}\frac{\partial}{\partial x} + mc^2\hat{\beta} + U(x), \\ \tilde{H} &= -i\hbar c\tilde{\alpha}\frac{\partial}{\partial x} + mc^2\tilde{\beta} + U(x) \end{aligned} \tag{10}$$

are the usual Dirac Hamiltonian operators ( $U(x)$  is the potential-energy function, and it is real and independent of time) and the Dirac matrices are related as shown in Eq. (6). Then, the Dirac wave functions  $\psi$  and  $\tilde{\psi}$  are related by

$$\tilde{\psi} = \hat{S}\psi. \tag{11}$$

If the operators  $\hat{H}$  and  $\tilde{H}$  in (10) are replaced by any of the operators  $\hat{h}_A$ , the result given by Eq. (11) remains true. In

the SR, a wave function is usually written as  $\psi = \psi(t, x) = [\varphi(t, x) \chi(t, x)]^\top$ , where  $\varphi$  is the so-called large component of  $\psi$  and  $\chi$  is the small component (for positive energies, the upper component is “larger” than the lower component in the nonrelativistic limit). In the WR, we write the wave function as  $\tilde{\psi} = \tilde{\psi}(t, x) = [\varphi_1(t, x) \varphi_2(t, x)]^\top$ . Using Eqs. (7) and (11), we can write the relation between the components of  $\psi$  and  $\tilde{\psi}$  as follows:

$$\begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} \varphi \\ \chi \end{bmatrix}. \tag{12}$$

Likewise, in the SSR, we write the wavefunction as  $\tilde{\psi} = \tilde{\psi}(t, x) = [\phi_1(t, x) \phi_2(t, x)]^\top$ . The relation between the components of the latter wave function and those of the wave function in the SR can be obtained using Eqs. (8) and (11):

$$\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix} \begin{bmatrix} \varphi \\ \chi \end{bmatrix}. \tag{13}$$

Using Eqs. (12) and (13), we can also write the following expression:

$$\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ 1+i & -(1-i) \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix}, \tag{14}$$

which expresses the relation between the components of the wave function in the SSR and those of the wave function in the WR. Note that because the matrix  $\hat{S}$  in Eq. (11) is unitary, the bilinear densities in one representation (see Eq. (5)) are the same in any other representation. In effect,  $\tilde{C}_A = c\tilde{\psi}^\dagger \tilde{\Gamma}_A \tilde{\psi} = c\psi^\dagger \hat{S}^\dagger \hat{S} \hat{\Gamma}_A \hat{S} \hat{S}^\dagger \psi = C_A$ . It is also worth mentioning that in the SSR, the free Dirac equation can be written as follows (see Eqs. (9) and (10)):

$$\begin{aligned} &-i\hbar c\hat{\sigma}_x\frac{\partial\tilde{\psi}}{\partial x} + mc^2\hat{\sigma}_y\tilde{\psi} \\ &= i\hbar\frac{\partial\tilde{\psi}}{\partial t} \Rightarrow \left(\frac{1}{c}\frac{\partial}{\partial t} + \hat{\sigma}_x\frac{\partial}{\partial x} + \frac{mc}{\hbar}i\hat{\sigma}_y\right)\tilde{\psi} = 0, \end{aligned}$$

that is to say, the latter equation is real, *i.e.*,  $\tilde{\psi}$  can be chosen to be real. In this regard, the SSR is also a Majorana representation (further details concerning the Majorana representation can be found, for example, in Ref. [5]). As expected, the physical predictions do not depend on the chosen representation, even though wave functions describing the same physical situation take different forms in different representations. For example, to simulate a penetrable barrier at  $x = a$  and  $x = b$  (the physical situation), we may choose the periodic boundary condition  $\psi(a) = \psi(b)$  in the SR, but then we should choose the same boundary condition in any other representation, *i.e.*,  $\tilde{\psi}(a) = \tilde{\psi}(b)$ . Naturally,  $\psi$  is not equal to  $\tilde{\psi}$ .

## 2. Dirac operators

In this section, we first present, together with the most essential results associated with the hermiticity of each operator  $\hat{h}_A$  (see also Ref. [6]), known families of general boundary conditions for  $\hat{h}_1$  and  $\hat{h}_2$  in the WR under the assumption that these operators are self-adjoint. Then, using only the general boundary condition for  $\hat{h}_2$  and changes of representation among the Dirac matrices, we also obtain general boundary conditions for  $\hat{h}_3$  and  $\hat{h}_4$  in the WR. In the latter procedure, we need only consider the SR, the WR and the SSR. At the end of the section, using these results, we also write general boundary conditions for each of these four operators in the SR.

(a) First, the operator  $\hat{h}_1$  is essentially the (Dirac) momentum operator  $\hat{P}$ ; in fact,

$$\hat{h}_1 = -i\hbar c \hat{1} \frac{\partial}{\partial x} (= c\hat{P} = c\hat{1}\hat{p}). \tag{15}$$

In the latter expression, we distinguish between  $\hat{P} = -i\hbar\hat{1}\partial/\partial x$ , which is, in the end, a  $2 \times 2$  matrix, and  $\hat{p} = -i\hbar\partial/\partial x$ , which is usually considered to be the momentum operator. Note that  $\hat{h}_1$  does not change if we change the representation (the identity matrix  $\hat{1}$  is manifestly independent of the representation). This operator satisfies the following relation:

$$\langle \psi, \hat{h}_1 \xi \rangle - \langle \hat{h}_1 \psi, \xi \rangle = -i\hbar c [\psi^\dagger \xi]_a^b, \tag{16}$$

where  $[f]_a^b = f(t, b) - f(t, a)$ , and  $\psi$  and  $\xi$  are vectors in  $\mathcal{H}$ . If the boundary conditions imposed on  $\psi$  and  $\xi$  lead to the cancellation of the term evaluated at the endpoints of the interval  $\Omega$ , we can write relation (16) as  $\langle \psi, \hat{h}_1 \xi \rangle = \langle \hat{h}_1 \psi, \xi \rangle$ . In this case,  $\hat{h}_1$  is a Hermitian operator. If we impose  $\psi = \xi$  in this last relation and in Eq. (16), we obtain the following condition:

$$[\psi^\dagger \psi]_a^b = [\varrho]_a^b = 0 \quad (\Rightarrow \varrho(b) = \varrho(a)), \tag{17}$$

*i.e.*,  $C_1(b) = C_1(a)$ . Furthermore,  $\langle \psi, \hat{h}_1 \psi \rangle = \langle \hat{h}_1 \psi, \psi \rangle = \langle \psi, \hat{h}_1 \psi \rangle$ ; therefore,  $\text{Im}\langle \psi, \hat{h}_1 \psi \rangle = 0$ , *i.e.*,  $\langle \psi, \hat{h}_1 \psi \rangle \equiv \langle \hat{h}_1 \psi, \psi \rangle \in \mathbb{R}$  (the bar represents complex conjugation). The requirement given in Eq. (17) implies that each wavefunction  $\psi$  that belongs to the domain  $D(\hat{h}_1)$  must obey only specific boundary conditions at the endpoints of the interval  $\Omega$  (under the assumption that  $\hat{h}_1$  is also a self-adjoint operator). Indeed, Eq. (17) is satisfied by imposing the following general boundary condition:

$$\psi(b) = \hat{U}_1 \psi(a), \tag{18}$$

where the matrix  $\hat{U}_1$  is unitary (and therefore, Eq. (18) is a 4-parameter family of boundary conditions) [7]. In fact, let us consider the following general relation,  $\psi(b) = \hat{M}\psi(a)$ , where  $\hat{M}$  is an arbitrary (complex) matrix. By substituting the latter relation into Eq. (17), we obtain  $\psi^\dagger(a)\hat{M}^\dagger\hat{M}\psi(a) - \psi^\dagger(a)\psi(a) = 0$ ; therefore,  $\hat{M}^\dagger\hat{M} = \hat{1}$ , *i.e.*,  $\hat{M}$  is unitary.

The latter result can also be obtained using the theory of self-adjoint extensions of symmetric operators [8]. In the WR, we write Eq. (18) as follows:

$$\begin{bmatrix} \varphi_1(b) \\ \varphi_2(b) \end{bmatrix} = \hat{U}_1 \begin{bmatrix} \varphi_1(a) \\ \varphi_2(a) \end{bmatrix}. \tag{19}$$

The latter result was derived in detail in Appendix A of Ref. [8].

(b) The operator  $\hat{h}_2$  can be written as

$$\hat{h}_2 = -i\hbar c \hat{\alpha} \frac{\partial}{\partial x} (= c\hat{\alpha}\hat{p}), \tag{20}$$

and it satisfies the following relation:

$$\langle \psi, \hat{h}_2 \xi \rangle - \langle \hat{h}_2 \psi, \xi \rangle = -i\hbar c [\psi^\dagger \hat{\alpha} \xi]_a^b, \tag{21}$$

where  $\psi$  and  $\xi$  are vectors in  $\mathcal{H}$ . Again, if the boundary conditions imposed on  $\psi$  and  $\xi$  lead to the cancellation of the boundary term on the right-hand side of Eq. (21), then the operator  $\hat{h}_2$  is Hermitian, *i.e.*,  $\langle \psi, \hat{h}_2 \xi \rangle = \langle \hat{h}_2 \psi, \xi \rangle$ . If we impose  $\psi = \xi$  in this last relation and in Eq. (21), we obtain the following condition:

$$c [\psi^\dagger \hat{\alpha} \psi]_a^b = [j]_a^b = 0 \quad (\Rightarrow j(b) = j(a)), \tag{22}$$

*i.e.*,  $C_2(b) = C_2(a)$ . Moreover,  $\langle \psi, \hat{h}_2 \psi \rangle = \langle \hat{h}_2 \psi, \psi \rangle = \langle \psi, \hat{h}_2 \psi \rangle$ ; therefore,  $\text{Im}\langle \psi, \hat{h}_2 \psi \rangle = 0$ , *i.e.*,  $\langle \psi, \hat{h}_2 \psi \rangle \equiv \langle \hat{h}_2 \psi, \psi \rangle \in \mathbb{R}$ . In addition, the operator  $\hat{h}_2$  is, essentially, self-adjoint on the domain  $D(\hat{h}_2)$  formed by the Dirac wave functions  $\psi$  such that  $\psi \in \mathcal{H}$  and  $\hat{h}_2 \psi \in \mathcal{H}$  and that satisfy, in the WR ( $\hat{\alpha} = \hat{\sigma}_z$ ), the following general boundary condition [9, 10]:

$$\begin{bmatrix} \varphi_1(b) \\ \varphi_2(b) \end{bmatrix} = \hat{U}_2 \begin{bmatrix} \varphi_2(b) \\ \varphi_1(a) \end{bmatrix}, \tag{23}$$

where the matrix  $\hat{U}_2$  is also unitary. Notice that the results (21)-(23), which are associated with the hermiticity and the self-adjointness of  $\hat{h}_2$ , are clearly also valid for the usual Hamiltonian operator  $\hat{H} = \hat{h}_2 + mc^2\hat{\beta} + U(x)$ . In other words, the matrix  $\hat{\beta}$  does not influence any of these results (it is also understood that the potential-energy function  $U(x)$  that is present in  $\hat{H}$  is bounded inside the interval  $\Omega$ ). Thus, the latter result allows us to ensure that the results associated with  $\hat{h}_2$  are also valid for a Hamiltonian that describes, for example, a massless Dirac fermion in 1+1 dimensions. In particular, the result given in Eq. (23) in combination with changes of representations provides all we require to obtain general boundary conditions for  $\hat{h}_3$  and  $\hat{h}_4$  in the WR, as outlined below.

(c) The operator  $\hat{h}_3$  can be written as

$$\hat{h}_3 = -i\hbar c \hat{\beta} \frac{\partial}{\partial x} (= c\hat{\beta}\hat{p}), \tag{24}$$

and it satisfies the following relation:

$$\langle \psi, \hat{h}_3 \xi \rangle - \langle \hat{h}_3 \psi, \xi \rangle = -i\hbar c [\psi^\dagger \hat{\beta} \xi]_a^b, \tag{25}$$

where  $\psi$  and  $\xi$  are vectors in  $\mathcal{H}$ . If, as a result of the boundary conditions imposed on  $\psi$  and  $\xi$ , the boundary term in Eq. (25) vanishes, then the operator  $\hat{h}_3$  is Hermitian, *i.e.*,  $\langle \psi, \hat{h}_3 \xi \rangle = \langle \hat{h}_3 \psi, \xi \rangle$ . By imposing  $\psi = \xi$  in this last relation and in Eq. (25), we obtain the following condition:

$$\left[ \psi^\dagger \hat{\beta} \psi \right]_a^b = [s]_a^b = 0 \quad (\Rightarrow s(b) = s(a)), \quad (26)$$

*i.e.*,  $C_3(b) = C_3(a)$ . Additionally,  $\langle \psi, \hat{h}_3 \psi \rangle = \langle \hat{h}_3 \psi, \psi \rangle = \langle \psi, \hat{h}_3 \psi \rangle$ ; therefore,  $\text{Im} \langle \psi, \hat{h}_3 \psi \rangle = 0$ , *i.e.*,  $\langle \psi, \hat{h}_3 \psi \rangle \equiv \langle \hat{h}_3 \rangle_\psi \in \mathbb{R}$ . However, the operator  $\hat{h}_3$  is also self-adjoint on the domain  $D(\hat{h}_3)$  formed by Dirac wave functions  $\psi$  such that  $\psi \in \mathcal{H}$  and  $\hat{h}_3 \psi \in \mathcal{H}$  and that also satisfy a general boundary condition. To obtain this general boundary condition in the WR for which the operator  $\hat{h}_3 = -i\hbar c \hat{\beta} \partial / \partial x$  is self-adjoint, we must exploit the fact that  $\hat{\beta}$  is precisely  $\hat{\sigma}_z$  in the SR. In other words,  $\hat{h}_3$  in the SR is simply the operator  $\hat{h}_2 = -i\hbar c \hat{\alpha} \partial / \partial x$  in the WR ( $\hat{\alpha} = \hat{\sigma}_z$ ). In this manner, we can immediately write the general boundary condition for  $\hat{h}_3$  as follows: first, in Eq. (23), we make the replacements  $\varphi_1 \rightarrow \varphi$ ,  $\varphi_2 \rightarrow \chi$ , and  $\hat{U}_2 \rightarrow \hat{U}_3$  (the latter because we are interested in the operator  $\hat{h}_3$ ), and then, we transform into the WR using the inverse of the unitary transformation given in Eq. (12), *i.e.*,  $\varphi = (\varphi_1 + \varphi_2) / \sqrt{2}$  and  $\chi = (\varphi_1 - \varphi_2) / \sqrt{2}$ . We obtain the result

$$\begin{bmatrix} \varphi_1(b) + \varphi_2(b) \\ \varphi_1(a) - \varphi_2(a) \end{bmatrix} = \hat{U}_3 \begin{bmatrix} \varphi_1(b) - \varphi_2(b) \\ \varphi_1(a) + \varphi_2(a) \end{bmatrix}, \quad (27)$$

where the matrix  $\hat{U}_3$  is unitary.

(d) The operator  $\hat{h}_4$  can be written as

$$\hat{h}_4 = -i\hbar c i\hat{\beta}\hat{\alpha} \frac{\partial}{\partial x} (= +ci\hat{\beta}\hat{\alpha}\hat{p}), \quad (28)$$

and it satisfies the following relation:

$$\langle \psi, \hat{h}_4 \xi \rangle - \langle \hat{h}_4 \psi, \xi \rangle = -i\hbar c \left[ \psi^\dagger i\hat{\beta}\hat{\alpha} \xi \right]_a^b, \quad (29)$$

where  $\psi$  and  $\xi$  are vectors in  $\mathcal{H}$ . If, because of the boundary conditions imposed on  $\psi$  and  $\xi$ , the boundary term in Eq. (29) vanishes, then the operator  $\hat{h}_4$  is Hermitian, *i.e.*,  $\langle \psi, \hat{h}_4 \xi \rangle = \langle \hat{h}_4 \psi, \xi \rangle$ . By imposing  $\psi = \xi$  in this last relation and in Eq. (29), we obtain:

$$\left[ \psi^\dagger i\hat{\beta}\hat{\alpha} \psi \right]_a^b = [w]_a^b = 0 \quad (\Rightarrow w(b) = w(a)), \quad (30)$$

*i.e.*,  $C_4(b) = C_4(a)$ . Moreover,  $\langle \psi, \hat{h}_4 \psi \rangle = \langle \hat{h}_4 \psi, \psi \rangle = \langle \psi, \hat{h}_4 \psi \rangle$ ; therefore,  $\text{Im} \langle \psi, \hat{h}_4 \psi \rangle = 0$ , *i.e.*,  $\langle \psi, \hat{h}_4 \psi \rangle \equiv \langle \hat{h}_4 \rangle_\psi \in \mathbb{R}$ . In the same manner as for the other operators we have introduced, the operator  $\hat{h}_4$  is also self-adjoint on the domain  $D(\hat{h}_4)$  formed by Dirac wave functions  $\psi$  such that  $\psi \in \mathcal{H}$  and  $\hat{h}_4 \psi \in \mathcal{H}$  and that satisfy a general boundary condition. To obtain this general boundary condition in the WR for which the operator  $\hat{h}_4 = -i\hbar c i\hat{\beta}\hat{\alpha} \partial / \partial x$  is self-adjoint, we must exploit the fact that  $i\hat{\beta}\hat{\alpha}$  is precisely  $\hat{\sigma}_z$  in

the SSR (*i.e.*,  $i\hat{\sigma}_y \hat{\sigma}_x = \hat{\sigma}_z$ ). In other words,  $\hat{h}_4$  in the SSR is simply the operator  $\hat{h}_2 = -i\hbar c \hat{\alpha} \partial / \partial x$  in the WR ( $\hat{\alpha} = \hat{\sigma}_z$ ). Thus, we can immediately write the general boundary condition for  $\hat{h}_4$  as follows: first, in Eq. (23), we make the replacements  $\varphi_1 \rightarrow \phi_1$ ,  $\varphi_2 \rightarrow \phi_2$ , and  $\hat{U}_2 \rightarrow \hat{U}_4$  (the latter because we are interested in the operator  $\hat{h}_4$ ), and then, we transform into the WR using the unitary transformation given in Eq. (14), *i.e.*,  $\phi_1 = ((1+i)\varphi_1 + (1-i)\varphi_2) / 2$  and  $\phi_2 = ((1+i)\varphi_1 - (1-i)\varphi_2) / 2$ . After some simplifications, we obtain

$$\begin{bmatrix} \varphi_1(b) - i\varphi_2(b) \\ \varphi_1(a) + i\varphi_2(a) \end{bmatrix} = \hat{U}_4 \begin{bmatrix} \varphi_1(b) + i\varphi_2(b) \\ \varphi_1(a) - i\varphi_2(a) \end{bmatrix}, \quad (31)$$

where the matrix  $\hat{U}_4$  is unitary. Incidentally, the latter boundary condition was obtained in Ref. [11], although that discussion concerned a Dirac Hamiltonian, which is essentially the same operator  $\hat{h}_4$  in the WR plus a certain matrix potential.

Likewise, we can explicitly write the most general boundary condition for each of these operators in the SR, which is the most frequently used representation, in part because it is very convenient for studying the non-relativistic limit [12]. Our results are as follows:

(a) In the SR, we write the boundary condition that belongs to  $D(\hat{h}_1)$  as follows:

$$\begin{bmatrix} \varphi(b) \\ \chi(b) \end{bmatrix} = \hat{T}_1 \begin{bmatrix} \varphi(a) \\ \chi(a) \end{bmatrix}, \quad (32)$$

where  $\hat{T}_1 = \hat{S}\hat{U}_1\hat{S}$  and  $\hat{S}$  is given in Eq. (7). The result expressed by (32) is expected because  $\hat{h}_1$  is independent of the representation (see Eq. (15)).

(b) Likewise, inside  $D(\hat{h}_2)$ , we have the following boundary condition:

$$\begin{bmatrix} \varphi(b) + \chi(b) \\ \varphi(a) - \chi(a) \end{bmatrix} = \hat{T}_2 \begin{bmatrix} \varphi(b) - \chi(b) \\ \varphi(a) + \chi(a) \end{bmatrix}, \quad (33)$$

where  $\hat{T}_2 = \hat{U}_2$ . This result is easily obtained because we know the general boundary condition for  $\hat{h}_2$  in the WR (see Eq. (23)); thus, all that is necessary is to transform from the latter representation into the SR (using Eq. (12)). In the non-relativistic limit, Eq. (33) provides the most general boundary condition for which the Schrödinger Hamiltonian is self-adjoint. See Ref. [10] for further details and Ref. [13] for the confirmation of this result (although in the latter, the equivalent problem of a particle moving on a real line with a point interaction at the origin was considered). Let us also note in passing that the usual Dirichlet boundary condition,  $\psi(a) = \psi(b) = 0$ , *i.e.*,  $\varphi(a) = \varphi(b) = 0$  and  $\chi(a) = \chi(b) = 0$ , is not included in Eq. (33). In other words, the operator  $\hat{h}_2$  and the Dirac Hamiltonian  $\hat{H}$  (see Eq. (10)) are not self-adjoint when this boundary condition is within their domains; in any case, these two operators can be made Hermitian by imposing the boundary condition in question (this particular topic was discussed in Ref. [14]). However, the following boundary conditions, for example, are contained in Eq. (33):  $\varphi(a) = \varphi(b) = 0$  ( $\hat{T}_2 = -\hat{1}$ ),

$\chi(a) = \chi(b) = 0$  ( $\hat{T}_2 = +\hat{1}$ ),  $\psi(a) = \psi(b)$  ( $\hat{T}_2 = +\hat{\sigma}_x$ ), and  $\psi(a) = -\psi(b)$  ( $\hat{T}_2 = -\hat{\sigma}_x$ ).

(c) Similarly, inside  $D(\hat{h}_3)$ , we have the following boundary condition:

$$\begin{bmatrix} \varphi(b) \\ \chi(a) \end{bmatrix} = \hat{T}_3 \begin{bmatrix} \chi(b) \\ \varphi(a) \end{bmatrix}, \tag{34}$$

where  $\hat{T}_3 = \hat{U}_3$ . We can immediately write this result because we know the general boundary condition for  $\hat{h}_3 = -i\hbar c \hat{\beta} \partial/\partial x$  when  $\hat{\beta} = \hat{\sigma}_z$  (see Eq. (23)), *i.e.*, for  $\hat{h}_3$  in the SR.

(d) Finally, in the domain  $D(\hat{h}_4)$ , we have the following boundary condition:

$$\begin{bmatrix} \varphi(b) + i\chi(b) \\ i\varphi(a) + \chi(a) \end{bmatrix} = \hat{T}_4 \begin{bmatrix} i\varphi(b) + \chi(b) \\ \varphi(a) + i\chi(a) \end{bmatrix}, \tag{35}$$

where  $\hat{T}_4 = \hat{U}_4$ . We can obtain this result because we know the general boundary condition for  $\hat{h}_4 = -i\hbar c i\hat{\beta}\hat{\alpha} \partial/\partial x$  when  $i\hat{\beta}\hat{\alpha} = \hat{\sigma}_z$  (see Eq. (23)), *i.e.*, for  $\hat{h}_4$  in the SSR. Thus, all that is necessary is to transform from the latter representation into the SR (using Eq. (13)).

At this point, certain remarks are in order. Indeed, we could construct different types of general boundary conditions for each of the operators considered here (some could also be dependent of four parameters). However, the families of general boundary conditions presented herein possess the advantage that none of the coefficients in the unitary matrices need be equal to infinity. In addition, each of these general boundary conditions is the most general that can be written with only one single matrix boundary condition. These features have been noted in the literature, especially in the study of the (equivalent) problem of a particle in a line with a point interaction at the origin (see, for example, Refs. [10, 13, 15]).

### 3. The standard and the Foldy-Wouthuysen representations

Thus far, we have considered representations of the Dirac equation that are related to the SR via trivial unitary transformations, *i.e.*, transformations that do not involve the momentum operator (see Ref. [16] for further discussion). As in Eq. (9), let us consider the following two (relativistic) wave equations, each in its own representation:

$$\hat{H}\psi = i\hbar \frac{\partial\psi}{\partial t}, \quad \tilde{H}\tilde{\psi} = i\hbar \frac{\partial\tilde{\psi}}{\partial t}. \tag{36}$$

Here,  $\hat{H}$  is the usual Dirac Hamiltonian operator with  $U(x) = 0$  (*i.e.*, the Hamiltonian for a free Dirac particle in 1+1 dimensions):

$$\hat{H} = c\hat{\alpha}\hat{p} + mc^2\hat{\beta}, \tag{37}$$

where, as we know,  $\hat{p} = -i\hbar\partial/\partial x$ . Moreover, using the relations of Eq. (3), we can show that  $\hat{H}^2 = (c\hat{p})^2 + (mc^2)^2$ , as expected. On the other hand, let  $\tilde{H}$  be the following operator:

$$\tilde{H} = \hat{\beta}\sqrt{(c\hat{p})^2 + (mc^2)^2}, \tag{38}$$

which also satisfies the expression  $\tilde{H}^2 = (c\hat{p})^2 + (mc^2)^2$ . It is that there exists a matrix, more specifically, a unitary matrix  $\hat{U}$  that is dependent on  $\hat{p}$  such that

$$\tilde{H} = \hat{U}\hat{H}\hat{U}^\dagger \tag{39}$$

and such that the wave functions  $\psi$  and  $\tilde{\psi}$  in (36) are related by

$$\tilde{\psi} = \hat{U}\psi. \tag{40}$$

In effect, by first using the equation on the right-hand side in (36) and also Eqs. (39) and (40), we can write the following:

$$\begin{aligned} \tilde{H}\tilde{\psi} &= i\hbar \frac{\partial\tilde{\psi}}{\partial t} \Rightarrow \tilde{H}\hat{U}\psi = i\hbar\hat{U} \frac{\partial\psi}{\partial t} \Rightarrow \hat{U}^\dagger \tilde{H}\hat{U}\psi \\ &= i\hbar\hat{U}^\dagger \hat{U} \frac{\partial\psi}{\partial t} = i\hbar \frac{\partial\psi}{\partial t}, \end{aligned}$$

and therefore (after applying the remaining equation in (36)),

$$\hat{H} = \hat{U}^\dagger \tilde{H}\hat{U}$$

(the operators  $\hat{H}$  and  $\tilde{H}$  as well as  $\hat{U}$  are time independent). Moreover, to transform operators from one representation into the other, we can use expressions similar to that given in (39) for  $\hat{H}$  and  $\tilde{H}$ . For example, we can write  $\hat{\alpha} = \hat{U}\hat{\alpha}\hat{U}^\dagger$  and also  $\hat{\beta} = \hat{U}\hat{\beta}\hat{U}^\dagger$ ; in any case, we do not need to explicitly calculate the matrices  $\{\hat{\alpha}, \hat{\beta}\}$  in this paper.

The exact transformation  $\hat{U}$  was obtained for the first time by Foldy and Wouthuysen [17] and can be written as follows (see, for example, Ref. [2], p. 277, and for a rather unusual calculation of  $\hat{U}$ , see Ref. [18]):

$$\begin{aligned} \hat{U} &= \frac{\hat{\beta}\hat{H} + E}{\sqrt{2E(E + mc^2)}} \\ \left( \Rightarrow \hat{U}^\dagger &= \frac{\hat{H}\hat{\beta} + E}{\sqrt{2E(E + mc^2)}} \right), \end{aligned} \tag{41}$$

where  $E \equiv \sqrt{(c\hat{p})^2 + (mc^2)^2} > 0$  is an eigenvalue of the operator  $\hat{H}$  ( $-E$  is also an eigenvalue of  $\hat{H}$ ), such that  $E^2$  is an eigenvalue of the operator  $\hat{H}^2$ . Naturally,  $E$  is also an eigenvalue of  $\tilde{H}$  (and  $-E$  is also an eigenvalue of  $\tilde{H}$ ). It is worth mentioning that to verify the relation  $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{1}$ , we have made use of the relation  $\hat{H}^2 = E^2$ , *i.e.*, we must assume that  $\hat{H}^2$  acts on plane waves or linear combinations of plane waves with the same energy. The same assumption is applied, for example, in the demonstration that the momentum operator when transformed into a new representation is the momentum operator itself, *i.e.*,  $\tilde{p} = \hat{p}$ . By substituting the matrix  $\hat{U}$  given by Eq. (41) into the expression (39) and using the relation  $\hat{H}^2 = E^2$  once again (along with some equations in (3)), we obtain

$$\tilde{H} = \hat{\beta}E. \tag{42}$$

It is clear that  $\tilde{U}$  permits us to transform quantities from a trivial representation (the SR, the WR, etc) into a new representation (represented by quantities marked with a tilde). However, the new representation can be regarded as the usual Foldy-Wouthuysen representation (FWR) only when  $\hat{\beta}$  is diagonal. Thus, we choose to use the SR to express  $\tilde{H}$  and  $\tilde{U}$ , *i.e.*,  $\{\hat{\alpha}, \hat{\beta}\} = \{\hat{\sigma}_x, \hat{\sigma}_z\}$ , as usual. From Eqs. (40) and (41), we can obtain the explicit relation between wave functions in these two representations, *i.e.*, we can write  $\psi = \tilde{U}\tilde{\psi}$  as follows:

$$\begin{bmatrix} \varphi \\ \chi \end{bmatrix} = \frac{1}{\sqrt{2E(E + mc^2)}} \times \begin{bmatrix} E + mc^2 & -c\hat{p} \\ c\hat{p} & E + mc^2 \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}. \quad (43)$$

Henceforth, we will write the Foldy-Wouthuysen wave function as  $\tilde{\psi} \equiv \psi_{FW} = [\psi_1 \ \psi_2]^T$ . Some aspects of the relation between wave functions in the SR and the FWR have been recently studied [19, 20]. However, to the best of our knowledge, no specific discussion of the connections between possible boundary conditions in these two representations is present in the literature.

First, we have noticed that (i) for positive energies,  $E$ , the wave function in the FWR has the form  $\psi_{FW} = [\psi_1 \ 0]^T$  (this result have also been noted in Ref. [20]). In effect,

$$\tilde{H}\psi_{FW} = E\psi_{FW} \Rightarrow \begin{bmatrix} E\psi_1 \\ -E\psi_2 \end{bmatrix} = \begin{bmatrix} E\psi_1 \\ E\psi_2 \end{bmatrix} \Rightarrow \psi_2 = 0,$$

where we have made use of Eq. (42). Thus, because  $\psi_2(x) = 0$ , the spatial derivative also vanishes, *i.e.*,  $\psi_2'(x) = 0$ , for all  $x \in \Omega$ . Therefore, from Eq. (43), we also have the following expressions:

$$\begin{aligned} \varphi(x) &= \frac{E + mc^2}{\sqrt{2E(E + mc^2)}}\psi_1(x), \\ \chi(x) &= \frac{-i\hbar c}{\sqrt{2E(E + mc^2)}}\psi_1'(x). \end{aligned} \quad (44)$$

Note that by writing  $\chi(x)$  in (44) in terms of  $\varphi(x)$  (by eliminating  $\psi_1'(x)$  using the first derivative of the other equation in (44)), we can write  $\psi(x)$  in the SR in terms of only  $\varphi(x)$  and  $\varphi'(x)$ , as follows:

$$\psi(x) = \begin{bmatrix} \varphi(x) \\ \chi(x) \end{bmatrix} = \begin{bmatrix} \varphi(x) \\ \frac{-i\hbar c}{E+mc^2}\varphi'(x) \end{bmatrix}. \quad (45)$$

Second, we have found that (ii) for negative energies,  $-E$ , we have  $\psi_{FW} = [0 \ \psi_2]^T$  [20]. In effect,

$$\begin{aligned} \tilde{H}\psi_{FW} &= -E\psi_{FW} \Rightarrow \begin{bmatrix} E\psi_1 \\ -E\psi_2 \end{bmatrix} \\ &= \begin{bmatrix} -E\psi_1 \\ -E\psi_2 \end{bmatrix} \Rightarrow \psi_1 = 0, \end{aligned}$$

where we have made use of Eq. (42). Thus, because  $\psi_1(x) = 0$ , its spatial derivative also vanishes for all  $x \in \Omega$  (*i.e.*,

$\psi_1'(x) = 0$ ). Therefore, from Eq. (43), we also have the following expressions:

$$\begin{aligned} \varphi(x) &= \frac{i\hbar c}{\sqrt{2E(E + mc^2)}}\psi_2'(x), \\ \chi(x) &= \frac{E + mc^2}{\sqrt{2E(E + mc^2)}}\psi_2(x). \end{aligned} \quad (46)$$

Note that by writing  $\varphi(x)$  in (46) in terms of  $\chi(x)$  (by eliminating  $\psi_2'(x)$  using the first derivative of the other equation in (46)), we can write  $\psi(x)$  in the SR in terms of only  $\chi(x)$  and  $\chi'(x)$ , as follows:

$$\psi(x) = \begin{bmatrix} \varphi(x) \\ \chi(x) \end{bmatrix} = \begin{bmatrix} \frac{i\hbar c}{E+mc^2}\chi'(x) \\ \chi(x) \end{bmatrix}. \quad (47)$$

Therefore, in the non-relativistic limit  $E \approx mc^2$ , *i.e.*,  $p/mc \ll 1$ , (i) when the energies are positive, we know from Eq. (45) that  $\chi = -i\hbar c\varphi'/(E + mc^2) \approx \hat{p}\varphi/2mc = O(v/c)$  (for this reason  $\chi$  is called the small component, and  $\varphi$  is the large component), and the entire wave function in the SR tends toward  $\psi = [\varphi \ 0]^T$ . Likewise, (ii) when the energies are negative, we know from Eq. (47) that  $\varphi = i\hbar c\chi'/(E + mc^2) \approx -\hat{p}\chi/2mc = O(v/c)$  (for this reason,  $\varphi$  is called the small component in this case, and  $\chi$  is the large component), and the wave function tends toward  $\psi = [0 \ \chi]^T$ . Thus, the wave function in the SR in the non-relativistic limit and the wave function in the FWR exhibit a clear similarity. (i) For positive energies,  $\psi = [\varphi \ 0]^T$  and  $\psi_{FW} = [\psi_1 \ 0]^T$ , where the latter  $\varphi$  and  $\psi_1$  differ by a constant factor (see Eq. (44)). (ii) For negative energies,  $\psi = [0 \ \chi]^T$  and  $\psi_{FW} = [0 \ \psi_2]^T$ , and the latter  $\chi$  and  $\psi_2$  differ by a constant factor (see Eq. (46)).

Now, we present some examples of boundary conditions in the FWR that correspond to physically acceptable boundary conditions in the SR. For example, let us impose the usual Dirichlet boundary condition upon the entire Foldy-Wouthuysen wave function at the ends of the interval  $\Omega = [a, b]$ , *i.e.*,

$$\psi_{FW}(a) = \psi_{FW}(b) = 0. \quad (48)$$

This boundary condition appears to be acceptable because the operator  $\tilde{H}$  in Eq. (38) contains a second derivative with respect to  $x$  (although this derivative is under the square root sign). (i) For positive energies, the latter boundary condition implies that  $\psi_1(a) = \psi_1(b) = 0$  (remember that  $\psi_2(x) = \psi_2'(x) = 0$ ). On the other hand, using the equation on the left-hand side in (44), we find that the upper component of the wave function in the SR (*i.e.*, the large component, in this case) satisfies the Dirichlet boundary condition, *i.e.*,  $\varphi(a) = \varphi(b) = 0$ . This boundary condition is included in Eq. (33), and therefore, the Dirac Hamiltonian  $\tilde{H}$  is self-adjoint [10]. (ii) For negative energies, the boundary condition in (48) implies that  $\psi_2(a) = \psi_2(b) = 0$  (remember that  $\psi_1(x) = \psi_1'(x) = 0$ ). On the other hand, from the equation

on the right-hand side in (46), we find that the lower component of the wavefunction in the SR (*i.e.*, the large component again in this case) satisfies the Dirichlet boundary condition, *i.e.*,  $\chi(a) = \chi(b) = 0$ . This boundary condition is also included in Eq. (33), and hence, the Dirac Hamiltonian  $\hat{H}$  is self-adjoint [10].

Now, let us consider the usual periodic boundary condition for the Foldy-Wouthuysen wave function, *i.e.*,

$$\psi_{\text{FW}}(a) = \psi_{\text{FW}}(b), \quad \psi'_{\text{FW}}(a) = \psi'_{\text{FW}}(b). \quad (49)$$

In the SR (and also in the other trivial representations), the periodic boundary condition is defined only by the condition  $\psi(a) = \psi(b)$ , *i.e.*, the derivative of  $\psi(x)$  need not satisfy the periodicity condition (this is true because the corresponding Hamiltonian is considered to be self-adjoint [10]). Then, using the periodic boundary condition for  $\psi_{\text{FW}}(x)$ , we obtain the following results: (i) For positive energies, we obtain from Eq. (44) the conditions  $\varphi(a) = \varphi(b)$  and  $\chi(a) = \chi(b)$ , and therefore,  $\psi(a) = \psi(b)$ . Likewise, (ii) for negative energies, we obtain from Eq. (46) the conditions  $\varphi(a) = \varphi(b)$  and  $\chi(a) = \chi(b)$ , and hence,  $\psi(a) = \psi(b)$ , *i.e.*, the periodic boundary condition. A similar analysis considering the antiperiodic boundary condition, *i.e.*,  $\psi_{\text{FW}}(a) = -\psi_{\text{FW}}(b)$  and  $\psi'_{\text{FW}}(a) = -\psi'_{\text{FW}}(b)$ , yields the antiperiodic boundary condition for  $\psi$ , *i.e.*,  $\psi(a) = -\psi(b)$  (for both positive and negative energies). Naturally, both the condition  $\psi(a) = \psi(b)$  as well as the condition  $\psi(a) = -\psi(b)$  are included in Eq. (33), and hence, the Dirac Hamiltonian  $\hat{H}$  is self-adjoint [10].

We can also consider a slightly less common example, the Neumann boundary condition for the Foldy-Wouthuysen wave function, *i.e.*,

$$\psi'_{\text{FW}}(a) = \psi'_{\text{FW}}(b) = 0. \quad (50)$$

(i) For positive energies, the latter boundary condition leads to  $\psi'_1(a) = \psi'_1(b) = 0$  (remember that  $\psi_2(x) = \psi'_2(x) = 0$ ), and from Eq. (44), we find that the lower component of the wave function in the SR (*i.e.*, the small component, in this case) satisfies the Dirichlet boundary condition, *i.e.*,  $\chi(a) = \chi(b) = 0$ . (ii) For negative energies, the boundary condition in (50) leads to  $\psi'_2(a) = \psi'_2(b) = 0$  (remember that  $\psi_1(x) = \psi'_1(x) = 0$ ), and from Eq. (46), we find that the upper component of the wavefunction in the SR (*i.e.*, the small component again in this case) satisfies the Dirichlet boundary condition, *i.e.*,  $\varphi(a) = \varphi(b) = 0$ . As we know, both the condition  $\chi(a) = \chi(b) = 0$  and the condition  $\varphi(a) = \varphi(b) = 0$  are included in Eq. (33), and hence the Dirac Hamiltonian  $\hat{H}$  is self-adjoint [10].

To summarize, we have imposed certain boundary conditions on the wave function  $\psi_{\text{FW}}$ . These boundary conditions lead to physically acceptable boundary conditions for the (self-adjoint) Dirac Hamiltonian  $\hat{H}$  in its standard form, *i.e.*, the Hamiltonian given by Eq. (37) with general boundary conditions given by Eq. (33) (because we have precisely considered  $\hat{H}$  in the SR). On the other hand, a physically acceptable boundary condition for  $\hat{H}$  can lead to different

boundary conditions for the Hamiltonian in the FWR. For example, the boundary condition  $\varphi(a) = \varphi(b) = 0$  ( $\hat{T}_2 = -\hat{1}$  in Eq. (33)) leads to  $\psi_{\text{FW}}(a) = \psi_{\text{FW}}(b) = 0$  for positive energies but leads to  $\psi'_{\text{FW}}(a) = \psi'_{\text{FW}}(b) = 0$  for negative energies. However, the periodic boundary condition  $\psi(a) = \psi(b)$  in the SR ( $\hat{T}_2 = \hat{\sigma}_x$  in Eq. (33)) also leads to the periodic boundary condition in the FWR,  $\psi_{\text{FW}}(a) = \psi_{\text{FW}}(b)$  and  $\psi'_{\text{FW}}(a) = \psi'_{\text{FW}}(b)$ , for both positive and negative energies. Thus, we can propose general boundary conditions for  $\psi_{\text{FW}}$  based on the family of self-adjoint general boundary conditions for  $\psi$  given in Eq. (33). (i) For positive energies, using the fact that, in this case, the wavefunction in the FWR has the form  $\psi_{\text{FW}} = [\psi_1 \ 0]^T$ , we obtain the following family of general boundary conditions from Eqs. (44) and (33):

$$\begin{aligned} &\psi_{\text{FW}}(b) - i\lambda\psi'_{\text{FW}}(b) + \hat{\sigma}_x [\psi_{\text{FW}}(a) + i\lambda\psi'_{\text{FW}}(a)] \\ &= \hat{T}_2 \{ \psi_{\text{FW}}(b) + i\lambda\psi'_{\text{FW}}(b) + \hat{\sigma}_x [\psi_{\text{FW}}(a) \\ &- i\lambda\psi'_{\text{FW}}(a)] \}, \end{aligned} \quad (51)$$

where  $\lambda \equiv \hbar c/(E + mc^2)$ . Likewise, (ii) for negative energies, using the fact that, in this case, the wave function in the FWR has the form  $\psi_{\text{FW}} = [0 \ \psi_2]^T$ , we obtain the following family of general boundary conditions from Eqs. (46) and (33):

$$\begin{aligned} &-\psi_{\text{FW}}(a) + i\lambda\psi'_{\text{FW}}(a) + \hat{\sigma}_x [\psi_{\text{FW}}(b) + i\lambda\psi'_{\text{FW}}(b)] \\ &= \hat{T}_2 \{ \psi_{\text{FW}}(a) + i\lambda\psi'_{\text{FW}}(a) \\ &+ \hat{\sigma}_x [-\psi_{\text{FW}}(b) + i\lambda\psi'_{\text{FW}}(b)] \}. \end{aligned} \quad (52)$$

Notice that some of the boundary conditions in (51) and (52) are energy dependent, *i.e.*, these boundary conditions should be applied only to a stationary state with definite energy. We will not elaborate further on the consequences of this energy dependence in this article.

## 4. Conclusions

In summary, we have studied several essential properties associated with the hermiticity and self-adjointness of four differential Dirac operators,  $\hat{h}_A = -i\hbar c \hat{\Gamma}_A \partial/\partial x$ , for  $x \in \Omega = [a, b]$ . The hermiticity leads to  $C_A(b) = C_A(a)$ , where  $C_A = c\psi^\dagger \hat{\Gamma}_A \psi$ . The self-adjointness additionally leads to specific families of boundary conditions, each to be included in its respective domain  $D(\hat{h}_A)$ . In general, because in any trivial representation the matrices  $\hat{\Gamma}_2 = \hat{\alpha}$ ,  $\hat{\Gamma}_3 = \hat{\beta}$ , and  $\hat{\Gamma}_4 = i\hat{\beta}\hat{\alpha}$  are (essentially) the three (anticommuting) Pauli matrices (the latter satisfy  $\hat{\sigma}_j \hat{\sigma}_k = i\hat{\sigma}_l$  for cyclic  $\{j, k, l\}$ ), the families of general boundary conditions for the operators  $\hat{h}_2$ ,  $\hat{h}_3$ , and  $\hat{h}_4$  are linked. In particular, we obtained the families of general boundary conditions for  $\hat{h}_3$  and  $\hat{h}_4$  from the general family for  $\hat{h}_2$  in the WR. To transform these families of boundary conditions into any other trivial representation, such as the SR, is a simple task. We were also able

to obtain boundary conditions for the free Dirac Hamiltonian in the FWR from boundary conditions for the free (self-adjoint) Dirac Hamiltonian in the SR. In fact, these boundary conditions can be obtained because they are consistent with the self-adjointness of the standard free Dirac Hamiltonian. However, given a boundary condition for the standard Dirac

Hamiltonian, we could obtain (in certain cases) two different boundary conditions for the Dirac Hamiltonian in the FWR depending on the sign of the energy of the state in question. We hope that this article will be of interest to those interested in the mathematical aspects of relativistic quantum mechanics, presented in a simple and pedagogical fashion.

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1. B. Thaller, *Advanced Visual Quantum Mechanics* (New York: Springer 2005) p. 325.
  2. W. Greiner, *Relativistic Quantum Mechanics* 3rd Edition (Berlin Heidelberg: Springer-Verlag 2000).
  3. V. Alonso, S. De Vincenzo, and L. Mondino, *Found. Phys.* **29** (1999) 231-50.
  4. C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics* (Reading, MA: Addison-Wesley 1977) p. 300.
  5. B. Thaller, *The Dirac Equation* (New York: Springer 1992). p. 36.
  6. S. De Vincenzo, *Operators and bilinear densities in the Dirac formal 1D Ehrenfest theorem*. (Submitted for publication 2014).
  7. W. Bulla, P. Falkensteiner, and H. Grosse, *Phys. Lett. B* **215** (1988) 359-63.
  8. V. Alonso and S. De Vincenzo, *J. Phys. A: Math. Gen.* **32** (1999) 5277-84.
  9. P. Falkensteiner and H. Grosse, *J. Math. Phys.* **28** (1987) 850-54.
  10. V. Alonso and S. De Vincenzo, *J. Phys. A: Math. Gen.* **30** (1997) 8573-85.
  11. S. M. Roy and V. Singh, *Phys. Lett.* **143B** (1984) 179-82.
  12. P. Holland and H. R. Brown, *Studies in History and Philosophy of Modern Physics* **34** (2003) 161-87.
  13. Z. Brzezniak and B. Jefferies, *J. Phys. A: Math. Gen.* **34** (2001) 2977-83.
  14. V. Alonso S. De Vincenzo and L. Mondino, *Eur. J. Phys.* **18** (1997) 315-320.
  15. V. Alonso and S. De Vincenzo, *Int. J. Theor. Phys.* **39** (2000) 1483-98.
  16. J. P. Costella and B. H. J. McKellar, *Am. J. Phys.* **63** (1995) 1119-21.
  17. L. L. Foldy and S. A. Wouthuysen, *Phys. Rev.* **78** (1950) 29-36.
  18. D. Atkinson and P. W. Johnson, *Exercises in Quantum Field Theory* Vol 4 (Princeton: Rinton Press 2003) p. 62.
  19. A. J. Silenko, *Phys. Part. Nucl. Lett.* **5** (2008) 501-5.
  20. V. P. Neznamov and A. J. Silenko, *J. Math. Phys.* **50** (2009) 122302.