# On changes of representation and general boundary conditions for Dirac operators in (1+1) dimensions

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#### ESSAY

#### I. Introduction

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

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

where  $x \in \Omega = [a, b]$ . We assume that each  $\hat{h}_A$  acts on two-component column vectors (or Dirac wave functions in (1+1) dimensions)  $\psi = \psi(t, x) = [\psi_1(t, x) \psi_2(t, x)]^{\mathsf{T}}$  (where the symbol  $\mathsf{T}$ 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. Note: in this essay we use the term Hermitian to refer to differential operators that are called symmetric (or formally self-adjoint) in the mathematical jargon. The 2 × 2 (Hermitian) matrices  $\hat{\Gamma}_A = \hat{\Gamma}_A^{\dagger}$  are given by

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

$$\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha} = 0, \quad \hat{\alpha}^2 = \hat{\beta}^2 = \hat{1}.$$
(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)  $\operatorname{tr}(\hat{\Gamma}_A) = 0$  (where 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

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

where  $C_A = \operatorname{tr}(\hat{\Gamma}_A \hat{C})/2$  (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:

$$C_A = c\psi^{\dagger} \hat{\Gamma}_A \psi. \tag{5}$$

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 essay, 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)  $(\hat{C}/2c\rho)^{\dagger} = \hat{C}/2c\rho$ , (ii)  $(\hat{C}/2c\rho)^2 = \hat{C}/2c\rho$ , and (iii)  $\text{tr}(\hat{C}/2c\rho)^2 = 1$ . Hence,  $\hat{C}/2c\rho$  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  $(c\rho)^2 = (cs)^2 + j^2 + (cw)^2$ , 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  $\{\hat{\alpha}', \hat{\beta}'\}$ , 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

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

(and therefore also  $\hat{\Gamma}'_A = \hat{S} \hat{\Gamma}_A \hat{S}^{-1}$ ). 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 essay, 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),  $\{\hat{\alpha}', \hat{\beta}'\} = \{\hat{\sigma}_z, \hat{\sigma}_x\}$ ; and (iii) the supersymmetric representation (SSR),  $\{\hat{\alpha}', \hat{\beta}'\} = \{\hat{\sigma}_x, \hat{\sigma}_y\}$ . As we will see below, in (1+1) dimensions the last could also be considered to be a Majorana representation [5]. 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:

$$\hat{H}\psi = i\hbar \frac{\partial \psi}{\partial t}, \quad \hat{H}'\psi' = i\hbar \frac{\partial \psi'}{\partial t},$$
(9)

where, for example,

$$\hat{H} = -i\hbar c\hat{\alpha}\frac{\partial}{\partial x} + mc^2\hat{\beta} + U(x), \quad \hat{H}' = -i\hbar c\hat{\alpha}'\frac{\partial}{\partial x} + mc^2\hat{\beta}' + U(x)$$
(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  $\psi'$  are related by

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

If the operators  $\hat{H}$  and  $\hat{H}'$  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  $\psi = \psi(t, x) = [\varphi(t, x)\chi(t, x)]^{\mathsf{T}}$ , 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  $\psi' = \psi'(t, x) = [\varphi_1(t, x) \varphi_2(t, x)]^{\mathsf{T}}$ . Using Eqs. (7) and (11), we can write the relation between the components of  $\psi$  and  $\psi'$  as follows:

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

Likewise, in the SSR, we write the wavefunction as  $\psi' = \psi'(t, x) = [\phi_1(t, x) \phi_2(t, x)]^{\intercal}$ . 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):

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

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

$$\begin{bmatrix} \phi_1 \\ \phi_2 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1+i & 1-i \\ 1+i & -(1-i) \end{bmatrix} \begin{bmatrix} \varphi_1 \\ \varphi_2 \end{bmatrix},$$
(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,  $C'_A = c\psi'^{\dagger} \hat{\Gamma}'_A \psi' = c\psi^{\dagger} \hat{S}^{\dagger} \hat{S} \hat{\Gamma}_A \hat{S}^{\dagger} \hat{S} \psi = C_A$ . It is also worth mentioning that in the SSR, the free Dirac equation can be written as follows (see Eqs. (9) and (10)):

$$-\mathrm{i}\hbar c\hat{\sigma}_x \frac{\partial \psi'}{\partial x} + \mathrm{m}c^2 \hat{\sigma}_y \psi' = \mathrm{i}\hbar \frac{\partial \psi'}{\partial t} \Rightarrow \left(\frac{1}{c}\frac{\partial}{\partial t} + \hat{\sigma}_x \frac{\partial}{\partial x} + \frac{\mathrm{m}c}{\hbar}\mathrm{i}\hat{\sigma}_y\right)\psi' = 0,$$

that is to say, the latter equation is real, i.e.,  $\psi'$  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.

#### II. 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,

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

$$\langle \psi, \hat{h}_1 \xi \rangle - \langle \hat{h}_1 \psi, \xi \rangle = -i\hbar c \left[ \psi^{\dagger} \xi \right] \Big|_a^b,$$
 (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:

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

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,  $\operatorname{Im} \langle \psi, \hat{h}_1 \psi \rangle = 0$ , i.e.,  $\langle \psi, \hat{h}_1 \psi \rangle \equiv \langle \hat{h}_1 \rangle_{\psi} \in \mathbb{R}$  (the asterisk 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:

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

$$\langle \psi, \hat{h}_2 \xi \rangle - \langle \hat{h}_2 \psi, \xi \rangle = -i\hbar c \left[ \psi^{\dagger} \hat{\alpha} \xi \right] \Big|_a^b,$$
 (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:

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

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,  $\operatorname{Im} \langle \psi, \hat{h}_2 \psi \rangle = 0$ , i.e.,  $\langle \psi, \hat{h}_2 \psi \rangle \equiv \langle \hat{h}_2 \rangle_{\psi} \in \mathbb{R}$ . 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]:

$$\begin{bmatrix} \varphi_1(b) \\ \varphi_2(a) \end{bmatrix} = \hat{U}_2 \begin{bmatrix} \varphi_2(b) \\ \varphi_1(a) \end{bmatrix},$$
(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  $\hat{H} = \hat{h}_2 + \mathrm{m}c^2\hat{\beta} + U(x)$ . 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:

$$\langle \psi, \hat{h}_3 \xi \rangle - \langle \hat{h}_3 \psi, \xi \rangle = -i\hbar c \left[ \psi^{\dagger} \hat{\beta} \xi \right] \Big|_a^b,$$
<sup>(25)</sup>

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:

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

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,  $\operatorname{Im} \langle \psi, \hat{h}_3 \psi \rangle = 0$ , 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  $\varphi_1 \to \varphi$ ,  $\varphi_2 \to \chi$ , and  $\hat{U}_2 \to \hat{U}_3$  (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

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

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

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

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

and it satisfies the following relation:

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

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:

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

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,  $\operatorname{Im} \langle \psi, \hat{h}_4 \psi \rangle = 0$ , 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

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

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

where  $\hat{T}_1 = \hat{S}\hat{U}_1\hat{S}^{-1}$  and  $\hat{S} (= \hat{S}^{-1})$  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:

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

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

### **III.** Conclusions

In summary, we have introduced 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  $x \in \Omega = [a, b]$ . 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. The hermiticity leads to  $C_A(x = b) = C_A(x = a)$ , 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,  $\hat{C}/2c\varrho$  is a density matrix ( $\varrho$  is the probability density). 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  $\hat{\Gamma}_2$ ,  $\hat{\Gamma}_3$ , and  $\hat{\Gamma}_4$  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, because the most general family of self-adjoint boundary conditions for  $\hat{h}_2$  in the WR (using only the aforementioned family for  $\hat{h}_2$  and changes of representation among the Dirac matrices) can be obtained. From these results, families of general boundary conditions for all these operators in the SR can also be determined.

Recently, we were also able to obtain boundary conditions for the free Dirac Hamiltonian in the Foldy-Wouthuysen representation (FWR) from boundary conditions for the free (self-adjoint) Dirac Hamiltonian in the SR [16]. 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.

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