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General boundary conditions for a Dirac particle in a box and their non-relativistic limits

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Abstract. The most general relativistic boundary conditions (BCs) for a 'free' Dirac particle in a one-dimensional box are discussed. It is verified that in the Weyl representation there is only one family of BCs, labelled with four parameters. This family splits into three sub-families in the Dirac representation. The energy eigenvalues as well as the corresponding non-relativistic limits of all these results are obtained. The BCs which are symmetric under space inversion P and those which are CPT invariant for a particle confined in a box, are singled out.

1. Introduction

A 'free' particle in a one-dimensional box is the canonical example of elementary non-relativistic quantum mechanics. Recently, at least in the physical literature [1], the boundary conditions (BCs) that force the energy eigenfunctions to vanish at the walls of the box were generalized to a four-parameter family of BCs for which the Schrödinger 'free' Hamiltonian is self-adjoint. These authors claim that this family of BCs is the general one for a particle in a box. However, by using von Neumann's theory of self-adjoint extensions of symmetric operators, as exposed for example in [2], it was shown [3] that by maintaining the column vectors of the BCs that relate linearly the wavefunction and its derivatives at the wall of the box, there are three inequivalent families of self-adjoint extensions, one of which is that of [1]. Moreover, these families represent the most general manifold of self-adjoint extensions for a 'free' non-relativistic particle in a box [4].

In this paper, we examine, from the relativistic point of view, this problem by using the Dirac equation. In the Weyl representation (WR), the most general BCs may be written using only one family which splits into three families in the Dirac representation (DR). This is the appropriate representation in order to take the non-relativistic limit.

On the other hand, the vanishing of the whole spinor at the walls yields to incompatibility, that is to say, the problem has only the trivial solution [6]. The same result has been obtained in the relativistic scattering on an impenetrable cylindrical solenoid of finite radius [5, 6]. This is not actually surprising, inasmuch as the spinor has four complex components which are coupled in a system of first-order differential equations. So, to force all the components to vanish at the boundary is too restrictive. Something similar occurs in electromagnetism by requiring that the field tensor vanish at the walls of a wave guide, the only solution being the trivial one. Imposing less restrictive conditions,

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for example, by cancelling only parts of the electric and magnetic fields at the boundary, it is found that a non-trivial solution exists (stationary waves).

A particular solution may be obtained by considering the Dirac equation with a Lorentz scalar potential [7]; here the rest mass can be thought of as an x-dependent mass. This permits us to solve the infinite square well problem as if it is were a particle with a changing mass that becomes infinite out of the box, so avoiding the Klein paradox [8].

By considering the 'free' Dirac Hamiltonian along with appropriate BCs, we can simulate the presence of potentials that constrain the particle to be in a certain region, but these BCs should be such that the corresponding Hamiltonian be self-adjoint. For this, it is worth emphasizing that the specification of its domain, which includes the BCs, is an essential part of the definition of all operators in quantum mechanics. Moreover, different BCs lead to different physical consequences. For relativistic scattering problems [6, 9], it has been proposed that the vanishing of only the large component of the Dirac spinor is a physically acceptable BC. It can be easily seen that, for the 'free' particle in a box, in the non-relativistic limit this BC yields the well known Dirichlet BC. Furthermore, such a BC is only one of the infinite self-adjoint extensions of the 'free' Dirac Hamiltonian. This result, as well as the eigenvalues and eigenfunctions for the family of self-adjoint extensions of the 'free' Dirac Hamiltonian in the WR, was obtained in [10].

The problem of a Dirac fermion in a one-dimensional box interacting with a scalar solitonic potential, with periodic [11], as well as with more general BC [12], was considered earlier, in order to elucidate the phenomenon of the fractional fermion number. For the case of the Dirac 'free' massless operator, also in $(1 + 1)$ dimensions, eigenvalues and eigenfunctions have been obtained for a family of self-adjoint extensions in [13]. The case with a non-zero vector potential was examined in [14].

In section 2, and in appendix A, we verify that in the WR the self-adjoint extensions of the Hamiltonian of a 'free' Dirac particle in a one-dimensional box, may be written by means of only one family. This family leads to three non-equivalent families of self-adjoint extensions for this operator in the standard or DR. In the last part of section 2, for each family of self-adjoint extensions,, we give the energy eigenvalues as well as several examples of BCs which may be of physical interest. We also select the BCs according to their invariance under P and CPT transformations.

In section 3, the non-relativistic limit of each family of self-adjoint extensions in the DR is obtained, as well as their non-relativistic energy eigenvalues. We write the most general non-relativistic BCs obtained from the non-relativistic limit of the single relativistic family in the WR.

2. Self-adjoint extensions

The Dirac equation for a relativistic 'free' particle inside a one-dimensional box, with fixed walls at $x = 0$ and $x = L$, may be written as

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi(x,t) = \left(-\mathrm{i}\hbar c\alpha\frac{\partial}{\partial x} + mc^2\beta\right)\Psi(x,t) \tag{1}$$

where Ψ denotes a two-component spinor depending upon $x \in \Omega = [0, L]$ and upon time. The 2×2 matrices α and β satisfy: $\alpha\beta + \beta\alpha = 0$ and $\alpha^2 = \beta^2 = 1$. In the DR: $\alpha = \sigma_x$ and $\beta = \sigma_z$. In the WR: $\alpha = \sigma_z$ and $\beta = \sigma_x$.

The Dirac eigenvalue equation is given by

$$(H\psi)(x) = \left(-\mathrm{i}\hbar c\alpha\frac{\mathrm{d}}{\mathrm{d}x} + mc^2\beta\right)\psi(x) = E\psi(x) \tag{2}$$

where ψ is related to Ψ by $\Psi(x,t) = \psi(x)\mathrm{e}^{-\mathrm{i}(E/\hbar)t}$.

The spinors $\psi(x)$ and $(H\psi)(x)$ belong to a dense proper subset of the Hilbert space $\mathcal{H} = L^2(\Omega) \oplus L^2(\Omega)$, with a scalar product denoted by $\langle , \rangle$. The domain of H and its adjoint H^* verify $\mathrm{Dom}(H) \subseteq \mathrm{Dom}(H^*)$; but H must be self-adjoint, so we look for self-adjoint extensions of the symmetric operator H (appendix A).

In the DR,

$$\psi_{\mathrm{D}}(x) = \begin{pmatrix} \phi(x) \\ \chi(x) \end{pmatrix}$$

where ϕ and χ are respectively, the spatial parts of the so-called large and small components of the Dirac spinor. On the other hand, in the WR we write

$$\psi_{\mathrm{w}}(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}.$$

In order to change representation, we use the transformation $\phi = (1/\sqrt{2})(\psi_1 + \psi_2)$ and $\chi = (1/\sqrt{2})(\psi_1 - \psi_2)$.

2.1. Self-adjoint extensions in the WR

In this representation there exists a four-parameter family of self-adjoint extensions of the formal Hamiltonian operator, $H_{\mathrm{w}} \equiv (H_{\mathrm{w}})_{\theta,\mu,\tau,\gamma}$

$$(H_{\mathrm{w}})_{\theta,\mu,\tau,\gamma} = -\mathrm{i}\hbar c\sigma_z \frac{\mathrm{d}}{\mathrm{d}x} + mc^2\sigma_x \tag{3}$$

with its domain given by [10, 12–14]

$$\mathrm{Dom}(H_{\mathrm{w}}) = \left\{ \psi_{\mathrm{w}} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \middle| \psi_{\mathrm{w}} \in \mathcal{H}, \text{a.c. in } \Omega, (H_{\mathrm{w}}\psi_{\mathrm{w}}) \in \mathcal{H}\ \psi_{\mathrm{w}} \text{ fulfils} \right.$$
$$\left. \begin{pmatrix} \psi_1(L) \\ \psi_2(0) \end{pmatrix} = U \begin{pmatrix} \psi_2(L) \\ \psi_1(0) \end{pmatrix}, \ U^{-1} = U^{\dagger} \right\} \tag{4}$$

where hereafter a.c. means absolutely continuous functions and the symbol '$\dagger$' denotes the adjoint of a vector or a matrix. The unitary matrix U may be written as

$$U = \begin{pmatrix} v & u \\ s & w \end{pmatrix} \tag{5}$$

where $v = \mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{\mathrm{i}\tau}\cos\theta$, $u = \mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{\mathrm{i}\gamma}\sin\theta$, $s = \mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{-\mathrm{i}\gamma}\sin\theta$ and $w = -\mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{-\mathrm{i}\tau}\cos\theta$, with $0 \leqslant \theta < \pi$, $0 \leqslant \mu, \tau, \gamma < 2\pi$.

It is worth noting that with this parametrization the self-adjoint extensions are not labelled in a single form, that is to say, the same boundary condition may be given by a sub-family of parameters. Let us also point out that the same four-parameter family of self-adjoint extensions is valid when a bounded potential is present inside the box.

It can be shown that for every spinor $\psi_{\mathrm{w}} \in \mathrm{Dom}(H_{\mathrm{w}})$, the current density $j(x) = c\psi_{\mathrm{w}}^{\dagger}\sigma_z\psi_{\mathrm{w}}$ satisfies at the walls of the box $j(0) = j(L)$, and for some of the extensions ($\theta = 0$) it is verified that $j(0) = j(L) = 0$, which leads to the relativistic impenetrability condition at the walls of the box.

In appendix A, we briefly verify that in the domain of H_{w} are included all BCs that make H_{w} self-adjoint.

In the WR the general solution of (2) can be written as

$$\psi_{\mathrm{w}} = c_1 \begin{pmatrix} 1 \\ \frac{E - \hbar ck}{mc^2} \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + c_2 \begin{pmatrix} \frac{E - \hbar ck}{mc^2} \\ 1 \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \tag{6}$$

where $k = (E^2 - (mc^2)^2)^{1/2}/\hbar c$ and c_1, c_2 are arbitrary complex constants. Imposing upon this spinor the BCs given in (4), an homogeneous algebraic system for c_1, c_2 is obtained, whose determinant must be zero, and from which the following transcendental equation for the energy eigenvalues follows:

$$\cos(\mu - kL) - \left(\frac{E - \hbar ck}{mc^2}\right)^2 \cos(\mu + kL) - \left[1 - \left(\frac{E - \hbar ck}{mc^2}\right)^2\right] \cos\gamma \sin\theta \\ +2\left(\frac{E - \hbar ck}{mc^2}\right) \sin\tau \cos\theta \sin(kL) = 0. \tag{7}$$

2.2. Self-adjoint extensions in the DR

In order to obtain the non-relativistic families of BCs, let us first change to the DR. From H_{w}, with its domain given in (4), and using the transformation from the WR to DR we have

$$\begin{pmatrix} 1+v & u \\ s & 1+w \end{pmatrix} \begin{pmatrix} -\chi(L) \\ \chi(0) \end{pmatrix} = \begin{pmatrix} 1-v & -u \\ -s & 1-w \end{pmatrix} \begin{pmatrix} \phi(L) \\ \phi(0) \end{pmatrix}. \tag{8}$$

Then, three families of self-adjoint extensions of H_{D} are obtained. Firstly

$$H_{\mathrm{D}}^{(1)} \equiv (H_{\mathrm{D}}^{(1)})_{\theta,\mu,\tau,\gamma} = -\mathrm{i}\hbar c\sigma_x \frac{\mathrm{d}}{\mathrm{d}x} + mc^2\sigma_z \tag{9}$$

whose domain can be written as

$$\mathrm{Dom}(H_{\mathrm{D}}^{(1)}) = \left\{ \psi_{\mathrm{D}} = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \psi_{\mathrm{D}} \in \mathcal{H}, \text{a.c. in } \Omega, (H_{\mathrm{D}}^{(1)}\psi_{\mathrm{D}}) \in \mathcal{H}, \psi_{\mathrm{D}} \text{ fulfils} \right. \\ \left. \begin{pmatrix} -\chi(L) \\ \chi(0) \end{pmatrix} = A_1 \begin{pmatrix} \phi(L) \\ \phi(0) \end{pmatrix}, A_1 = -(A_1)^\dagger \right\} \tag{10}$$

where

$$A_1 = \mathrm{i}(\sin\mu - \sin\tau\cos\theta)^{-1} \begin{pmatrix} \cos\mu - \cos\tau\cos\theta & -\mathrm{e}^{\mathrm{i}\gamma}\sin\theta \\ -\mathrm{e}^{-\mathrm{i}\gamma}\sin\theta & \cos\mu + \cos\tau\cos\theta \end{pmatrix} \tag{11}$$

with the restriction $\sin\mu - \sin\tau\cos\theta \neq 0$.

Likewise,

$$H_{\mathrm{D}}^{(2)} \equiv (H_{\mathrm{D}}^{(2)})_{\theta,\mu,\tau,\gamma} = -\mathrm{i}\hbar c\sigma_x \frac{\mathrm{d}}{\mathrm{d}x} + mc^2\sigma_z \tag{12}$$

acting on the domain

$$\mathrm{Dom}(H_{\mathrm{D}}^{(2)}) = \left\{ \psi_{\mathrm{D}} = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \psi_{\mathrm{D}} \in \mathcal{H}, \text{a.c. in } \Omega, (H_{\mathrm{D}}^{(2)}\psi_{\mathrm{D}}) \in \mathcal{H}, \psi_{\mathrm{D}} \text{ fulfils} \right. \\ \left. \begin{pmatrix} \phi(L) \\ \phi(0) \end{pmatrix} = A_2 \begin{pmatrix} -\chi(L) \\ \chi(0) \end{pmatrix}, A_2 = -(A_2)^\dagger \right\} \tag{13}$$

where

$$A_2 = \mathrm{i}(\sin\mu + \sin\tau\cos\theta)^{-1} \begin{pmatrix} \cos\mu + \cos\tau\cos\theta & \mathrm{e}^{\mathrm{i}\gamma}\sin\theta \\ \mathrm{e}^{-\mathrm{i}\gamma}\sin\theta & \cos\mu - \cos\tau\cos\theta \end{pmatrix} \tag{14}$$

with the restriction $\sin\mu + \sin\tau\cos\theta \neq 0$.

Let us note that the boundary conditions included in (10) are not always equivalent to those given in (13), because $\det A_1$ and $\det A_2$ may be zero. Thus, $H_{\mathrm{D}}^{(1)}$ and $H_{\mathrm{D}}^{(2)}$ are two different families of self-adjoint extensions of the relativistic 'free' Hamiltonian.

Finally, let us consider the cases where the above two restrictions are changed to $\sin\mu - \sin\tau\cos\theta = 0$ and $\sin\mu + \sin\tau\cos\theta = 0$. This corresponds to the vanishing of the determinants of the matrices in (8). It can be shown that all BCs in this new family are obtained from (8), and are included in some of the following cases: (i) $\mu = 0$, $\tau = 0$; (ii) $\mu = 0$, $\tau = \pi$; (iii) $\mu = \pi$, $\tau = 0$; and (iv) $\mu = \pi$, $\tau = \pi$; where $0 \leqslant \theta < \pi$ and $0 \leqslant \gamma < 2\pi$. We write this family as

$$H_{\mathrm{D}}^{(3)} \equiv (H_{\mathrm{D}}^{(3)})_{\theta,\mu,\tau,\gamma} = -\mathrm{i}\hbar c\sigma_x \frac{\mathrm{d}}{\mathrm{d}x} + mc^2\sigma_z \tag{15}$$

with the domain given by

$$\mathrm{Dom}(H_{\mathrm{D}}^{(3)}) = \left\{ \psi_{\mathrm{D}} = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \psi_{\mathrm{D}} \in \mathcal{H}, \text{a.c. in } \Omega, (H_{\mathrm{D}}^{(3)}\psi_{\mathrm{D}}) \in \mathcal{H}, \psi_{\mathrm{D}} \text{ fulfils equation (8)} \right.$$
$$\text{with the following cases: (i) } \mu = 0, \tau = 0\text{; (ii) } \mu = 0, \tau = \pi\text{;}$$
$$\left. \text{(iii) } \mu = \pi, \tau = 0\text{; and (iv) } \mu = \pi, \tau = \pi \right\}. \tag{16}$$

In the DR we have three energy eigenvalue equations, one for each Hamiltonian operator $H_{\mathrm{D}}^{(1)}$, $H_{\mathrm{D}}^{(2)}$, $H_{\mathrm{D}}^{(3)}$. The general solution may be written as

$$\psi_{\mathrm{D}} = d_1 \begin{pmatrix} \sqrt{E + mc^2} \\ \sqrt{E - mc^2} \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} + d_2 \begin{pmatrix} \sqrt{E - mc^2} \\ -\sqrt{E + mc^2} \end{pmatrix} \mathrm{e}^{-\mathrm{i}kx} \tag{17}$$

with d_1, d_2 arbitrary complex constants. By imposing upon this solution the boundary conditions included in the domains of the operators $H_{\mathrm{D}}^{(1)}$, $H_{\mathrm{D}}^{(2)}$, $H_{\mathrm{D}}^{(3)}$, the following eigenvalue equations are obtained

$$\left\{ \frac{E + (-1)^j mc^2}{\hbar c} + \frac{E + (-1)^{j+1} mc^2}{\hbar c} D_j \right\} \sin(kL) + F_j k \cos(kL) - G_j k = 0 \tag{18}$$

where

$$D_j = \frac{\sin^2\theta - \cos^2\mu + \cos^2\tau\cos^2\theta}{(\sin\mu + (-1)^j \sin\tau\cos\theta)^2} \qquad F_j = \frac{2\cos\mu}{\sin\mu + (-1)^j \sin\tau\cos\theta}$$

and

$$G_j = \frac{2\sin\theta\cos\gamma}{\sin\mu + (-1)^j \sin\tau\cos\theta} \qquad \text{with } j = 1, 2.$$

The case $j = 1$ corresponds to the eigenvalue equation of $H_{\mathrm{D}}^{(1)}$ and $j = 2$ to $H_{\mathrm{D}}^{(2)}$. For the third family, the energy eigenvalues of $H_{\mathrm{D}}^{(3)}$ are obtained from

$$\cos(kL) = \pm\sin\theta\cos\gamma \tag{19}$$

where the upper sign corresponds to the cases (i) and (ii) and the lower sign to the cases (iii) and (iv).

2.3. Some typical BCs

BCs are frequently referred to spinors in the DR because of its non-relativistic limit. We therefore give several examples involving ψ_{D}, which also belong to $\mathrm{Dom}(H_{\mathrm{w}})$:

(a)

$$\theta = 0 \qquad \mu = \tau = \pi/2 \qquad 0 \leqslant \gamma < 2\pi$$
$$\text{BC}: \qquad \phi(0) = \phi(L) = 0 \in \mathrm{Dom}(H_{\mathrm{D}}^{(2)})$$

(b)

$$\theta = 0 \qquad \mu = \pi/2 \qquad \tau = 3\pi/2 \qquad 0 \leqslant \gamma < 2\pi$$
$$\text{BC}: \qquad \chi(0) = \chi(L) = 0 \in \mathrm{Dom}(H_{\mathrm{D}}^{(1)})$$

(c)

$$\begin{array}{l} \theta = 0 \qquad \mu = \tau = 0, \pi \qquad 0 \leqslant \gamma < 2\pi \\ \text{BC}: \qquad \phi(0) = \chi(L) = 0 \in \mathrm{Dom}(H_{\mathrm{D}}^{(3)}) \end{array}$$

(d)

$$\begin{array}{l} \theta = 0 \qquad \{\mu \neq \tau\} = 0, \pi \qquad 0 \leqslant \gamma < 2\pi \\ \text{BC}: \qquad \phi(L) = \chi(0) = 0 \in \mathrm{Dom}(H_{\mathrm{D}}^{(3)}) \end{array}$$

(e)

$$\begin{array}{l} \theta = 0 \qquad \mu = 0 \qquad \tau = \pi/2 \qquad 0 \leqslant \gamma < 2\pi \\ \text{BC}: \qquad \chi(L) = \mathrm{i}\phi(L) \text{ and } \chi(0) = -\mathrm{i}\phi(0) \in \mathrm{Dom}(H_{\mathrm{D}}^{(1)}) \cap \mathrm{Dom}(H_{\mathrm{D}}^{(2)}) \end{array}$$

(f)

$$\begin{array}{l} \theta = \pi/2 \qquad \mu = \gamma = 0, \pi \qquad \tau = 0, \pi \\ \text{BC}: \qquad \psi_{\mathrm{D}}(0) = \psi_{\mathrm{D}}(L) \in \mathrm{Dom}(H_{\mathrm{D}}^{(3)}) \end{array}$$

(g)

$$\begin{array}{l} \theta = \pi/2 \qquad \{\mu \neq \gamma\} = 0, \pi \qquad \tau = 0, \pi \\ \text{BC}: \qquad \psi_{\mathrm{D}}(0) = -\psi_{\mathrm{D}}(L) \in \mathrm{Dom}(H_{\mathrm{D}}^{(3)}). \end{array}$$

It is worth noting that all these BCs are obtained without making the matrices A_1 and A_2 singular, or those given in (8). On the other hand, the BCs (a)–(e), can be used if we consider the walls of the box as impenetrable barriers, that is, for the current density $j(x) = c\psi_{\mathrm{D}}^{\dagger}\sigma_x\psi_{\mathrm{D}}$ to be zero at the walls of the box. The vanishing of the normal component (to any surface) of the relativistic current density has been used in the MIT bag model of quarks confinement, see, for example, [15]. In $(1+1)$ dimensions this BC is $\pm(-\mathrm{i})\beta\alpha\psi = \psi$, where the minus sign corresponds to $x = 0$ and the plus sign to $x = L$. This BC in the DR is precisely (e).

2.4. Parity and CPT invariance

Let us single out the BCs which are symmetric under space inversion P, and those which are CPT invariant. The Dirac spinor transforms under the discrete transformations P, T, C in the Weyl representation according to

$$\begin{aligned} P\Psi_{\mathrm{w}}(x,t) &= \sigma_x\Psi_{\mathrm{w}}(L-x,t) \\ T\Psi_{\mathrm{w}}(x,t) &= -\sigma_x\overline{\Psi_{\mathrm{w}}(x,-t)} \\ C\Psi_{\mathrm{w}}(x,t) &= \sigma_z\overline{\Psi_{\mathrm{w}}(x,t)} \\ (CPT)\Psi_{\mathrm{w}}(x,t) &= -\sigma_z\Psi_{\mathrm{w}}(L-x,-t) \end{aligned} \tag{20}$$

where $\bar{\Psi}$ is the complex conjugate of Ψ. In order to change from the WR to the DR it is enough to replace $\Psi_{\mathrm{w}} \to \Psi_{\mathrm{D}}$ and $\sigma_x \leftrightarrow \sigma_z$.

If the Hamiltonian in the WR is invariant under the parity transformation we write

$$PH_{\mathrm{w}} = H_{\mathrm{w}}P. \tag{21}$$

Then, the spinor must satisfy $P\psi_{\mathrm{w}} \in \mathrm{Dom}(H_{\mathrm{w}})$, that is, the parity transformed spinor must obey the same BC as ψ_{w} does. Thus, the parameters γ and τ take the values $\gamma = 0$; $\tau = \pi/2$, $3\pi/2$ or $\gamma = \pi$; $\tau = \pi/2$, $3\pi/2$. For a particle confined in a box, $\theta = 0$ and the four-parameter unitary matrix becomes

$$U = \mathrm{e}^{\mathrm{i}(\mu\pm(\pi/2))}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{22}$$

Similarly, in order to obtain a CPT invariant Hamiltonian, we require

$$(CPT)H_{\mathrm{w}} = H_{\mathrm{w}}(CPT). \tag{23}$$

So, $(CPT)\psi_{\mathrm{w}} \in \mathrm{Dom}(H_{\mathrm{w}})$ if $\mu = 0$; $\gamma = 0$, π or $\mu = \pi$; $\gamma = 0, \pi$. In addition, for a particle confined in a box, $\theta = 0$ and

$$U = \pm \begin{pmatrix} \mathrm{e}^{\mathrm{i}\tau} & 0 \\ 0 & -\mathrm{e}^{-\mathrm{i}\tau} \end{pmatrix}. \tag{24}$$

In the DR the corresponding BCs are MIT bag-like which for $\tau = \pi/2$ become

$$\chi(L) = \mp\mathrm{i}\phi(L) \qquad \chi(0) = \pm\mathrm{i}\phi(0). \tag{25}$$

From those BCs given in section 2.3, the cases (a), (b), (e), (f), and (g) are invariant under the parity transformation, but only (e), (f), and (g) are CPT invariant.

3. Non-relativistic limits (NRLs)

As is well known, in the DR the Dirac equation (2) for stationary states is equivalent to the system

$$-\mathrm{i}\hbar c\frac{\mathrm{d}}{\mathrm{d}x}\phi = (E + mc^2)\chi \qquad -\mathrm{i}\hbar c\frac{\mathrm{d}}{\mathrm{d}x}\chi = (E - mc^2)\phi. \tag{26}$$

We achieve the NRL by letting $c \to \infty$. However, the Dirac operator, $H(c) - mc^2$, makes no sense for $c = \infty$. The correct way to analyse the NRL is to look at its resolvent. It has been proved [7, 16] that the NRL of the Dirac resolvent is the resolvent of a Schrödinger or Pauli operator times a projection to the upper components of the Dirac wavefunction. Then, the eigenvalues, $E(c) - mc^2$, are analytic in the parameter $1/c^2$. Likewise, the upper or large component is analytic in $1/c^2$. So, assuming that $\phi(x, c) = \phi(x, -c)$, $\chi(x, c) = -\chi(x, -c)$, and $E(c) = E(-c)$, the functions $\phi(x, -c)$ and $\chi(x, -c)$ satisfy equations (26) with $c \to -c$; consequently, we may write the following expansions in c for $\phi(x, c)$ and $\chi(x, c)$ [17]

$$\begin{aligned} \phi &= \phi_{\mathrm{NR}} + \frac{1}{c^2}\phi_1 + \frac{1}{c^4}\phi_2 + \cdots \\ \chi &= \frac{1}{c}\chi_{\mathrm{NR}} + \frac{1}{c^3}\chi_1 + \frac{1}{c^5}\chi_2 + \cdots \end{aligned} \tag{27}$$

and for the energy

$$E = mc^2 + E_{\mathrm{NR}} + \frac{1}{c^2}E_1 + \frac{1}{c^4}E_2 + \cdots. \tag{28}$$

Substituting relations (27) and (28) in (26) and comparing the terms of the lower order, the following system is obtained:

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\phi_{\mathrm{NR}} + \frac{2m}{\hbar}\chi_{\mathrm{NR}} = 0 \qquad \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\chi_{\mathrm{NR}} + \frac{E_{\mathrm{NR}}}{\hbar}\phi_{\mathrm{NR}} = 0. \tag{29}$$

Eliminating χ_{NR}, we obtain the eigenvalue Schrödinger equation

$$(H_{\mathrm{NR}}\phi_{\mathrm{NR}})(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi_{\mathrm{NR}}(x) = E_{\mathrm{NR}}\phi_{\mathrm{NR}}(x). \tag{30}$$

Here, ϕ_{NR} belongs to the Hilbert space $\mathcal{H}_{\mathrm{NR}} = L^2(\Omega)$, with scalar product denoted by $\langle, \rangle$.

In the NRL, the connection between the components ϕ and χ of the Dirac spinor ψ_{D}, and the Schrödinger eigenfunction ϕ_{NR}, is obtained by keeping only the first term of the expansions (27), and using the first equation of (29), that is

$$\phi \to \phi_{\mathrm{NR}} \qquad \chi \to -\lambda \mathrm{i} \frac{\mathrm{d}}{\mathrm{d}x} \phi_{\mathrm{NR}} \tag{31}$$

where $\lambda = \hbar/(2mc)$. With these relations we may calculate the NRL up to order $1/c$ of any quantum mechanical expression in $(1+1)$ spacetime dimensions, as well as of each relativistic family of self-adjoint extensions.

Let us now consider the operator $H_{\mathrm{D}}^{(1)}$. In the NRL, the matricial BC included in its domain becomes

$$\begin{pmatrix} -\lambda \phi'_{\mathrm{NR}}(L) \\ \lambda \phi'_{\mathrm{NR}}(0) \end{pmatrix} = \mathrm{i} A_1 \begin{pmatrix} \phi_{\mathrm{NR}}(L) \\ \phi_{\mathrm{NR}}(0) \end{pmatrix}$$

where the primes, hereafter, point out differentiation with respect to x. The matrix A_1 is anti-Hermitian, so $\mathrm{i}A_1 = M_1$ is Hermitian.

The first four-parameter family of self-adjoint extensions of the non-relativistic 'free' Hamiltonian operator consists of the operators

$$H_{\mathrm{NR}}^{(1)} \equiv (H_{\mathrm{NR}}^{(1)})_{\theta,\mu,\tau,\gamma} = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{32}$$

with domain

$$\begin{aligned} \mathrm{Dom}(H_{\mathrm{NR}}^{(1)}) = \Bigg\{ & \phi_{\mathrm{NR}} | \phi_{\mathrm{NR}} \in \mathcal{H}_{\mathrm{NR}}, \phi_{\mathrm{NR}} \text{ and } \phi'_{\mathrm{NR}} \text{ a.c. in} \Omega, (H_{\mathrm{NR}}^{(1)} \phi_{\mathrm{NR}}) \in \mathcal{H}_{\mathrm{NR}}, \phi_{\mathrm{NR}} \text{ fulfils} \\ & \begin{pmatrix} -\lambda \phi'_{\mathrm{NR}}(L) \\ \lambda \phi'_{\mathrm{NR}}(0) \end{pmatrix} = M_1 \begin{pmatrix} \phi_{\mathrm{NR}}(L) \\ \phi_{\mathrm{NR}}(0) \end{pmatrix}, M_1 = (M_1)^{\dagger} \Bigg\}. \end{aligned} \tag{33}$$

In appendix B, we obtain, as an example, the NRL of the Hermiticity condition imposed upon the operator $H_{\mathrm{D}}^{(1)}$. This, leads to the Hermiticity condition for the operator $H_{\mathrm{NR}}^{(1)}$.

Analogously, the NRL of the families $H_{\mathrm{D}}^{(2)}$ and $H_{\mathrm{D}}^{(3)}$ lead to the operators $H_{\mathrm{NR}}^{(2)}$ and $H_{\mathrm{NR}}^{(3)}$ respectively, with their domains

$$H_{\mathrm{NR}}^{(2)} \equiv (H_{\mathrm{NR}}^{(2)})_{\theta,\mu,\tau,\gamma} = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{34}$$

$$\begin{aligned} \mathrm{Dom}(H_{\mathrm{NR}}^{(2)}) = \Bigg\{ & \phi_{\mathrm{NR}} | \phi_{\mathrm{NR}} \in \mathcal{H}_{\mathrm{NR}}, \phi_{\mathrm{NR}} \text{ and } \phi'_{\mathrm{NR}} \text{ a.c. in } \Omega, (H_{\mathrm{NR}}^{(2)} \phi_{\mathrm{NR}}) \in \mathcal{H}_{\mathrm{NR}}, \phi_{\mathrm{NR}} \text{ fulfils} \\ & \begin{pmatrix} \phi_{\mathrm{NR}}(L) \\ \phi_{\mathrm{NR}}(0) \end{pmatrix} = M_2 \begin{pmatrix} -\lambda \phi'_{\mathrm{NR}}(L) \\ \lambda \phi'_{\mathrm{NR}}(0) \end{pmatrix}, M_2 = (M_2)^{\dagger} \Bigg\} \end{aligned} \tag{35}$$

where $M_2 = -\mathrm{i}A_2$, and finally

$$H_{\mathrm{NR}}^{(3)} \equiv (H_{\mathrm{NR}}^{(3)})_{\theta,\mu,\tau,\gamma} = -\frac{\hbar^2}{2m} \frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{36}$$

$$\begin{aligned} \mathrm{Dom}(H_{\mathrm{NR}}^{(3)}) = \{ & \phi_{\mathrm{NR}} | \phi_{\mathrm{NR}} \in \mathcal{H}_{\mathrm{NR}}, \phi_{\mathrm{NR}} \text{ and } \phi'_{\mathrm{NR}} \text{ a.c. in } \Omega, (H_{\mathrm{NR}}^{(3)} \phi_{\mathrm{NR}}) \in \mathcal{H}_{\mathrm{NR}}, \phi_{\mathrm{NR}} \\ & \text{fulfils equation (8) with relations (31) for the cases given in (16)} \}. \end{aligned} \tag{37}$$

The energy eigenvalue equations for $H_{\mathrm{HR}}^{(1)}$ and $H_{\mathrm{NR}}^{(2)}$, obtained from the NRL of (18) are given respectively by

$$\{(\lambda k_{\mathrm{NR}})^2 + D_1\} \sin(k_{\mathrm{NR}} L) + F_1 \lambda k_{\mathrm{NR}} \cos(k_{\mathrm{NR}} L) - G_1 \lambda k_{\mathrm{NR}} = 0 \tag{38}$$

$$\{(\lambda k_{\mathrm{NR}})^2 D_2 + 1\} \sin(k_{\mathrm{NR}} L) + F_2 \lambda k_{\mathrm{NR}} \cos(k_{\mathrm{NR}} L) - G_2 \lambda k_{\mathrm{NR}} = 0 \tag{39}$$

with $\hbar k_{\rm NR} = \sqrt{2mE_{\rm NR}}$. Likewise, the energy eigenvalues of $H_{\rm NR}^{(3)}$ are

$$\cos(k_{\rm NR}L) = \pm \sin\theta \cos\gamma \tag{40}$$

where the plus sign corresponds to the cases (i) and (ii) and the minus sign to the cases (iii) and (iv). The transcendental equation for the eigenvalues of $H_{\rm NR}^{(1)}$ is a function $f(k_{\rm NR}) = 0$, similar to that obtained by da Luz and Cheng [1].

The BCs given in the $\mathrm{Dom}(H_{\rm NR}^{(1)})$ are similar to those in the literature [1]. In order to have the most general BC for a non-relativistic 'free' particle inside a box, we have to consider all these three families with domains given by, $\mathrm{Dom}(H_{\rm NR}^{(1)})$, $\mathrm{Dom}(H_{\rm NR}^{(2)})$, and $\mathrm{Dom}(H_{\rm NR}^{(3)})$ [3]. However, it is possible to have only one matricial condition that includes all possible BCs for which the self-adjointness of $H_{\rm NR}$ is maintained. This condition is precisely the NRL of the matricial BC included in $\mathrm{Dom}(H_{\rm w})$.

In fact, this family of four-parameter Hamiltonians is

$$H_{\rm NR} \equiv (H_{\rm NR})_{\theta,\mu,\tau,\gamma} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{41}$$

with domain

$$\begin{aligned}\mathrm{Dom}(H_{\rm NR}) = \Bigg\{&\phi_{\rm NR}|\phi_{\rm NR} \in \mathcal{H}_{\rm NR}, \phi_{\rm NR} \text{ and } \phi'_{\rm NR} \text{ a.c. in } \Omega, (H_{\rm NR}\phi_{\rm NR}) \in \mathcal{H}_{\rm NR}, \phi_{\rm NR} \text{ fulfils} \\ &\begin{pmatrix} \phi_{\rm NR}(L) - \lambda \mathrm{i}\phi'_{\rm NR}(L) \\ \phi_{\rm NR}(0) + \lambda \mathrm{i}\phi'_{\rm NR}(0)\end{pmatrix} = U \begin{pmatrix} \phi_{\rm NR}(L) + \lambda \mathrm{i}\phi'_{\rm NR}(L) \\ \phi_{\rm NR}(0) - \lambda \mathrm{i}\phi'_{\rm NR}(0)\end{pmatrix}, U^{-1} = U^\dagger \Bigg\}\end{aligned} \tag{42}$$

with U given by (5).

All possible BCs for which $H_{\rm NR}$ is self-adjoint are included in $\mathrm{Dom}(H_{\rm NR})$. It is worth noting that, as opposed to the results given in [1], all these BCs are obtained without making infinite the elements of U. The NRLs of the BCs given in section 2.3 are

(a) 'Dirichlet condition'

$$\phi_{\rm NR}(0) = \phi_{\rm NR}(L) = 0 \in \mathrm{Dom}(H_{\rm NR}^{(2)})$$

(b) 'Neumann condition'

$$\phi'_{\rm NR}(0) = \phi'_{\rm NR}(L) = 0 \in \mathrm{Dom}(H_{\rm NR}^{(1)})$$

(c) 'Mixed condition'

$$\phi_{\rm NR}(0) = \phi'_{\rm NR}(L) = 0 \in \mathrm{Dom}(H_{\rm NR}^{(3)})$$

(d) 'Another mixed condition'

$$\phi_{\rm NR}(L) = \phi'_{\rm NR}(0) = 0 \in \mathrm{Dom}(H_{\rm NR}^{(3)})$$

(e) 'NRL in the MIT bag model'

$$-\lambda\phi'_{\rm NR}(L) = \phi_{\rm NR}(L) \text{ and } \lambda\phi'_{\rm NR}(0) = \phi_{\rm NR}(0) \in \mathrm{Dom}(H_{\rm NR}^{(1)}) \cap \mathrm{Dom}(H_{\rm NR}^{(2)})$$

(f) 'Periodic condition'

$$\phi_{\rm NR}(0) = \phi_{\rm NR}(L) \text{ and } \phi'_{\rm NR}(0) = \phi'_{\rm NR}(L) \in \mathrm{Dom}(H_{\rm NR}^{(3)})$$

(g) 'Anti-periodic condition'

$$\phi_{\rm NR}(0) = -\phi_{\rm NR}(L) \text{ and } \phi'_{\rm NR}(0) = -\phi'_{\rm NR}(L) \in \mathrm{Dom}(H_{\rm NR}^{(3)}).$$

Obviously, these BCs represent different physical situations, in fact, (a)–(e) correspond to different definitions of barrier impenetrability and, with them, $j_{\rm NR}$ vanishes at the walls of the box.

4. Conclusions

The most general BCs to be satisfied by the Dirac spinor of a relativistic 'free' particle in a one-dimensional box in the WR, can be given in terms of only one family of self-adjoint extensions of four parameters of the 'free' Dirac Hamiltonian. In order to obtain the NRL, one must change to the DR. However, this procedure leads to three families of self-adjoint extensions for the Hamiltonian; that is to say, there are three types of BC for which the 'free' Hamiltonian of the DR is self-adjoint. Taking the non-relativistic limit of each one of these families, we have obtained three families of self-adjoint extensions for the non-relativistic 'free' Hamiltonian. It is worth stressing that only the three families together provide all possible BCs for a non-relativistic 'free' particle in a one-dimensional box, and that the matrix parameters connecting the spinor components at the walls of the box take only finite values. The corresponding eigenvalue equations depending on four parameters were also obtained, as well as their non-relativistic limits. Since in the WR it is possible to write down all self-adjoiint extensions in a single family, we have written the three previously found non-relativistic families in terms of only one family. Among the infinite BCs for which the Dirac 'free' hamiltonian is self-adjoint, we have singled out those which are invariant under the space inversion P and under the CPT transformation. We emphasize that only the MIT bag model-like BCs remain valid after imposing the CPT invariance.

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Appendix A

According to Von Neumann's theory of deficiency indices, a symmetric operator H has self-adjoint extensions if the solutions $\psi_\pm$ of the eigenvalues problem $H^*\psi_\pm = \pm \mathrm{i}\omega\psi_\pm$, $\omega \in \mathbb{R}$, belong to $\mathcal{H}$, and if the dimensions of the solution spaces $n_\pm$ verify $n_+ = n_- \neq 0$. In our case, it is not difficult to check that $n_+ = n_- = 2$. Therefore, there exist families of $2^2 = 4$ parameters of self-adjoint extensions.

Without using the machinery of Von Neumann's theory of self-adjoint extensions of symmetric operators [2], and without intending to be rigorous, let us briefly consider the construction of a self-adjoint operator from the formal Hamiltonian

$$H_\mathrm{w} = -\mathrm{i}\hbar c\sigma_z \frac{\mathrm{d}}{\mathrm{d}x} + mc^2\sigma_x \tag{A1}$$

whose dense domain may be written as

$$\mathrm{Dom}(H_\mathrm{w}) = \left\{ \psi_\mathrm{w} = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \middle| \psi_\mathrm{w} \in \mathcal{H}, \text{a.c. in } \Omega, (H_\mathrm{w}\psi_\mathrm{w}) \in \mathcal{H}, \text{with } \psi_\mathrm{w}(0) = \psi_\mathrm{w}(L) = 0 \right\}. \tag{A2}$$

With the BC $\psi_\mathrm{w}(0) = \psi_\mathrm{w}(L) = 0$, H_w is certainly a Hermitian operator, that is, for all $\zeta, \eta \in \mathrm{Dom}(H_\mathrm{w})$

$$\langle H_\mathrm{w}\zeta, \eta\rangle - \langle\zeta, H_\mathrm{w}\eta\rangle = \mathrm{i}\hbar c[(\zeta^\dagger\sigma_z\eta)(L) - (\zeta^\dagger\sigma_z\eta)(0)] = 0 \tag{A3}$$

and since $\mathrm{Dom}(H_\mathrm{w})$ is dense, H_w is a symmetric operator. Nevertheless, its eigenvalue equation has only the trivial solution $\psi_\mathrm{w} = 0$. This suggests that the BC on the wavefunctions in $\mathrm{Dom}(H_\mathrm{w})$ are too restrictive.

Then, it is necessary to extend the set of functions in $\mathrm{Dom}(H_\mathrm{w})$ by allowing more general BCs. A wider and simple domain of functions is obtained just by requiring $\psi_\mathrm{w}(0) = \psi_\mathrm{w}(L)$. With this BC the eigenvalue equation of H_w now has non-trivial solutions, and as we have seen in section 2.3, H_w with this BC is one of the infinite self-adjoint extensions of the initial symmetric operator (A1).

On the other hand, the quantum dynamics requires that H_w be a self-adjoint operator. For this it is necessary that $\mathrm{Dom}(H_\mathrm{w}) = \mathrm{Dom}(H_\mathrm{w}^*)$, where H_w^*, defined by the same formal operator (A1) is the adjoint of the differential operator H_w. Its domain is defined as [2]

$$\mathrm{Dom}(H_\mathrm{w}^*) = \left\{ \nu = \begin{pmatrix} \nu_1 \\ \nu_2 \end{pmatrix} \middle| \nu \in \mathcal{H}, \text{a.c. in } \Omega, (H_\mathrm{w}^*\nu) \in \mathcal{H} \right\}$$

with

$$\langle H_\mathrm{w}\zeta, \nu\rangle - \langle \zeta, H_\mathrm{w}^*\nu\rangle = \mathrm{i}\hbar c[(\zeta^\dagger\sigma_z\nu)(L) - (\zeta^\dagger\sigma_z\nu)(0)] = 0 \tag{A4}$$

for all

$$\zeta = \begin{pmatrix} \zeta_1 \\ \zeta_2 \end{pmatrix} \in \mathrm{Dom}(H_\mathrm{w}) \qquad \text{and} \qquad \nu = \begin{pmatrix} \nu_1 \\ \nu_2 \end{pmatrix} \in \mathrm{Dom}(H_\mathrm{w}^*).$$

Here, $\mathrm{Dom}(H_\mathrm{w}) \subseteq \mathrm{Dom}(H_\mathrm{w}^*)$. Now the problem is choosing a sufficiently general set of boundary conditions for which $\mathrm{Dom}(H_\mathrm{w}) = \mathrm{Dom}(H_\mathrm{w}^*)$. If $\mathrm{Dom}(H_\mathrm{w})$ is fixed, H_w^* will be the adjoint of H_w if it has the maximal domain consistent with the vanishing of $(\zeta^\dagger\sigma_z\nu)(L) - (\zeta^\dagger\sigma_z\nu)(0)$, for all $\zeta \in \mathrm{Dom}(H_\mathrm{w})$.

In order to enlarge the initial domain of H_w, let us consider a pair of sufficiently general linear relations among $\zeta_1(0)$, $\zeta_1(L)$, $\zeta_2(0)$, $\zeta_2(L)$

$$N_1 \begin{pmatrix} \zeta_1(L) \\ \zeta_2(0) \end{pmatrix} = N_2 \begin{pmatrix} \zeta_2(L) \\ \zeta_1(0) \end{pmatrix} \tag{A5}$$

where N_1 and N_2 are matrices with complex elements.

If both determinants do not vanish, we write

$$\begin{pmatrix} \zeta_1(L) \\ \zeta_2(0) \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \zeta_2(L) \\ \zeta_1(0) \end{pmatrix}. \tag{A6}$$

If $\det N_1 = \det N_2 = 0$, without loss of generality we can write

$$\begin{pmatrix} 0 & 0 \\ \delta_1 & \delta_2 \end{pmatrix} \begin{pmatrix} \zeta_1(L) \\ \zeta_2(0) \end{pmatrix} = \begin{pmatrix} \delta_3 & \delta_4 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \zeta_2(L) \\ \zeta_1(0) \end{pmatrix} \tag{A7}$$

with δ_1, δ_2, δ_3, δ_4 being non-zero complex numbers. Nevertheless, with this BC H_w must be a symmetric operator, and this implies that all δ_i must be zero, so, $\zeta_1(L)$ and $\zeta_2(0)$ are 'independent', as well as $\zeta_2(L)$ and $\zeta_1(0)$.

Thus, by replacing the relation (A6) in (A4) it may be verified that a necessary and sufficient condition for the vanishing of $(\zeta^\dagger\sigma_z\nu)(L) - (\zeta^\dagger\sigma_z\nu)(0)$ is

$$\begin{pmatrix} \nu_2(L) \\ \nu_1(0) \end{pmatrix} = \begin{pmatrix} \bar{a} & \bar{c} \\ \bar{b} & \bar{d} \end{pmatrix} \begin{pmatrix} \nu_1(L) \\ \nu_2(0) \end{pmatrix}. \tag{A8}$$

To make sure that $\mathrm{Dom}(H_\mathrm{w}) = \mathrm{Dom}(H_\mathrm{w}^*)$, this condition must be equivalent to (A6) and this is satisfied if

$$a\bar{a} + c\bar{c} = 1 \qquad b\bar{b} + d\bar{d} = 1 \qquad a\bar{b} + c\bar{d} = 0. \tag{A9}$$

These relations imply that the matrix in (A6) is unitary, so it has an inverse. Its general form depends on four parameters.

In this way the chosen family of self-adjoint extensions of H_w is the most general one and consists of the operators $(H_\mathrm{w})_{\theta,\mu,\tau,\gamma}$ given by (3) acting on the domain given by (4).

Appendix B

The relativistic formal Hamiltonian $H_{\mathrm{D}}^{(1)}$ in the DR is a Hermitian operator, and therefore satisfies the condition

$$\langle H_{\mathrm{D}}^{(1)}\zeta,\eta\rangle - \langle\zeta, H_{\mathrm{D}}^{(1)}\eta\rangle = \mathrm{i}\hbar c[(\zeta^{\dagger}\sigma_x\eta)(L) - (\zeta^{\dagger}\sigma_x\eta)(0)] = 0 \qquad \text{(B1)}$$

for all ζ and η in the domain of $H_{\mathrm{D}}^{(1)}$. Taking the NRL of the right-hand side term in (B1), that is, making

$$\zeta = \begin{pmatrix}\zeta_l\\ \zeta_s\end{pmatrix} \to \begin{pmatrix}\zeta_{\mathrm{NR}}\\ -\mathrm{i}\lambda\zeta'_{\mathrm{NR}}\end{pmatrix} \qquad \text{and} \qquad \eta = \begin{pmatrix}\eta_l\\ \eta_s\end{pmatrix} \to \begin{pmatrix}\eta_{\mathrm{NR}}\\ -\mathrm{i}\lambda\eta'_{\mathrm{NR}}\end{pmatrix}$$

one obtains

$$-\frac{\hbar^2}{2m}\left[(\overline{\zeta'_{\mathrm{NR}}}\eta_{\mathrm{NR}} - \overline{\zeta_{\mathrm{NR}}}\eta'_{\mathrm{NR}})(L) - (\overline{\zeta'_{\mathrm{NR}}}\eta_{\mathrm{NR}} - \overline{\zeta_{\mathrm{NR}}}\eta'_{\mathrm{NR}})(0)\right] = 0. \qquad \text{(B2)}$$

This last relation is precisely $\langle H_{\mathrm{NR}}^{(1)}\zeta_{\mathrm{NR}},\eta_{\mathrm{NR}}\rangle - \langle\zeta_{\mathrm{NR}}, H_{\mathrm{NR}}^{(1)}\eta_{\mathrm{NR}}\rangle = 0$, that is, $H_{\mathrm{NR}}^{(1)}$ is Hermitian. Relation (B2) is valid for all ζ_{NR} and η_{NR} in the domain of $H_{\mathrm{NR}}^{(1)}$.

Likewise, the NRL of the current density in the DR, $j(x) = c\psi_{\mathrm{D}}^{\dagger}\sigma_x\psi_{\mathrm{D}}$, yields

$$j_{\mathrm{NR}}(x) = -\frac{\hbar}{2\mathrm{i}m}\left(\overline{\phi'_{\mathrm{NR}}}\phi_{\mathrm{NR}} - \overline{\phi_{\mathrm{NR}}}\phi'_{\mathrm{NR}}\right).$$

Certainly, we can extend this procedure to the operator $H_{\mathrm{D}}^{(1)*}$, in order to obtain the corresponding domain of the operator

$$H_{\mathrm{NR}}^{(1)*} = -\frac{\hbar}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}.$$

Its domain is

$$\mathrm{Dom}(H_{\mathrm{NR}}^{(1)*}) = \{\nu_{\mathrm{NR}} | \nu_{\mathrm{NR}} \in \mathcal{H}_{\mathrm{NR}}, \text{a.c. in } \Omega, (H_{\mathrm{NR}}^{(1)*}\nu_{\mathrm{NR}}) \in \mathcal{H}_{\mathrm{NR}}\}$$

with

$$\langle H_{\mathrm{NR}}^{(1)}\zeta_{\mathrm{NR}},\nu_{\mathrm{NR}}\rangle - \langle\zeta_{\mathrm{NR}}, H_{\mathrm{NR}}^{(1)*}\nu_{\mathrm{NR}}\rangle = 0 \qquad \text{(B3)}$$

for all $\zeta_{\mathrm{NR}} \in \mathrm{Dom}(H_{\mathrm{NR}}^{(1)})$ and $\nu_{\mathrm{NR}} \in \mathrm{Dom}(H_{\mathrm{NR}}^{(1)*})$.

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