

General boundary conditions for a Dirac particle in a box*

*Vidal Alonso** and Salvatore De Vincenzo*

*Escuela de Física, Facultad de Ciencias, Universidad Central de Venezuela,
Apartado 47145. Caracas 1041-A, Venezuela.*

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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 subfamilies in the Dirac representation. The energy eigenvalues as well as the corresponding non-relativistic limits of all these results are obtained.

Key words: Boundary conditions; Dirac particle; quantum mechanics; Weyl representation.

Condiciones de fronteras más generales para una partícula de Dirac en una caja

Resumen

Se discuten las condiciones de frontera (BC) relativísticas más generales para una partícula “libre” de Dirac en una caja unidimensional. Se verifica que en la representación de Weyl existe sólo una familia de BC, representadas por cuatro parámetros. Esta familia se divide en tres subfamilias en la representación de Dirac. Se obtienen los autovalores de la energía así como los correspondientes límites no-relativísticos.

Palabras clave: Condiciones de frontera; mecánica cuántica; partícula de Dirac; representación de Weyl.

1. Introduction

A “free” particle in a one-dimensional box is certainly the canonical example of elementary non-relativistic quantum mechanics. Recently, at least in the physical literature (1), the boundary conditions (BCs) that forces the energy eigenfunctions to vanish at the walls of the box were generalized to a 4-

parameters family of BCs for which the Schrödinger “free” hamiltonian is self-adjoint. These authors claim that this family of BCs is the most general one for a particle in a box. However, by using von Neumann's theory of self-adjoint extensions of symmetric operators, as is exposed for example in (2), it was shown (3) that maintaining the column vectors of the BC that relate linearly

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** To whom correspondence should be addressed. E-mail: valonso@tierra.ciens.ucv.ve

the wave function and its derivatives at the wall of the box, there are three inequivalent families of self-adjoint extensions one of which is that of reference (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 note, 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), which 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 by itself 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 a finite radius (5, 6).

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 were a particle with a changing mass that becomes infinite out of the box, so avoiding the Klein paradox (8).

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 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 BCs (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 (4).

In section 2, we write in the WR the self-adjoint extensions of the hamiltonian of a "free" Dirac particle in a one-dimensional box. 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.

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

$$(H\psi)(x) = \left(-i\hbar c\alpha \frac{d}{dx} + c^2\beta \right) \psi(x) = E\psi(x) \quad [1]$$

where ψ denotes a two-components spinor depending upon $x \in \Omega = [0, L]$. In the DR: $\alpha = \sigma_x$ and $\beta = \sigma_z$. In the WR: $\alpha = \sigma_z$ and $\beta = \sigma_x$.

The spinors $\psi(x)$ and $(H\psi)(x)$ belong to a dense proper subset of the Hilbert space

$H = L^2(\Omega) \oplus L^2(\Omega)$, with a scalar product denoted by \langle, \rangle . The domains of H and its adjoint H^* verify $Dom(H) \subseteq Dom(H^*)$; but H must be self-adjoint, so, we look for self-adjoint extensions of the symmetric operator H .

In the DR, $\psi_D(x) = \begin{pmatrix} \phi(x) \\ \chi(x) \end{pmatrix}$, in the WR we

write: $\psi_w(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \end{pmatrix}$. In order to change representation, we use the transformation: $\phi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$ and $\chi = \frac{1}{\sqrt{2}}(\psi_1 - \psi_2)$.

2.1. Self-adjoint extensions in the WR

In this representation there exists a four-parameters family of self-adjoint extensions of the formal hamiltonian operator $H_w \equiv (H_w)_{\theta, \mu, \tau, \gamma}$

$$(H_w)_{\theta, \mu, \tau, \gamma} = -i\hbar c \sigma_z \frac{d}{dx} + mc^2 \sigma_x \quad [2]$$

with domain given by (10, 12-14)

$$Dom(H_w) = \left\{ \psi_w = \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \mid \psi_w \in H, \text{ a.c. in } \Omega, \right. \\ \left. (H_w \psi_w) \in H, \psi_w \text{ fulfils:} \right. \\ \left. \begin{pmatrix} \psi_1(L) \\ \psi_2(0) \end{pmatrix} = U \begin{pmatrix} \psi_2(L) \\ \psi_1(0) \end{pmatrix}, U^{-1} = U^\dagger \right\} \quad [3]$$

where hereafter a.c. means absolutely continuous functions and the symbol “†” denotes the adjoint of a vector or a matrix. The unitary matrix U may be written as:

$$U = \begin{pmatrix} v & u \\ s & w \end{pmatrix} \quad [4]$$

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

Let us also point out that the same four-parameters family of self-adjoint exten-

sions is valid when a bounded potential is present inside the box.

It can be shown that for every spinor $\psi_w \in Dom(H_w)$, the current density $j(x) = c\psi_w^\dagger \sigma_z \psi_w$ 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 the WR the general solution of [1] can be written as

$$y_w = c_1 \begin{pmatrix} 1 \\ \frac{E - \hbar ck}{mc^2} \end{pmatrix} e^{ikx} + c_2 \begin{pmatrix} E - \hbar ck \\ mc^2 \end{pmatrix} e^{-ikx} \quad [5]$$

where $k = \frac{\sqrt{E^2 - (mc^2)^2}}{\hbar c}$ and c_1, c_2 are arbitrary complex constants. The transcendental equation for the energy eigenvalues is

$$\cos(\mu - kL) - \left(\frac{E - \hbar ck}{mc^2} \right)^2 \cos(\mu + kL) - \\ \left[1 - \left(\frac{E - \hbar ck}{mc^2} \right)^2 \right] \cos\gamma \sin\theta + \\ 2 \left(\frac{E - \hbar ck}{mc^2} \right) \sin\tau \cos\theta \sin(kL) = 0 \quad [6]$$

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 domain given in [3], and using the transformation from the WR to DR we have

$$\begin{pmatrix} 1+v & u \\ s & 1+w \end{pmatrix} \begin{pmatrix} -\chi(L) \\ \chi(0) \end{pmatrix} = \begin{pmatrix} 1-v & -u \\ -s & 1-w \end{pmatrix} \begin{pmatrix} \phi(L) \\ \phi(0) \end{pmatrix} \quad [7]$$

Then, three families of self-adjoint extensions of H_D are obtained. Firstly

$$H_D^{(1)} \equiv (H_D^{(1)})_{\theta, \mu, \tau, \gamma} = -i\hbar c \sigma_x \frac{d}{dx} + mc^2 \sigma_z \quad [8]$$

whose domain can be written as

$$\begin{aligned}
 \text{Dom}(H_D^{(1)}) &= \left\{ \psi_D = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \mid \psi_D \in H, \text{ a.c. in } \Omega, \right. \\
 &\quad \left. (H_D^{(1)} \psi_D) \in H, \psi_D \text{ fulfils:} \right. \\
 &\quad \left. \begin{pmatrix} -\chi(L) \\ \chi(0) \end{pmatrix} = A_1 \begin{pmatrix} \phi(L) \\ \phi(0) \end{pmatrix}, A_1 = -(A_1)^\dagger \right\} \quad [9]
 \end{aligned}$$

where

$$\begin{aligned}
 A_1 &= i(\sin \mu - \sin \tau \cos \theta)^{-1} \\
 &\begin{pmatrix} \cos \mu - \cos \tau \cos \theta & -e^{-\tau} \sin \theta \\ -e^{-\tau} \sin \theta & \cos \mu + \cos \tau \cos \theta \end{pmatrix} \\
 &\hspace{15em} [10]
 \end{aligned}$$

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

Likewise

$$H_D^{(2)} \equiv (H_D^{(2)})_{\theta, \mu, \tau, \gamma} = -i\hbar c \sigma_x \frac{d}{dx} + mc^2 \sigma_z \quad [11]$$

acting on the domain

$$\begin{aligned}
 \text{Dom}(H_D^{(2)}) &= \left\{ \psi_D = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \mid \psi_D \in H, \text{ a.c. in } \Omega, \right. \\
 &\quad \left. (H_D^{(2)} \psi_D) \in H, \psi_D \text{ fulfils:} \right. \\
 &\quad \left. \begin{pmatrix} \phi(L) \\ \phi(0) \end{pmatrix} = A_2 \begin{pmatrix} -\chi(L) \\ \chi(0) \end{pmatrix}, A_2 = -(A_2)^\dagger \right\} \\
 &\hspace{15em} [12]
 \end{aligned}$$

where

$$\begin{aligned}
 A_{21} &= i(\sin \mu + \sin \tau \cos \theta)^{-1} \\
 &\begin{pmatrix} \cos \mu + \cos \tau \cos \theta & e^{-\tau} \sin \theta \\ e^{-\tau} \sin \theta & \cos \mu - \cos \tau \cos \theta \end{pmatrix} \\
 &\hspace{15em} [13]
 \end{aligned}$$

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

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 [7]. It can be shown that all BCs in this new family are obtained from [7], 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 $0 \leq \theta < \pi$, but $\theta \neq \frac{\pi}{2}$, and $0 \leq \gamma < 2\pi$. If $\theta = \frac{\pi}{2}$ then $\mu = 0, \pi$ and $0 \leq \tau < 2\pi$. We write this family as

$$H_D^{(3)} \equiv (H_D^{(3)})_{\theta, \mu, \tau, \gamma} = -i\hbar c \sigma_x \frac{d}{dx} + mc^2 \sigma_z \quad [14]$$

with the domain given by

$$\begin{aligned}
 \text{Dom}(H_D^{(3)}) &= \left\{ \psi_D = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \mid \psi_D \in H, \text{ a.c. in } \Omega, \right. \\
 &\quad \left. (H_D^{(3)} \psi_D) \in H, \psi_D \text{ fulfils equation} \right. \\
 &\quad \left. [7] \text{ with the following cases:} \right. \\
 &\quad \text{i) } \mu = 0, \tau = 0, \text{ ii) } \mu = 0, \tau = \pi, \\
 &\quad \text{iii) } \mu = \pi, \tau = 0, \text{ and} \\
 &\quad \text{iv) } \mu = \pi, \tau = \pi; \text{ whith } \theta \neq \frac{\pi}{2}. \text{ If } \theta = \frac{\pi}{2} \\
 &\quad \left. \text{then } \mu = 0, \pi \text{ and } 0 \leq \tau < 2\pi \right\} \quad [15]
 \end{aligned}$$

In the DR we have three energy eigenvalues equations, one for each hamiltonian operator $H_D^{(1)}, H_D^{(2)}, H_D^{(3)}$. The general solution may be written as

$$\psi_D = d_1 \begin{pmatrix} \sqrt{E + mc^2} \\ \sqrt{E - mc^2} \end{pmatrix} e^{ikx} + d_2 \begin{pmatrix} \sqrt{E - mc^2} \\ -\sqrt{E + mc^2} \end{pmatrix} e^{-ikx} \quad [16]$$

with d_1, d_2 arbitrary complex constants. The eigenvalues equations are

$$\begin{aligned}
 &\left\{ \frac{E + (-1)^j mc^2}{\hbar c} + \frac{E + (-1)^{j-1} mc^2}{\hbar c} D_j \right\} \sin(kL) + \\
 &F_j k \cos(kL) - G_j k = 0 \quad [17]
 \end{aligned}$$

$$\text{where } D_j = \frac{\sin^2 \theta - \cos^2 \mu + \cos^2 \tau \cos^2 \gamma}{(\sin \mu + (-1)^j \sin \tau \cos \theta)^2},$$

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

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

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

$$\cos(kL) = \pm \sin \theta \cos \gamma \quad [18]$$

where the upper sign corresponds to the cases i) and ii) and the lower sign to the cases iii) and iv), for all θ .

2.3. Some typical BCs

BCs are frequently referred to spinors in the DR because of its non-relativistic limit. So, we give several examples of them involving ψ_D that also belong to $Dom(H_w)$

- a) $\theta = 0 \quad \mu = \tau = \frac{\pi}{2} \quad 0 \leq \gamma < 2\pi$
BC: $\phi(0) = \phi(L) = 0 \in Dom(H_D^{(2)})$
- b) $\theta = 0 \quad \mu = \frac{\pi}{2} \quad \tau = \frac{3\pi}{2} \quad 0 \leq \gamma < 2\pi$
BC: $\chi(0) = \chi(L) = 0 \in Dom(H_D^{(1)})$
- c) $\theta = 0 \quad \mu = \tau = 0, \pi \quad 0 \leq \gamma < 2\pi$
BC: $\phi(0) = \chi(L) = 0 \in Dom(H_D^{(3)})$
- d) $\theta = 0 \quad \mu = 0 \quad \tau = \frac{\pi}{2} \quad 0 \leq \gamma < 2\pi$
BC: $\chi(L) = \psi(L)$ and $\chi(0) = \psi(0) \in Dom(H_D^{(1)}) \cap Dom(H_D^{(2)})$
- e) $\theta = \frac{\pi}{2} \quad \mu = \gamma = 0, \pi$
BC: $\psi_D(0) = \psi_D(L) \in Dom(H_D^{(3)})$

The BCs a), b), c), and d), can be used if we consider the walls of the box as impenetrable barriers, that is, for the current density: $j(x) = c\psi_D^\dagger \sigma_x \psi_D$ to be zero at the walls of the box. The vanishing of the normal component (to any surface) of the relativistic cur-

rent density, has been used in the MIT bag model of quarks confinement, see, e.g. [15]. In 1 + 1 dimensions this BC is: $\pm(-i)\beta\alpha\psi = \psi$, where the minus sign corresponds to $x = 0$ and the plus sign to $x = L$. This BC in the DR is precisely d).

3. Non-relativistic limits (NRLs)

As is well known, in the DR the Dirac equation [1] for stationary states is equivalent to the system.

$$-i\hbar c \frac{d}{dx} \phi = (E + mc^2)\chi$$

$$-i\hbar c \frac{d}{dx} \chi = (E + mc^2)\phi \quad [19]$$

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 eqns. [19] with $c \rightarrow -c$; consequently we may write the following expansions in c for $\phi(x, c)$ and $\chi(x, c)$ (16)

$$\phi = \phi_{NR} + \frac{1}{c^2} \phi_1 + \frac{1}{c^4} \phi_2 + \dots$$

$$\chi = \frac{1}{c} \chi_{NR} + \frac{1}{c^3} \chi_1 + \frac{1}{c^5} \chi_2 + \dots \quad [20]$$

and for the energy

$$E = mc^2 + E_{NR} + \frac{1}{c^2} E_1 + \frac{1}{c^4} E_2 + \dots \quad [21]$$

Substituting relations [20] and [21] in [19] and comparing the terms of lower order, the following system is obtained

$$i \frac{d}{dx} \phi_{NR} + \frac{2m}{\hbar} \chi_{NR} = 0$$

$$i \frac{d}{dx} \chi_{NR} + \frac{E_{NR}}{\hbar} \phi_{NR} = 0 \quad [22]$$

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

$$(H_{NR} \phi_{NR})(x) = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \phi_{NR}(x) = E_{NR} \phi_{NR}(x) [23]$$

Here, ϕ_{NR} belongs to the Hilbert space $H_{NR} = L^2(\Omega)$ 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 [20], and using the first equation of [22], that is

$$\phi \rightarrow \phi_{NR}$$

$$\chi \rightarrow -\lambda i \frac{d}{dx} \phi_{NR} \quad [24]$$

where: $\lambda = \frac{\hbar}{2mc}$

Let us now consider the operator $H_D^{(1)}$. In the NRL, the matricial BC included in its domain becomes: $\begin{pmatrix} -\lambda \phi'_{NR}(L) \\ \lambda \phi'_{NR}(0) \end{pmatrix} = iA_1 \begin{pmatrix} \phi_{NR}(L) \\ \phi_{NR}(0) \end{pmatrix}$ where the primes, hereafter, point out differentiation with respect to x . The matrix A_1 is anti-hermitian, then $iA_1 = M_1$ is hermitian.

The first four-parameters family of self-adjoint extensions of the non-relativistic "free" hamiltonian operator consists of the operators

$$H_{NR}^{(1)} \equiv (H_{NR}^{(1)})_{\theta, \mu, \tau, \gamma} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \quad [25]$$

with domain

$$\begin{aligned} Dom(H_{NR}^{(1)}) = \{ & \phi_{NR} \mid \phi_{NR} \in H_{NR}, \phi_{NR} \text{ and } \phi'_{NR} \\ & \text{a.c. in } \Omega, (H_{NR}^{(1)} \phi_{NR}) \in H_{NR}, \\ & \phi_{NR} \text{ fulfils:} \\ & \begin{pmatrix} -\lambda \phi'_{NR}(L) \\ \lambda \phi'_{NR}(0) \end{pmatrix} = M_1 \begin{pmatrix} \phi_{NR}(L) \\ \phi_{NR}(0) \end{pmatrix}, \\ & M_1 = (M_1)^\dagger \} \quad [26] \end{aligned}$$

Analogously, the NRL of the families: $H_D^{(2)}$ and $H_D^{(3)}$, lead respectively the operators $H_{NR}^{(2)}$ and $H_{NR}^{(3)}$, with their domains

$$H_{NR}^{(2)} \equiv (H_{NR}^{(2)})_{\theta, \mu, \tau, \gamma} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \quad [27]$$

$$\begin{aligned} Dom(H_{NR}^{(2)}) = \{ & \phi_{NR} \mid \phi_{NR} \in H_{NR}, \phi_{NR} \text{ and } \phi'_{NR} \\ & \text{a.c. in } \Omega, (H_{NR}^{(2)} \phi_{NR}) \in H_{NR}, \\ & \phi_{NR} \text{ fulfils:} \\ & \begin{pmatrix} \phi_{NR}(L) \\ \phi_{NR}(0) \end{pmatrix} = M_2 \begin{pmatrix} -\lambda \phi'_{NR}(L) \\ \lambda \phi'_{NR}(0) \end{pmatrix}, \\ & M_2 = (M_2)^\dagger \} \quad [28] \end{aligned}$$

where $M_2 = -iA_2$, and finally

$$H_{NR}^{(3)} \equiv (H_{NR}^{(3)})_{\theta, \mu, \tau, \gamma} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \quad [29]$$

$$\begin{aligned} Dom(H_{NR}^{(3)}) = \{ & \phi_{NR} \mid \phi_{NR} \in H_{NR}, \phi_{NR} \text{ and } \phi'_{NR} \\ & \text{a.c. in } \Omega, (H_{NR}^{(3)} \phi_{NR}) \in H_{NR}, \\ & \phi_{NR} \text{ fulfils: equation [7] with} \\ & \text{relations [24] for the cases} \\ & \text{given in [15]} \} \quad [30] \end{aligned}$$

The energy eigenvalues equations for $H_D^{(1)}$ and $H_D^{(2)}$, obtained from the NRL of [17] are respectively given by

$$\begin{aligned} \{ & (\lambda k_{NR})^2 + D_1 \} \sin(k_{NR}L) + F_1 \lambda k_{NR} \cos(k_{NR}L) \\ & -G_1 \lambda k_{NR} = 0 \quad [31] \end{aligned}$$

$$\begin{aligned} \{ & (\lambda k_{NR})^2 + D_2 + 1 \} \sin(k_{NR}L) + F_2 \lambda k_{NR} \cos(k_{NR}L) \\ & -G_2 \lambda k_{NR} = 0 \quad [32] \end{aligned}$$

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

$$\cos(k_{NR}L) = \pm \sin \theta \cos \gamma \quad [33]$$

for the cases given in [18]. The transcendental equation for the eigenvalues of $H_D^{(1)}$ is a

function $f(k_{NR}) = 0$, similar to that obtained by da Luz and Cheng (1).

The BC given in the $Dom(H_D^{(1)})$ are similar to those known 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: $Dom(H_D^{(1)})$, $Dom(H_D^{(2)})$ and $Dom(H_D^{(3)})$ (3). However, it is possible to have only one matricial condition that includes all possible BC for which the self-adjointness of H_{NR} is maintained. This condition is precisely the NRL of the matricial BC included in $Dom(H_w)$.

In fact, this family of four-parameters hamiltonians is

$$H_{NR} \equiv (H_{NR})_{\theta, \mu, \tau, \gamma} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \quad [34]$$

with domain

$$\begin{aligned} Dom(H_{NR}) = \{ & \phi_{NR} \mid \phi_{NR} \in H_{NR}, \phi_{NR} \text{ and } \phi'_{NR} \\ & \text{a.c. in } \Omega, (H_{NR} \phi_{NR}) \in H_{NR}, \\ & \phi_{NR} \text{ fulfils:} \\ & \begin{pmatrix} \phi_{NR}(L) - \lambda i \phi'_{NR}(L) \\ \phi_{NR}(0) + \lambda i \phi'_{NR}(0) \end{pmatrix} = \\ & U \begin{pmatrix} \phi_{NR}(L) + \lambda i \phi'_{NR}(L) \\ \phi_{NR}(0) - \lambda i \phi'_{NR}(0) \end{pmatrix}, U^{-1} = U^\dagger \} \end{aligned} \quad [35]$$

with U given by [4].

All possible BC for which H_{NR} is self-adjoint, are included in $Dom(H_{NR})$. It is worth to note that, as opposed to the results given in references (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”
 $\phi_{NR}(0) = \phi_{NR}(L) = 0 \in Dom(H_{NR}^{(2)})$
- b) “Neumann condition”
 $\phi'_{NR}(0) = \phi'_{NR}(L) = 0 \in Dom(H_{NR}^{(1)})$

- c) “Mixed condition”
 $\phi_{NR}(0) = \phi'_{NR}(L) = 0 \in Dom(H_{NR}^{(3)})$
- d) “NRL in the MIT bag model”
 $-\lambda \phi'_{NR}(L) = \phi_{NR}(L) \text{ and } \lambda \phi'_{NR}(0) = \phi_{NR}(0) \\ \in Dom(H_{NR}^{(1)}) \cap Dom(H_{NR}^{(2)})$
- e) “Periodic condition”
 $\phi_{NR}(0) = \phi_{NR}(L) \text{ and } \phi'_{NR}(0) = \phi'_{NR}(L) \\ \in Dom(H_{NR}^{(3)})$

Obviously, these BC represent different physical situations, in fact, a), b), c), d) and e) correspond to different definitions of barrier impenetrability, with them, j_{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 NRLs, 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 BCs 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 eigenvalues equations depending on four-parameters were also obtained, as well as their non-relativistic limits. Since in the WR it was possible to write down all self-adjoint extensions in a single family, we have written the three previously found non-relativistic families in terms of only one family.

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