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On the boundary conditions for the Dirac equation

Vidal Alonso†, Salvatore De Vincenzo‡ and Luigi Mondino§

Escuela de Física y Matemáticas, Facultad de Ciencias, Universidad Central de Venezuela, AP 47399, Caracas 1041-A, Venezuela

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Abstract. A relativistic 'free' particle in a one-dimensional box is studied. The impossibility of the wavefunction vanishing completely at the walls of the box is proven. Various physically acceptable boundary conditions that allow non-trivial solutions for this problem are proposed. The non-relativistic limits of these results are obtained. The problem of a particle in a spherical box, which presents the same type of difficulties as the one-dimensional problem, is also considered.

Resumen. Se considera el problema de una partícula 'libre' relativista en una caja unidimensional. Se comprueba la imposibilidad de anular completamente la función de onda en las paredes de la caja. Se proponen diversas condiciones de frontera físicamente aceptables que permiten encontrar soluciones no triviales para este problema. Se discute el límite no relativista de estos resultados. También consideramos el problema de una partícula en una caja esférica, el cual presenta el mismo tipo de dificultades que el problema unidimensional.

1. Introduction

In non-relativistic quantum mechanics a vanishing normal component of the probability current is a sufficient condition to obtain an impenetrable boundary surface. This might be accomplished by imposing Dirichlet, Neumann or mixed boundary conditions upon the wavefunction. In the well known problem that we all learn in elementary quantum mechanics, the 'free' particle in a one-dimensional box, the Dirichlet boundary condition, $\psi = 0$, is the simplest one. With this boundary condition the formal 'free Schrödinger Hamiltonian' is a well defined self-adjoint operator. However, besides the above boundary condition, there exists a family of self-adjoint extensions each labelled by four parameters [1, 2].

In relativistic quantum mechanics the wavefunction is a spinor of four complex components, which are coupled in a system of first-order differential equations. Imposing the Dirichlet condition at the boundary is too restrictive; it leads to incompatibility in the relativistic scattering [3] as well as in the energy eigenvalues problem, as will be shown below. However, non-trivial solutions may be obtained by using appropriate boundary conditions for the wavefunction [4, 5], in such a way that self-adjointness of the formal Dirac operator is maintained.

† E-mail address: valonso@tierra.ciens.ucv.ve
‡ E-mail address: svincenz@tierra.ciens.ucv.ve
§ E-mail address: lmondino@tierra.ciens.ucv.ve

According to the principles of quantum mechanics, for each quantum mechanical system one defines a Hilbert space $\mathcal{H}$. Every measurable quantity is called an 'observable' (e.g. energy, momentum, angular momentum, etc) and has to be represented by a self-adjoint operator acting on $\mathcal{H}$. One might be interested in studying the Lorentz-covariant Dirac equation with covariant boundary conditions, but without losing any generality, the formal Lorentz covariance of a dynamical equation can be used to choose the privileged frame in which the intrinsic nature of the physical system is the simplest one. For a particle in a box, if we want to know its energy eigenvalues, the convenient privileged frame is that in which the space–time Lorentz transformations are frozen and the box is at rest in a determined space region. Once we have obtained the energy spectrum in the privileged frame, the energy–momentum 4-vector may be calculated in any inertial frame. So, the state of the system is a normalized spinor, i.e. a four-component vector $\Psi \in \mathcal{H}$. Its time evolution is determined by the family of operators $U(t) = e^{-iHt/\hbar}$. Conservation of probability requires the operator $U(t)$ to be unitary and, consequently, the Hamiltonian H to be self-adjoint.

H is a very special observable because it generates the time evolution of the states and its spectrum represents the energy of the system. To define the Hamiltonian properly, besides the formal expression as a differential operator, its domain, in particular the boundary conditions, must be specified. In fact, by changing the boundary conditions of a given operator, one modifies the operator itself without changing its formal expression, not to mention the risk of losing the self-adjointness property (see appendix A). For example, in the Aharonov–Bohm effect, by choosing different boundary conditions, which preserve self-adjointness, one obtains different cross sections [4]; aside from other considerations, it is the experimental arrangement which selects the appropriate observable.

In section 2 we give several physically acceptable boundary conditions, some of which were already proposed in scattering problems [4, 5]. We find non-trivial solutions of the Dirac equation for a particle with a fixed mass localized in a box. These results, as well as the eigenvalues and eigenfunctions for a family of self-adjoint extensions of the 'free' Dirac Hamiltonian were obtained in [6].

It is worth pointing out that, as far as we know, the problem of the several boundary conditions that may be imposed for a 'free' particle inside a box in relativistic quantum mechanics, has not been considered in the widely used textbooks for exact solutions of the Dirac equation [7–9]. However, the problem of a Dirac fermion in a one-dimensional box interacting with a scalar solitonic potential was considered earlier with periodic [10], as well as with more general boundary conditions [11] to elucidate the phenomenon of fractional fermion number. For the case of the Dirac 'free' massless operator, also in $1+1$ dimensions, eigenvalues and eigenfunctions were obtained for a family of self-adjoint extensions in [12] and the case with a non-zero vector potential was examined in [13]. Another particular solution to this problem has been obtained by considering the Dirac equation with a Lorentz scalar potential; here the rest mass can be thought of as an x-dependent mass [9]. This allows us to solve the infinite square well problem as a particle with a changing mass that becomes infinite outside the box, which avoids the Klein paradox [14]. A detailed study of the possible boundary conditions, i.e. self-adjoint extensions, for a relativistic particle inside a box, as well as their non-relativistic limits, has been considered by two of us (VA and SDeV) and will be submitted for publication elsewhere.

The principal motivation in this pedagogical note is to call attention to the fact that the boundary conditions used in non-relativistic quantum mechanics should not be extrapolated to the relativistic case, without proving beforehand that the relativistic Hamiltonian will be self-adjoint for them.

In section 2 we verify that the Dirac spinor cannot vanish at the boundary of a non-permitted region—in our case, the walls of a one-dimensional box. We find non-trivial solutions upon imposing several boundary conditions on the wavefunction. The non-relativistic limit of these results is also discussed. In section 3 we solve the problem of a particle in a spherical box using a boundary condition that cancels the large component of the spinor at the walls of the box. We propose various boundary conditions that lead to non-trivial solutions.

2. One-dimensional box

Let us consider a 'free' electron in a one-dimensional box in the interval $\Omega = [0, L]$. The three-dimensional Dirac equation for stationary states reads

$$H_0\psi = (-\mathrm{i}\hbar c\alpha\cdot\nabla + mc^2\beta)\psi = E\psi \tag{1}$$

where α, β are the well known Dirac matrices.

In this paper we restrict ourselves to positive relativistic energies. In the Dirac representation, the four-valued Dirac spinor ψ can be expressed in terms of the large and small two-valued semi-spinors, $\phi = \binom{\phi_1}{\phi_2}$ and $\chi = \binom{\chi_1}{\chi_2}$, respectively; that is

$$\psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix}. \tag{2}$$

Equation (1) is equivalent to the following coupled equations:

$$-\mathrm{i}\hbar c\sigma\cdot\nabla\chi + mc^2\phi = E\phi \tag{3}$$

$$-\mathrm{i}\hbar c\sigma\cdot\nabla\phi - mc^2\chi = E\chi \tag{4}$$

where σ are the Pauli matrices.

Eliminating χ from (3) and (4), and taking $\phi = \phi(x)$ and $\chi = \chi(x)$, with $k = \left[E^2 - \left(mc^2\right)^2\right]^{1/2}/\hbar c$, one obtains

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + k^2\right)\phi_i = 0 \qquad i = 1, 2 \tag{5}$$

which is independently satisfied by the large components.

The small components may be obtained by means of (4)

$$\begin{pmatrix}\chi_1\\ \chi_2\end{pmatrix} = \frac{-\mathrm{i}\hbar c}{E + mc^2}\begin{pmatrix}0 & \dfrac{\mathrm{d}}{\mathrm{d}x}\\ \dfrac{\mathrm{d}}{\mathrm{d}x} & 0\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}. \tag{6}$$

One of the positive energy solutions is obtained by taking $\phi_2 = 0$ and therefore $\chi_1 = 0$. From equation (5), the general solution for ϕ_1 is

$$\phi_1 = A_1\phi_1^{(1)} + B_1\phi_1^{(2)} = A_1\mathrm{e}^{\mathrm{i}kx} + B_1\mathrm{e}^{-\mathrm{i}kx} \tag{7}$$

where A_1 and B_1 are complex constants. The solutions $\phi_1^{(1)}$ and $\phi_1^{(2)}$ are independent and verify the following relation in the interval Ω:

$$\phi_1^{(1)}\frac{\mathrm{d}\phi_1^{(2)}}{\mathrm{d}x} - \phi_1^{(2)}\frac{\mathrm{d}\phi_1^{(1)}}{\mathrm{d}x} \neq 0. \tag{8}$$

From equation (6) one gets

$$\chi_2 = \frac{-\mathrm{i}\hbar c}{E + mc^2}\left(A_1\frac{\mathrm{d}\phi_1^{(1)}}{\mathrm{d}x} + B_1\frac{\mathrm{d}\phi_1^{(2)}}{\mathrm{d}x}\right) = \frac{\hbar ck}{E + mc^2}\left(A_1\mathrm{e}^{\mathrm{i}kx} - B_1\mathrm{e}^{-\mathrm{i}kx}\right). \tag{9}$$

If $\phi(0) = \binom{\phi_1(0)}{0} = 0$ and $\chi(0) = \binom{0}{\chi_2(0)} = 0$ one obtains the homogeneous system

$$A_1\phi_1^{(1)}\big|_{x=0} + B_1\phi_1^{(2)}\big|_{x=0} = 0 \tag{10}$$

$$A_1\frac{\mathrm{d}\phi_1^{(1)}}{\mathrm{d}x}\bigg|_{x=0} + B_1\frac{\mathrm{d}\phi_1^{(2)}}{\mathrm{d}x}\bigg|_{x=0} = 0 \tag{11}$$

the determinant of which cannot be zero due to (8). Thus $A_1 = B_1 = 0$, that is, the only solution is the trivial one. A similar result is obtained if $\psi = 0$ at $x = L$.

From equation (6), it can be seen that the vanishing of the small component χ_2 at $x = 0$ is equivalent to $\mathrm{d}\phi_1/\mathrm{d}x|_{x=0} = 0$. The non-existence of non-trivial solutions for the given boundary condition is certainly a consequence of the fact that (5) is an elliptic equation, so that there are no non-trivial solutions if the function ϕ_1 and its derivative χ_2 have to vanish simultaneously at the boundaries of the interval Ω. Certainly, the vanishing of the entire relativistic wavefunction at the beginning of an impenetrable barrier is not admissible. Though in non-relativistic quantum mechanics a vanishing wavefunction at the boundaries is one of the self-adjoint extensions of the 'free' Hamiltonian, in relativistic quantum mechanics it is not so. Indeed, the formal Dirac 'free' Hamiltonian does not have this boundary condition as one of its self-adjoint extensions. However, taking only the large component as zero is a physically acceptable boundary condition, because this condition is a self-adjoint extension of H_0.

In the problem of an electron inside a one-dimensional box, by imposing upon the large component

$$\phi_1(0) = \phi_1(L) = 0 \tag{12}$$

one obtains inside the interval Ω

$$\psi = 2A_1\begin{pmatrix} \mathrm{i}\sin(kx) \\ 0 \\ 0 \\ \dfrac{\hbar ck}{E+mc^2}\cos(kx) \end{pmatrix} \tag{13}$$

with $k = N\pi/L$, $N = 1, 2, \ldots$.

From appendix B, it can be seen that condition (12) corresponds, in the non-relativistic limit, to the familiar condition of a vanishing wavefunction at the walls of the box; that is, $\phi_1^{(\mathrm{NR})}(0) = \phi_1^{(\mathrm{NR})}(L) = 0$. Likewise, and according to the Schrödinger–Pauli problem, the small components of (13) are of the order of $v^{(\mathrm{NR})}/c$ and $k^{(\mathrm{NR})} = \left(2mE^{(\mathrm{NR})}\right)^{1/2}/\hbar$, from which one obtains the energy $E^{(\mathrm{NR})} = (\hbar^2/2m)(N\pi/L)^2$.

The Dirac probability density and current are given by

$$\rho = \bar{\phi}_1\phi_1 + \bar{\chi}_2\chi_2 \tag{14}$$

$$j = ec\psi^\dagger\alpha_x\psi = ec\left(\bar{\phi}_1\chi_2 + \bar{\chi}_2\phi_1\right) \tag{15}$$

where $\psi^\dagger$ is the Hermitian conjugate spinor and $\bar{\phi}$ is the complex conjugate of ϕ. With the boundary condition (12), these quantities verify

$$\rho(0) = \rho(L) \tag{16}$$

$$j(0) = j(L) = 0. \tag{17}$$

In this case, the electron is actually enclosed inside the box—there is no particle for $x < 0$ or $x > L$.

There are a variety of other ways of satisfying (17), even though the four components of the Dirac spinor cannot be equal to zero simultaneously. In fact, in addition to (12), the impenetrability condition $j = 0$ can be achieved, for example, in any of the following three cases: $\phi_1(0) = \chi_2(L) = 0$, $\phi_1(L) = \chi_2(0) = 0$ and $\chi_2(0) = \chi_2(L) = 0$. The vanishing of the relativistic current density at the walls of the box has been used in the MIT bag model, see e.g. [15]. The relativistic boundary condition used in this model is $\pm(-\mathrm{i})\beta\alpha_x\psi = \psi$, where the minus sign corresponds to $x = 0$ and the plus sign to $x = L$. This boundary condition in the Dirac representation is precisely $\chi_2(L)/\phi_1(L) = -\chi_2(0)/\phi_2(0) = \mathrm{i}$. All these conditions, which can be used if we consider the walls of the box to be impenetrable barriers, are self-adjoint extensions for the 'free' Dirac Hamiltonian.

It may argued that the mixed boundary conditions $\phi_1(0) = \chi_2(L) = 0$ and $\phi_1(L) = \chi_2(0) = 0$ are not physical because their symmetry is not the same at the walls of the box. In fact, the probability density ρ is such that $\rho(0) \neq \rho(L)$; therefore these boundary conditions are not symmetric and consequently the corresponding wavefunctions exhibit a set of eigenvalues, $k = \left(N - \frac{1}{2}\right)\pi/L$ with $N = 1, 2, 3\ldots$, which are different from those of the wavefunction (13). In the non-relativistic limit these conditions correspond to a vanishing of $\phi_1^{(\mathrm{NR})}$ at $x = 0$ ($x = L$) and a vanishing of $\mathrm{d}\phi_1^{(\mathrm{NR})}/\mathrm{d}x$ in $x = L$ ($x = 0$).

On the other hand, the boundary condition

$$\chi_2(0) = \chi_2(L) = 0 \tag{18}$$

yields the eigenfunction in Ω

$$\psi = 2A_1\begin{pmatrix} \cos(kx) \\ 0 \\ 0 \\ \dfrac{\mathrm{i}\hbar ck}{E+mc^2}\sin(kx) \end{pmatrix} \tag{19}$$

which has the same eigenvalues as the wavefunction (13) and satisfies the same relations (16) and (17). In the non-relativistic limit this state corresponds to a vanishing of $\mathrm{d}\phi_1^{(\mathrm{NR})}/\mathrm{d}x$ at $x = 0$ and $x = L$. The spinor (19) describes a positive energy electron; however, one may consider the charge conjugate of this spinor which has a vanishing large component, which may be regarded as describing a negative energy positron.

It is important to emphasize that by taking into account only the physical symmetry (16), the requirement of impenetrability (17) and the corresponding energy spectrum, one cannot distinguish between the boundary conditions (12) and (18); that is, $\phi_1(0) = \phi_1(L) = 0$ and $\chi_2(0) = \chi_2(L) = 0$. Hence, the wavefunctions (13) and (19) should be regarded as equivalent, although not trivially equivalent inasmuch as they cannot be taken one into the other by means of a symmetry operation which commutes with the Hamiltonian. Indeed, we consider that it is not possible to distinguish physically between these two solutions, despite the fact that they exhibit different probability densities. We assume that the probability prediction can be verified experimentally only in regions of size Δx sufficiently large so as to comply with the uncertainty relation $\Delta x\,\Delta p \geq \hbar/2$, with Δp corresponding to the quantum state not perturbed by the measurement of localization. According to this criterion, the localization of the points, which in the non-relativistic limit corresponds to a zero probability of the stationary wave, is not possible—not to mention that, in relativistic quantum mechanics, one cannot localize the electron in a region of size less than the Compton wavelength, because otherwise the electron energy would be sufficient for pair production. Clearly, L must be much larger than the Compton wavelength.

Finally, the boundary condition

$$\frac{\chi_2(L)}{\phi_1(L)} = -\frac{\chi_2(0)}{\phi_1(0)} = \mathrm{i} \tag{20}$$

yields the following eigenfunction in Ω:

$$\psi = 2A_1 \mathrm{e}^{\mathrm{i}\delta/2} \begin{pmatrix} \cos(kx - \delta/2) \\ 0 \\ 0 \\ \dfrac{\mathrm{i}\hbar ck}{E + mc^2}\sin(kx - \delta/2) \end{pmatrix} \tag{21}$$

where $\delta = \arctan(-\hbar k/mc)$. In this case the eigenvalues are obtained from the transcendental equation $\tan(kL) + (\hbar k/mc) = 0$.

It is worth pointing out that these results are the same as those obtained in [14]. There the authors give a mathematical justification for treating the problem of a particle absolutely confined in a box, without requiring the continuity of the wavefunction at the wall of the box. In [14] where a scalar potential is used, the particle mass becomes infinite in the external region of the box. However, we just impose adequate boundary conditions such that the Hamiltonian be self-adjoint.

Taking the non-relativistic limit of (20), as is done in appendix B, we obtain $\lambda\big(\mathrm{d}\phi_1^{(\mathrm{NR})}/\mathrm{d}x\big)(L) = -\big(\phi_1^{(\mathrm{NR})}\big)(L)$ and $\lambda\big(\mathrm{d}\phi_1^{(\mathrm{NR})}/\mathrm{d}x\big)(0) = \big(\phi_1^{(\mathrm{NR})}\big)(0)$. The non-relativistic energy eigenvalues are obtained from $\tan(k^{(\mathrm{NR})}L) + (\hbar k^{(\mathrm{NR})}/mc) = 0$. Obviously, by eliminating the term of order $v^{(\mathrm{NR})}/c$ and allowing the size of the box to grow, we obtain that the spectrum, the wavefunction and the boundary condition tend to their usual non-relativistic values [14].

Another way of getting a well defined self-adjoint problem is by extending the domain of H_0 to that of periodic or anti-periodic functions in the interval Ω. In fact, we may consider

$$\psi(0) = \pm\psi(L). \tag{22}$$

The corresponding plane-wave eigenfunctions have the form

$$\psi = C_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dfrac{\hbar ck}{E + mc^2} \end{pmatrix} \mathrm{e}^{\mathrm{i}kx} \tag{23}$$

and the energy eigenvalues are obtained from $k = 2n\pi/L$ with $n = 0, \pm 1, \pm 2, \ldots$ for the periodic condition and from $k = (2n-1)\pi/L$ for the anti-periodic one. On the other hand, taking the non-relativistic limit of these boundary conditions, we obtain $\phi_1^{(\mathrm{NR})}(0) = \pm\phi_1^{(\mathrm{NR})}(L)$, $\big(\mathrm{d}\phi_1^{(\mathrm{NR})}/\mathrm{d}x\big)(0) = \pm\big(\mathrm{d}\phi_1^{(\mathrm{NR})}/\mathrm{d}x\big)(L)$, where the plus (minus) sign corresponds to the non-relativistic periodic (anti-periodic) condition.

For these boundary conditions the density current in $x = 0$ and $x = L$ is not zero, and satisfies $j(0) = j(L)$. In this case the current at the box walls must be interpreted physically. One may say that the walls of the box are transparent to the particle, which is travelling through the box in a condition of resonance.

3. Spherical box

Let $V = 0$, $\boldsymbol{A} = \boldsymbol{0}$ in a spherical interval $a \leq r \leq b$ with

$$\begin{pmatrix} \phi \\ \chi \end{pmatrix} = \frac{1}{r}\begin{pmatrix} F(r)\, Y_{j,l,j_z}(\theta,\varphi) \\ \mathrm{i}G(r)\, Y_{j,l',j_z}(\theta,\varphi) \end{pmatrix}$$

where the two-valued semi-spinors Y are 'spinorial spherical harmonics' of order l, with $l = j + \frac{1}{2}\mu$, $l' = j - \frac{1}{2}\mu$, $\mu = \pm 1$, $j = \frac{1}{2}, \frac{3}{2}, \ldots$ and $j_z = -j, -j+1, \ldots, j$ [16].

The equation for the large components in this case is

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\kappa(\kappa+1)}{r^2} + k^2\right] F(r) = 0 \tag{24}$$

where $k = \big[E^2 - \big(mc^2\big)^2\big]^{1/2}/\hbar c$, $\kappa = \pm\big(j + \frac{1}{2}\big)$ and $\kappa(\kappa+1) = \big(j + \frac{1}{2}\big)\big(j + \mu + \frac{1}{2}\big) = l(l+1)$. In the non-relativistic limit equation (24) is the radial Schrödinger equation for free waves.

Equation (4) gives

$$G(r) = \frac{\hbar c}{E + mc^2}\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\kappa}{r}\right) F(r). \tag{25}$$

Solving equations (24) and (25), one finds

$$\psi = \begin{pmatrix} [Aj_l(kr) + B\eta_l(kr)]Y_{j,l,j_z} \\ \dfrac{\mathrm{i}\hbar ck\mu}{E + mc^2}[Aj_{l'}(kr) + B\eta_{l'}(kr)]Y_{j,l',j_z} \end{pmatrix} \tag{26}$$

where j_l and η_l are spherical Bessel functions and $l' = l - \mu$.

Also in this case, it is not admissible to make the spinor vanish at $r = a$ or $r = b$. If one sets $\psi(a) = 0$ explicitly, one obtains a homogeneous system, the determinant of which is not zero due to

$$j_v(z)\eta_{v+1}(z) - j_{v+1}(z)\eta_v(z) = -\frac{1}{z^2}. \tag{27}$$

If we want to find a non-trivial solution for this problem, by analogy with the previous one, we can propose the boundary condition that cancels the large component of the spinor at the walls of the spherical box, $\phi(a) = \phi(b) = 0$. This boundary condition is physically acceptable and verifies the vanishing of the radial component of the probability current. So, one obtains

$$\frac{j_l(ka)}{\eta_l(ka)} = \frac{j_l(kb)}{\eta_l(kb)} \tag{28}$$

and the wavefunction may then be written as

$$\psi = C \begin{pmatrix} [j_l(ka)\eta_l(kr) - \eta_l(ka)j_l(kr)]Y_{j,l,j_z} \\ \frac{\mathrm{i}\hbar ck\mu}{E+mc^2}[j_l(ka)\eta_{l'}(kr) - \eta_l(ka)j_{l'}(kr)]Y_{j,l',j_z} \end{pmatrix}$$
$$a \le r \le b. \tag{29}$$

In this case we can take the limit when $a \to 0$: $j_l(ka)/\eta_l(ka) \to (ka)^{2l+1} \to 0$, so the energy eigenvalues are obtained from $j_l(kb) = 0$. In this way, the solution for a particle localized in a sphere of radius b is

$$\psi = D \begin{pmatrix} j_l(kr)Y_{j,l,j_z} \\ \frac{\mathrm{i}\hbar ck\mu}{E+mc^2} j_{l-\mu}(kr)Y_{j,l-\mu,j_z} \end{pmatrix} \quad 0 \le r \le b. \tag{30}$$

Since in the non-relativistic limit the small components of (30) are of the order of $v^{(\mathrm{NR})}/c$, the well known non-relativistic energy eigenvalues, which are obtained from $j_l(k^{(\mathrm{NR})}b) = 0$, are recovered.

We may also consider other boundary conditions that satisfy the vanishing of the radial component of the probability current at the walls of the spherical region: $\chi(a) = \chi(b) = 0$, $\phi(a) = \chi(b) = 0$, $\phi(b) = \chi(a) = 0$.

Choosing one of these conditions is again a problem of symmetry or physical convenience.

4. Conclusions

As distinguished from the non-relativistic problem, the relativistic wavefunction at the boundaries of a non-permitted region cannot vanish entirely. A necessary and sufficient condition in order to find non-trivial solutions is to impose on the wavefunction boundary conditions that make the Hamiltonian self-adjoint. For some of these conditions the probability current vanishes at the walls of the box; they are just the conditions which can be used in a model of an impenetrable barrier in place of the continuity of the wavefunction. By taking the non-relativistic limit of the boundary conditions that we have considered, some already known results are recovered. We believe that the subject of this paper may be of interest to teachers and students of relativistic quantum mechanics; as far as we know, it has not been sufficiently discussed in textbooks and journals.

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Appendix A

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

$$(H_0\psi)(x) = \left(-\mathrm{i}\hbar c\alpha_x \frac{\mathrm{d}}{\mathrm{d}x} + mc^2\beta\right)\psi(x) = E\psi(x) \tag{A1}$$

where ψ is the four-component column Dirac spinor depending on $x \in \Omega = [0, L]$ and

$$\alpha_x = \begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The spinors $\psi(x)$ and $(H_0\psi)(x)$ belong to a dense proper subset of the Hilbert space $\mathcal{H} = L^2(\Omega)\oplus L^2(\Omega)\oplus L^2(\Omega) \oplus L^2(\Omega)$; that is, in this subset there exists a basis in which to expand every $\psi \in \mathcal{H}$, with a scalar product denoted by $\langle\, ,\rangle$. Generally the domains of H_0 and its adjoint H_0^* verify $\mathrm{Dom}(H_0) \subseteq \mathrm{Dom}(H_0^*)$, but H_0 must be self-adjoint, so we look for self-adjoint extensions of the symmetric operator H_0 (as we shall define below).

Without using the machinery of Von Neumann's theory of self-adjoint extensions of symmetric operators [17] and without intending to be rigorous, let us briefly consider the construction of a self-adjoint operator from the formal Hamiltonian

$$H_0 = -\mathrm{i}\hbar c\alpha_x \frac{\mathrm{d}}{\mathrm{d}x} + mc^2\beta \tag{A2}$$

whose initial dense domain may be written as

$$\mathcal{D} = \{\psi \in \mathcal{H}, \text{a.c. in } \Omega, (H_0\psi) \in \mathcal{H}, \text{ with } \psi(0) = \psi(L) = 0\} \tag{A3}$$

where a.c. means absolutely continuous functions. With this domain H_0 is a symmetric operator; that is, for all $\zeta, \eta \in \mathcal{D}$,

$$\langle H_0\zeta, \eta\rangle - \langle\zeta, H_0\eta\rangle = \mathrm{i}\hbar c[(\zeta^\dagger a_x\eta)(L) - (\zeta^\dagger a_x\eta)(0)] = 0. \tag{A4}$$

Since the quantum dynamics requires H_0 to be a self-adjoint operator, it must be fulfilled that $\mathrm{Dom}(H_0) = \mathrm{Dom}(H_0^*)$, where H_0^*, defined by the same formal operator (A2), is the adjoint of the differential operator H_0. Its domain is defined by $\mathrm{Dom}(H_0^*) = \{v \in \mathcal{H}, \text{a.c. in } \Omega, (H_0^*v) \in \mathcal{H}\}$ with

$$\langle H_0\zeta, v\rangle - \langle\zeta, H_0^*v\rangle = \mathrm{i}\hbar c[(\zeta^\dagger a_x v)(L) - (\zeta^\dagger a_x v)(0)] = 0 \tag{A5}$$

for all $\zeta \in \mathrm{Dom}(H_0)$ and $v \in \mathrm{Dom}(H_0^*)$. Clearly, H_0^* is defined on a manifold of spinors taking arbitrary values at the end points of the interval Ω. So, the boundary conditions (BC) defined by equation (A3) are incompatible with the required self-adjointness of H_0.

Now the problem consists in choosing a sufficiently general set of BC for which $\mathrm{Dom}(H_0) = \mathrm{Dom}(H_0^*)$. If $\mathrm{Dom}(H_0)$ is fixed, H_0^* will be the adjoint of H_0 if its maximal domain is consistent with the vanishing of $(\zeta^\dagger\alpha_x v)(L) - (\zeta^\dagger a_x v)(0)$, for all $\zeta \in \mathrm{Dom}(H_0)$.

Taking into account our study on the general BC for this problem, we write here, as an example, the form of one of the families of BC,

$$\begin{pmatrix} \phi_1(L) \\ \phi_1(0) \end{pmatrix} = A \begin{pmatrix} -\chi_2(L) \\ \chi_2(0) \end{pmatrix} \qquad A = -A^\dagger \quad \text{and} \quad \phi_2 = \chi_1 = 0 \tag{A6}$$

where

$$A = \mathrm{i}(\sin\mu + \sin\tau\cos\theta)^{-1} \times \begin{pmatrix} \cos\mu + \cos\tau\cos\theta & \mathrm{e}^{\mathrm{i}\gamma}\sin\theta \\ \mathrm{e}^{-\mathrm{i}\gamma}\sin\theta & \cos\mu - \cos\tau\cos\theta \end{pmatrix} \tag{A7}$$

with the restrictions that $\sin\mu + \sin\tau\cos\theta \neq 0$ and $0 \le \theta < \pi$, $0 \le \mu, \tau, \gamma < 2\pi$.

Among the BC included in this family are $\phi_1(L) = \phi_1(0) = 0$ and $\chi_2(L)/\phi_1(L) = -\chi_2(0)/\phi_1(0) = \mathrm{i}$. These BC and all the others discussed in this paper are self-adjoint extensions for the 'free' Dirac Hamiltonian. The eigenvalues and eigenfunctions for the most general BC of the Dirac Hamiltonian have been calculated in [6].

With respect to the problem of completeness, we remark that the set of eigenfunctions of a self-adjoint operator with a non-degenerate spectrum constitutes a basis of the Hilbert space. In our case we found eigenfunctions of positive energy, from which those of negative energy can easily be obtained.

Appendix B

By considering $\phi = \binom{\phi_1(x)}{0}$ and $\chi = \binom{0}{\chi_2(x)}$, equations (3) and (4) lead to the system

$$\begin{aligned} -\mathrm{i}\hbar c\frac{\mathrm{d}}{\mathrm{d}x}\phi_1 &= \left(E + mc^2\right)\chi_2 \\ -\mathrm{i}\hbar c\frac{\mathrm{d}}{\mathrm{d}x}\chi_2 &= \left(E - mc^2\right)\phi_1. \end{aligned} \tag{B1}$$

Assuming that $\phi_1(x,c) = \phi_1(x,-c)$, $\chi_2(x,c) = -\chi_2(x,-c)$ and $E(c) = E(-c)$, the functions $\phi_1(x,-c)$ and $\chi_2(x,-c)$ satisfy equations (B1) with $c \to -c$; consequently, we may write the following expansions in c for $\phi_1(x,c)$ and $\chi_2(x,c)$ [9]:

$$\begin{aligned} \phi_1 &= \phi_1^{(\mathrm{NR})} + \frac{1}{c^2}\phi_{1(1)} + \frac{1}{c^4}\phi_{1(2)} + \cdots \\ \chi_2 &= \frac{1}{c}\chi_2^{(\mathrm{NR})} + \frac{1}{c^3}\chi_{2(1)} + \frac{1}{c^5}\chi_{2(2)} + \cdots \end{aligned} \tag{B2}$$

and for the energy

$$E = mc^2 + E^{(\mathrm{NR})} + \frac{1}{c^2}E_{(1)} + \frac{1}{c^4}E_{(2)} + \cdots. \tag{B3}$$

Substituting relations (B2) and (B3) in (B1) and comparing the terms of lower order, we obtain the following system:

$$\begin{aligned} \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\phi_1^{(\mathrm{NR})} + \frac{2m}{\hbar}\chi_2^{(\mathrm{NR})} &= 0 \\ \mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\chi_2^{(\mathrm{NR})} + \frac{E^{(\mathrm{NR})}}{\hbar}\phi_1^{(\mathrm{NR})} &= 0. \end{aligned} \tag{B4}$$

Eliminating $\chi_2^{(\mathrm{NR})}$, we obtain the eigenvalue Schrödinger equation

$$\left[\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \left(k^{(\mathrm{NR})}\right)^2\right]\phi_1^{(\mathrm{NR})} = 0 \tag{B5}$$

where $\left(k^{(\mathrm{NR})}\right)^2 = 2mE^{(\mathrm{NR})}/\hbar^2$.

In the non-relativistic limit, the connection between the components ϕ_1 and χ_2 of the Dirac spinor ψ and the Schrödinger–Pauli function $\phi_1^{(\mathrm{NR})}$, is obtained keeping only the first term of the expansions (B2), and using the first equation of (B4); that is

$$\begin{aligned} \phi_1 &\to \phi_1^{(\mathrm{NR})} \\ \chi_2 &\to -\lambda\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}x}\phi_1^{(\mathrm{NR})} \end{aligned} \tag{B6}$$

where $\lambda = \hbar/2mc$.

With these relations, we may calculate the non-relativistic limit up to the order of $v^{(\mathrm{NR})}/c$ for any quantum mechanical expression in one spatial dimension.

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