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1999 J. Phys. A: Math. Gen. 32 5277

(http://iopscience.iop.org/0305-4470/32/28/307)

J. Phys. A: Math. Gen. **32** (1999) 5277–5284. Printed in the UK PII: S0305-4470(99)99668-3

Some remarks about the 'free' Dirac particle in a one-dimensional box

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Received 26 November 1998, in final form 6 April 1999

Abstract. The problem of a relativistic 'free' Dirac particle in a one-dimensional box, i.e., at the box, but not confined to the box, is considered. A four-parameter family of self-adjoint extensions of the momentum operator $P = -\mathrm{i}\hbar 1_2 \frac{\mathrm{d}}{\mathrm{d}x}$ is obtained, as well as sub-families of boundary conditions for which this operator transforms as a vector. Physical conditions (self-adjointness and not spontaneously broken $C\Pi T$ symmetry in the subspace of positive energies) imposed upon the Hamiltonian operator, which is a function of the momentum operator, give the physical Hamiltonian operator for this problem. The physical self-adjoint extension of H corresponds to the periodic boundary condition.

1. Introduction

The free particle (i.e., $V(x) = 0$) in one dimension is certainly the simplest example of non-relativistic quantum mechanics. However, a free particle in a one-dimensional box is not so simple due to mathematical subtleties appearing with boundary conditions, operator domains, and self-adjointness of the involved operators. As was shown in [1], only for the boundary conditions $\phi(0) = \phi(L) \neq 0$, $\phi'(0) = \phi'(L) \neq 0$, the momentum operator transforms as a vector and the parity symmetry operation of the Hamiltonian is not spontaneously broken. So, a non-relativistic particle in a box is 'free' (i.e., at the box, but not confined to the box) if the domain of the Hamiltonian operator consists of functions satisfying these boundary conditions. In this case the Hamiltonian is the kinetic energy, being this operator the only self-adjoint extension which is a function of the momentum operator in a box. Clearly, this quantum case does not correspond to the classical motion of a particle bouncing between the walls.

In relativistic quantum mechanics the mathematical subtleties are also present. The relativistic Dirac particle in a finite or infinite square well, has been considered in the literature using different approaches [2]. A detailed study of the possible boundary conditions for a relativistic Dirac particle inside a box, as well as their non-relativistic limits, has recently been considered [3]. In this problem, there are two types of boundary conditions. A necessary condition in order to have a confined particle in a box is that the probability current density $j(x) = \Psi^{+}\alpha\Psi$ vanishes at the walls: $j(0) = j(L) = 0$. Likewise, a necessary condition in order to have a 'free' particle in a box is that the probability current density must satisfy: $j(0) = j(L) \neq 0$, which would permit us to say that the walls are transparent to the current.

0305-4470/99/285277+08$30.00

However, the question about what is really a relativistic 'free' Dirac particle in a box, i.e., which boundary condition defines the domain of its Hamiltonian?, as far as we know, has not been considered in the literature. It is important to note that, for the quantum system consisting of a relativistic 'free' Dirac particle on a line with a hole (point interactions), we have a similar story. We can imagine bringing the extremities of the box close to each other, making it look like a circle with a hole [4]. So our results are also applied to this system. Physically, since a very localized interaction can be due to the interaction of the particle with an impurity or a local defect in a solid, for example, the case 'free' obviously corresponds to a particle that it is not disturbed by the point interaction.

The aim of this paper is to characterize a 'free' Dirac particle in a one-dimensional box, that is, we want to obtain the Hamiltonian operator which answers to the minimal questions for a 'free' particle in a box, i.e., which boundary condition defines its domain. We choose the Hamiltonian operator H as a function of the momentum operator. The domain of P essentially induces the domain of H.

One might be interested in studying covariant boundary conditions for this problem, 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. If we want to know the 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 two-vector (in 1+1 dimensions) may be calculated in any inertial frame.

In section 2, we first obtain the most general four-parameter family of boundary conditions for which the momentum operator $P = -\mathrm{i}\hbar 1_2 \frac{\mathrm{d}}{\mathrm{d}x}$ is self-adjoint, but this is only a necessary condition for having a momentum operator in quantum mechanics. It can be seen that for all these extensions, the probability current density does not vanish at the walls of the box. In second place, of all these infinite number of extensions we select those for which the momentum operator transforms as a vector under the parity operation. Even though this operator P corresponds to a physical self-adjoint momentum operator, we demand that the Hamiltonian operator, function of it, be also self-adjoint. However, there still exist infinite boundary conditions included in the domain of H. In the third place, we choose those boundary conditions for which the Hamiltonian is $C\Pi T$ invariant. So, we have only the periodic and antiperiodic boundary conditions. Finally, of these two boundary conditions we select the periodic boundary condition since for it, the $C\Pi T$ symmetry of the self-adjoint Dirac Hamiltonian operator, in the subspace of positive energies, is not spontaneously broken.

2. Relativistic results in a box

For a relativistic Dirac particle inside a one-dimensional box in the interval $\Omega = [0, L]$, the momentum operator P in Ω is defined by

$$P\psi(x) = \left(-\mathrm{i}\hbar 1_2 \frac{\mathrm{d}}{\mathrm{d}x}\right)\psi(x). \tag{1}$$

Using the Dirac representation we write $\psi = \binom{\phi}{\chi}$, which denotes a two-component wavefunction ('spinor') with $x \in \Omega$ and 1_2 the 2×2 unit matrix. The relevant Hilbert space is $\mathsf{H} = \mathsf{L}^2(\Omega) \oplus \mathsf{L}^2(\Omega)$, with the scalar product denoted by $\langle\psi_1, \psi_2\rangle = \int_0^L \psi_1^+ \psi_2 \,\mathrm{d}x$, where ψ^+ is the adjoint of ψ.

Let us choose the domain of P as

$$\mathrm{Dom}(P) = \left\{\psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix}\right\} \Bigg| \psi \in \mathbf{H},\ \text{a.c. in } \Omega,\ P\psi \in \mathbf{H},\ \psi \text{ fulfils } \psi(L) = U\psi(0),\ U^{-1} = U^{+}\Bigg\} \tag{2}$$

where hereafter a.c. means absolutely continuous functions. Since $\mathrm{Dom}(P)$ is dense and

$$\langle P\psi, \eta\rangle - \langle \psi, P\eta\rangle = \mathrm{i}\hbar[(\psi^{+}\eta)(L) - (\psi^{+}\eta)(0)] = 0 \tag{3}$$

then, P is symmetric for all $\psi, \eta \in \mathrm{Dom}(P)$, and self-adjoint because $\mathrm{Dom}(P) = \mathrm{Dom}(P^{*})$, where $P^{*} = -\mathrm{i}\hbar 1_2 \frac{\mathrm{d}}{\mathrm{d}x}$ is the adjoint of P [5]. In appendix A, the domain of P is directly obtained using the von Neumann theory of self-adjoint extensions of symmetric operators.

Thus, there exists a four-parameter family of boundary conditions, or equivalently, a four-parameter family of self-adjoint extensions of $P \equiv P_{\theta,\mu,\tau,\gamma} = -\mathrm{i}\hbar 1_2 \frac{\mathrm{d}}{\mathrm{d}x}$ with its domain given by (2), where the unitary matrix may be written as $U = \left(\begin{smallmatrix} v & u \\ s & w \end{smallmatrix}\right)$ 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 $0 \leqslant \theta < \pi$, $0 \leqslant \mu, \tau, \gamma < 2\pi$ (see appendix A). It is worth pointing out that for all these self-adjoint extensions, $j(0) = j(L) \neq 0$.

Among the boundary conditions included in $\mathrm{Dom}(P)$ we have the periodic condition $\psi(0) = \psi(L)$, obtained by making $\theta = 0$, $\{\mu \neq \tau\} = \pi/2, 3\pi/2$; and the antiperiodic one $\psi(0) = -\psi(L)$, with $\theta = 0$, $\mu = \tau = \pi/2, 3\pi/2$.

Let us define the parity operator as

$$\Pi\psi(x) = \beta\psi(L - x) \tag{4}$$

where $\beta = \sigma_z$ in the Dirac representation.

The momentum operator under the parity operation must transform as a vector, so,

$$\Pi P \Pi^{-1}\psi = -P\psi \tag{5}$$

for all $\psi \in \mathrm{Dom}(P)$. In addition, the parity-transformed spinor must verify $\Pi\psi \in \mathrm{Dom}(P)$, which implies that

$$\sigma_z = U\sigma_z U. \tag{6}$$

Thus, the parameters v, u, s, w, satisfy the following conditions

$$v^2 - us = 1 \qquad vu - uw = 0 \qquad vs - sw = 0 \qquad w^2 - us = 1.$$

Since U is a unitary matrix the parameters v, u, s, w, are related by (A.11), in which case we obtain two sub-families of unitary matrices:
Sub-family 1: $u \neq 0$, $s \neq 0$, $v = w$, $w^2 - us = 1$, $u\bar{u} = s\bar{s}$, $s\bar{s} + w\bar{w} = 1$, $w\bar{u} + s\bar{w} = 0$:

$$U = \begin{pmatrix} w & u \\ s & w \end{pmatrix}. \tag{7}$$

Sub-family 2: $u = 0$, $s = 0$, $v, w = \pm 1$, with U any of the matrices:

$$U = \pm 1_2 \qquad \pm\sigma_z. \tag{8}$$

As possible relativistic Hamiltonians for a 'free' particle in Ω we choose the following operators, functions of the momentum operator:

$$H(P_{\theta,\mu,\tau,\gamma}) \equiv H_{\theta,\mu,\tau,\gamma} = c\alpha P_{\theta,\mu,\tau,\gamma} + mc^2\beta \tag{9}$$

where $\alpha = \sigma_x$ and $\beta = \sigma_z$ in the Dirac representation. The momentum operator is $P_{\theta,\mu,\tau,\gamma}$ with domain given by (2) with the matrix U included in (7) or (8). In order to define the Hamiltonian operator properly, for a fixed set of parameters θ, μ, τ, γ, besides its formal expression (9), its domain must be specified. Since H is a function of P, the domain of H

is induced, essentially, by that of P. If ψ belongs to $\mathrm{Dom}(P)$, then ψ belongs to $\mathrm{Dom}(H)$ if $P\psi \in \mathrm{Dom}(\alpha)$ and $\psi \in \mathrm{Dom}(\beta)$. Since the domain of the matrices α and β is the whole space, all these conditions are satisfied. Finally, if $\psi \in \mathrm{Dom}(P)$ then $\psi \in \mathrm{Dom}(H(P))$.

Even though the operator P in (9) corresponds to a physical self-adjoint momentum operator, we must assure that with the boundary conditions $\psi(L) = U\psi(0)$ where U is given by (7) and (8), H is self-adjoint. For this, it is necessary that H be symmetric and also that $\mathrm{Dom}(H) = \mathrm{Dom}(H^*)$, where H^*, defined by the same formal operator (9) is the adjoint of the differential operator H. In appendix B, we show that this occurs only if

$$w = \bar{w} \qquad u = -\bar{u} \qquad s = -\bar{s} \tag{10}$$

for the sub-family 1, and without restrictions on the four matrices of the sub-family 2.

So, we write the domain of H as

$$\mathrm{Dom}(H) = \left\{ \psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \psi \in \mathbf{H}, \text{a.c. in } \Omega, H\psi \in \mathbf{H}, \psi \text{ fulfils } \psi(L) = U\psi(0), U^{-1}{=}U^{+}, \right.$$
$$\left. \text{with } U \text{ given by (7) with (10), and } U \text{ given by (8)} \right\}. \tag{11}$$

It can be verified that the boundary conditions given in (11) are included in the most general family of self-adjoint extensions of H, studied in [3].

Since we want to characterize a 'free' particle in a one-dimensional box, of all boundary conditions included in the domain of H, we choose those boundary conditions for which the Hamiltonian is $C\Pi T$ invariant. In analogy with the results in 3 + 1 dimensions, the Dirac wavefunction transforms under the discrete transformation Π in the Dirac representation according to (4), that is, $\Pi\Psi(x,t) = \sigma_z\Psi(L-x,t)$, and under the T, C and $C\Pi T$ transformations according to

$$\begin{aligned} &T\Psi(x,t) = \sigma_z\overline{\Psi(x,-t)} \\ &C\Psi(x,t) = \sigma_x\overline{\Psi(x,t)} \\ &C\Pi T\Psi(x,t) = \sigma_x\Psi(L-x,-t) \end{aligned} \tag{12}$$

where $\bar{\Psi}$ is the complex conjugate of Ψ.

We require

$$(C\Pi T)H(C\Pi T)^{-1}\psi = H\psi \tag{13}$$

for all $\psi \in \mathrm{Dom}(H)$ and $C\Pi T\psi \in \mathrm{Dom}(H)$, that is, the $C\Pi T$ transformed spinor must obey the same boundary conditions as ψ does, which implies that

$$\sigma_x = U\sigma_x U. \tag{14}$$

This matricial relation is not satisfied by the matrix U of the sub-family 1, but it is only satisfied by the two following matrices of the sub-family 2:

$$U = \pm 1_2$$

thus, the domain of H becomes

$$\mathrm{Dom}(H) = \left\{ \psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \psi \in \mathbf{H}, \text{a.c. in } \Omega, H\psi \in \mathbf{H}, \psi \text{ fulfils } \psi(L) = \pm\psi(0) \right\}. \tag{15}$$

In summary, we have the periodic and antiperiodic boundary conditions. The symmetry operation $C\Pi T$ commutes with the Hamiltonian, which is a function of the momentum operator, only if the operator P is any of the two self-adjoint extensions with periodic or antiperiodic boundary conditions.

As is well known, if a symmetry operation commutes with the Hamiltonian, then it generates a symmetry of the system if furthermore, the ground state of H is also an eigenstate of the symmetry operator. On the other hand, the symmetry operation is spontaneously broken if the ground state of H is not an eigenstate of the corresponding symmetry operator. For this to occur, it is necessary that the ground state be degenerate. In the following, we use this definition to select among the periodic and antiperiodic conditions.

The Dirac eigenvalue equation is given by

$$H(P)\psi_n(x) = \left[c\alpha\left(-\mathrm{i}\hbar 1_2 \frac{\mathrm{d}}{\mathrm{d}x}\right) + mc^2\beta\right]\psi_n(x) = E_n\psi_n(x). \tag{16}$$

The common eigenfunctions $\psi_n(x)$ of the formal Hamiltonian and momentum operators in (16), in the subspace of positive energies, have the form

$$\psi_n(x) \sim \begin{pmatrix} 1 \\ \frac{\hbar c k_n}{E_n + mc^2} \end{pmatrix} \mathrm{e}^{\mathrm{i}k_n x} \tag{17}$$

where the discrete momentum values are

$$k_n = \frac{2n\pi}{L} \qquad n = 0, \pm 1, \pm 2, \ldots$$

if $\{\mu \neq \tau\} = \pi/2, 3\pi/2$ (upper sign in (15): periodic boundary condition), and

$$k_n = \frac{(2n+1)\pi}{L} \qquad n = 0, \pm 1, \pm 2, \ldots$$

if $\mu = \tau = \pi/2, 3\pi/2$ (lower sign in (15): antiperiodic boundary condition).

The eigenvalues of the Hamiltonian are, respectively,

$$E_n = \left[\frac{\hbar^2 c^2}{L^2}(2n\pi)^2 + (mc^2)^2\right]^{1/2} \tag{18}$$

and

$$E_n = \left[\frac{\hbar^2 c^2}{L^2}((2n+1)\pi)^2 + (mc^2)^2\right]^{1/2}. \tag{19}$$

It can be seen that the ground state of (18) in the subspace of positive energies is not degenerate and corresponds to $n = 0$,

$$E_0 = mc^2. \tag{20}$$

Likewise, the ground state of (19) in the subspace of positive energies is degenerate and corresponds to $n = 0$ and $n = -1$,

$$E_0 = E_{-1} = \left[\frac{\hbar^2 c^2 \pi^2}{L^2} + (mc^2)^2\right]^{1/2}. \tag{21}$$

Therefore, the $C\Pi T$ symmetry of $H(P)$ is not spontaneously broken only if its domain consists of functions satisfying the periodic boundary condition.

Finally, we can say that the physical momentum operator in Ω, is the operator $P = -\mathrm{i}\hbar 1_2 \frac{\mathrm{d}}{\mathrm{d}x}$ with the domain given by

$$\mathrm{Dom}(P) = \left\{\psi = \begin{pmatrix}\phi \\ \chi\end{pmatrix} \middle| \psi \in \mathsf{H}, \text{a.c. in } \Omega, P \in \mathsf{H}, \psi \text{ fulfils } \psi(L) = \psi(0) \neq 0\right\} \tag{22}$$

since the Hamiltonian operator which describes a 'free' particle in Ω is $H(P) = c\alpha P + mc^2\beta$, with

$$\mathrm{Dom}(H) = \left\{\psi = \begin{pmatrix}\phi \\ \chi\end{pmatrix} \middle| \psi \in \mathsf{H}, \text{a.c. in } \Omega, H\psi \in \mathsf{H}, \psi \text{ fulfils } \psi(L) = \psi(0) \neq 0\right\}. \tag{23}$$

Clearly, in the non-relativistic limit, the wavefunction and its derivative are also periodic.

3. Conclusions

We have shown that only for the periodic boundary condition $\psi(0) = \psi(L)$, obtained by making: $\theta = 0$, $\{\mu \neq \tau\} = \pi/2, 3\pi/2$, the momentum operator $P = P_{\theta=0,\{\mu\neq\tau\}=\pi/2,3\pi/2}$ transforms as a vector under parity, and the $C\Pi T$ symmetry of the self-adjoint Hamiltonian operator, function of P: $H(P) = c\alpha P + mc^2\beta$, in the subspace of positive energies, is not spontaneously broken. Therefore, this is the Hamiltonian operator in the interval Ω. Since the spectrum of the $C\Pi T$ invariant Hamiltonian operator has a negative part, the ground state only makes sense either in the subspace of positive or negative energies. We restrict ourselves to the subspace of positive energies because we want to describe a single 'free' electron.

Finally, we can say that a relativistic free Dirac particle in a one-dimensional box is 'free', that is, with transparent walls to the probability current, only if the Dirac spinor satisfies the periodic boundary condition at the walls. Likewise, for a 'free' particle on a line with a hole, the physical boundary condition, and self-adjoint extension of the Hamiltonian with point interaction [6], is the periodic boundary condition: $\psi(0+) = \psi(0-) \neq 0$ (in this case it is enough to replace: $0 \to 0-$ and $L \to 0+$). So, the particle is not disturbed by the point interaction at $x = 0$, that is, it is 'free'.

Appendix A

The domain of $P = -\mathrm{i}1_2\frac{\mathrm{d}}{\mathrm{d}x}$ (using $\hbar = 1$) must be chosen so that P be a symmetric operator, meaning that every state in the Hilbert space could be arbitrarily well approximated by states in the domain of P, and (using integration by parts)

$$\langle P\psi, \eta\rangle - \langle\psi, P\eta\rangle = \mathrm{i}[(\psi^+\eta)(L) - (\psi^+\eta)(0)] = 0 \tag{A.1}$$

for all $\psi, \eta \in \mathrm{Dom}(P)$.

Certainly, if we choose for the domain of P

$$D = \left\{\psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix}\middle|\psi \in \mathsf{H}, \text{a.c. in } \Omega, P\psi \in \mathsf{H}, \psi \text{ fulfils } \psi(0) = \psi(L) = 0\right\} \tag{A.2}$$

then P is symmetric. However, P is not self-adjoint since the domain of P^* is larger than that of P (recall that the domain of P^* is $\mathrm{Dom}(P^*) = \{\nu = \binom{\nu_1}{\nu_2}|\nu \in \mathsf{H}, \text{a.c. in } \Omega, (P^*\nu) \in \mathsf{H}\}$, with $\langle P\psi, \nu\rangle - \langle\psi P^*\nu\rangle = 0$, for all $\psi \in \mathrm{Dom}(P)$ and $\nu \in \mathrm{Dom}(P^*)$).

Widening the initial domain of P we achieve that both domains coincide, in which case P will be self-adjoint.

In order to verify if P has self-adjoint extensions we use the so-called von Neumann method of deficiency indices [5]: if the solutions $\psi_\pm$ of the eigenvalues problems

$$P^*\psi_\pm(x) = -\mathrm{i}1_2\frac{\mathrm{d}}{\mathrm{d}x}\psi_\pm(x) = \pm\mathrm{i}\psi_\pm(x) \tag{A.3}$$

belong to H and the dimensions of the space solutions $n_\pm$ verify $n_+ = n_- \neq 0$, then P has self-adjoint extensions. It is not difficult to check that in our case the following spinors are normalized independent solutions of (A.3) that belong to the Hilbert space:

$$\begin{aligned} \psi_+^{(1)}(x) &= \frac{\sqrt{2}\mathrm{e}^L}{\sqrt{\mathrm{e}^{2L}-1}}\begin{pmatrix}1\\0\end{pmatrix}\mathrm{e}^{-x} \qquad & \psi_+^{(2)}(x) &= \frac{\sqrt{2}\mathrm{e}^L}{\sqrt{\mathrm{e}^{2L}-1}}\begin{pmatrix}0\\1\end{pmatrix}\mathrm{e}^{-x} \\ \psi_-^{(1)}(x) &= \frac{\sqrt{2}}{\sqrt{\mathrm{e}^{2L}-1}}\begin{pmatrix}1\\0\end{pmatrix}\mathrm{e}^{x} \qquad & \psi_-^{(2)}(x) &= \frac{\sqrt{2}}{\sqrt{\mathrm{e}^{2L}-1}}\begin{pmatrix}0\\1\end{pmatrix}\mathrm{e}^{x}. \end{aligned} \tag{A.4}$$

Thus, the spaces of solutions ψ_+ have dimensions $n_+ = n_- = 2$, therefore, there exist families of $2^2 = 4$ parameters of self-adjoint extensions.

A general theorem of von Neumann states that if we specify a unitary 2×2 matrix M and then add to the domain of P all vectors of the form

$$\psi(x) = (a\ b)\begin{pmatrix}\psi_+^{(1)}(x)\\ \psi_+^{(2)}(x)\end{pmatrix} + (a'\ b')\begin{pmatrix}\psi_-^{(1)}(x)\\ \psi_-^{(2)}(x)\end{pmatrix} + \tilde{\psi}(x) \tag{A.5}$$

where $\tilde{\psi}(x)$ belongs to the domain D and

$$\begin{pmatrix}a'\\ b'\end{pmatrix} = M\begin{pmatrix}a\\ b\end{pmatrix} \tag{A.6}$$

with a, b, a' and b' arbitrary complex numbers, then P defined on this enlarged domain will be self-adjoint for each choice of M [5].

The vector $\psi(x)$ in the enlarged domain satisfies

$$\psi(0) = \begin{pmatrix}\phi(0)\\ \chi(0)\end{pmatrix} = \frac{\sqrt{2}}{\sqrt{\mathrm{e}^{2L}-1}}\begin{pmatrix}ae^{L}+a'\\ be^{L}+b'\end{pmatrix} \tag{A.7}$$

$$\psi(L) = \begin{pmatrix}\phi(L)\\ \chi(L)\end{pmatrix} = \frac{\sqrt{2}}{\sqrt{\mathrm{e}^{2L}-1}}\begin{pmatrix}a+a'\mathrm{e}^{L}\\ b+b'\mathrm{e}^{L}\end{pmatrix}. \tag{A.8}$$

Now, we assume that the boundary conditions can be written in the following form:

$$\begin{pmatrix}\phi(L)\\ \chi(L)\end{pmatrix} = A\begin{pmatrix}\phi(0)\\ \chi(0)\end{pmatrix} \tag{A.9}$$

where the 2×2 matrix A will be specified later.

Substituting relations (A.7) and (A.8) in (A.9) and using (A.6), we obtain, for all a and b,

$$A = \frac{1_2 + \mathrm{e}^{L}M}{1_2\mathrm{e}^{L} + M}. \tag{A.10}$$

It can be shown that if M is unitary, then matrix A fulfils $A^{+} = A^{-1}$, that is, $A \equiv U = \begin{pmatrix}v & u\\ s & w\end{pmatrix}$ is also unitary and the parameters v, u, s, w, satisfy the conditions

$$\begin{aligned}&v\bar{v} + u\bar{u} = s\bar{s} + w\bar{w} = v\bar{v} + s\bar{s} = u\bar{u} + w\bar{w} = 1\\ &v\bar{s} + u\bar{w} = v\bar{u} + s\bar{w} = 0.\end{aligned} \tag{A.11}$$

We may choose $v = \mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{\mathrm{i}\tau}\cos\theta$, $u = \mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{\mathrm{i}\gamma}\sin\theta$, $s = \mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{-\mathrm{i}\gamma}\sin\theta$ and $w = -\mathrm{e}^{\mathrm{i}\mu}\mathrm{e}^{\mathrm{i}\tau}\cos\theta$, with $0 \leqslant \theta < \pi$, $0 \leqslant \mu, \tau, \gamma < 2\pi$. Finally, we can say that the family of self-adjoint extensions of $P \equiv P_{\theta,\mu,\tau,\gamma} = -\mathrm{i}\hbar 1_2\frac{\mathrm{d}}{\mathrm{d}x}$, has indeed the domain given by (2).

Appendix B

As is well known, the quantum dynamics requires that H be a self-adjoint operator, that is $\mathrm{Dom}(H) = \mathrm{Dom}(H^*)$, where H^*, defined by the same formal operator H, is the adjoint of H. Its domain is defined as [5]:

$$\mathrm{Dom}(H^*) = \left\{\eta = \begin{pmatrix}\eta_1\\ \eta_2\end{pmatrix}\middle|\, \eta \in \mathbf{H}, \text{a.c. in } \Omega, (H^*\eta) \in \mathbf{H}\right\} \qquad \text{with}$$

$$\langle H\xi, \eta\rangle - \langle \xi, H^*\eta\rangle = \mathrm{i}\hbar c[(\xi^{+}\sigma_x\eta)(L) - (\xi^{+}\sigma_x\eta)(0)] = 0 \tag{B.1}$$

for all $\xi \in \mathrm{Dom}(H)$ and $\eta \in \mathrm{Dom}(H^*)$.

If $\mathrm{Dom}(H)$ is fixed, H^* will be the adjoint of H if it has the maximal domain consistent with the vanishing of $(\xi^{+}\sigma_x\eta)(L) - (\xi^{+}\sigma_x\eta)(0)$, but such that $\mathrm{Dom}(H^*) = \mathrm{Dom}(H)$. In order to obtain the common domain, let us suppose, for example, that the boundary conditions

$$\begin{pmatrix}\xi_1(L)\\ \xi_2(L)\end{pmatrix} = U\begin{pmatrix}\xi_1(0)\\ \xi_2(0)\end{pmatrix} \tag{B.2}$$

with U given by (7) (sub-family 1) or (8) (sub-family 2), are included in the domain of H. By replacing (B.2) in (B.1), and since the vanishing of the two components of ξ at the walls of the box cannot be made, it may be verified that a necessary and sufficient condition for the vanishing of $(\xi^{+}\sigma_{x}\eta)(L) - (\xi^{+}\sigma_{x}\eta)(0)$ is

$$\begin{pmatrix} \eta_1(L) \\ \eta_2(L) \end{pmatrix} = \begin{pmatrix} \bar{w} & -\bar{u} \\ -\bar{s} & \bar{w} \end{pmatrix} \begin{pmatrix} \eta_1(0) \\ \eta_2(0) \end{pmatrix} \tag{B.3}$$

for the sub-family 1, and

$$\begin{pmatrix} \eta_1(L) \\ \eta_2(L) \end{pmatrix} = U \begin{pmatrix} \eta_1(0) \\ \eta_2(0) \end{pmatrix} \tag{B.4}$$

with U any of the matrices

$$U = \pm 1_2 \qquad \pm\,\sigma_z$$

for the sub-family 2.

To make sure that $\mathrm{Dom}(H^*) = \mathrm{Dom}(H)$, these boundary conditions, (B.3) and (B.4), must be equal in each case to (B.2), and this is satisfied only if

$$w = w \qquad u = -\bar{u} \qquad s = -\bar{s}$$

for the sub-family 1, and without restrictions on the four matrices of the sub-family 2. So, the 'free' Hamiltonian operator (9) corresponding to a 'free' particle has the domain given by (11).

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