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Boundary conditions and the Dirac spinor*

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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.

Key words: Dirac spinor; one-dimensional box; quantum mechanics.

Condiciones de frontera y el espinor de Dirac

Resumen

Se estudia la partícula "libre" en una caja unidimensional. Se prueba la imposibilidad de que se anule completamente la función de onda en la paredes de la caja. Se proponen varias condiciones de frontera aceptadas físicamente que permiten soluciones no triviales para este problema. De estos resultados se obtienen los límites no-relativísticos.

Palabras clave: Caja unidimensional; espinor de Dirac; mecánica cuántica.

1. Introduction

In non-relativistic quantum mechanics a vanishing normal component of the probability current is a sufficient condition in order to obtain an impenetrable boundary surface. This might be accomplished by imposing Dirichlet, Neumann or mixed boundary conditions upon the wave function. In the well known problem 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 wave function 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 it will be shown below. However, non-trivial solutions may be obtained by using appropriate boundary conditions for the wave function (4, 5), in such a way that self-adjointness of the formal Dirac operator be maintained.

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To define properly the Hamiltonian, 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 loosing the self-adjointness property. For example, in the Aharonov-Bohm effect, by choosing different boundary conditions, which preserve self-adjointness, one obtains different cross sections (4). By the way, aside other considerations, it is the experiment arrangement what selects the appropriate observable.

In this note in the section II 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 reference (6).

It is worth to point 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 about 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 reference (12) and the case with a non-zero vector potential was examined in reference (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 allow to solve the infinite square well problem as a particle with a changing mass that becomes infinite out of the box, which avoids the Klein paradox (14).

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

In the section II we verify that it cannot be annulled the Dirac spinor at the boundary of a not permitted region, in our case the walls of a one-dimensional box. We find non-trivial solutions upon imposing several boundary conditions on the wave function. The non-relativistic limit of these results are also discussed.

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 is equivalent to the following coupled equations

$$-i\hbar c\sigma \cdot \nabla\chi + mc^2\phi = E\phi \quad [1]$$

$$-i\hbar c\sigma \cdot \nabla\chi - mc^2\chi = E\chi \quad [2]$$

where σ are the Pauli matrices and $\phi = \begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix}$ and $\chi = \begin{pmatrix}\chi_1\\ \chi_2\end{pmatrix}$ respectively, that is

$$\psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix} \quad [3]$$

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

$$\left(\frac{d^2}{dx^2}+k^2\right)\phi_i = 0, \quad i=1,2 \qquad [4]$$

which is independently satisfied by the large components.

The small components may be obtained by means of [2]

$$\begin{pmatrix}\chi_1\\ \chi_2\end{pmatrix} = \frac{-i\hbar c}{E+mc^2}\begin{pmatrix}0 & \frac{d}{dx}\\ \frac{d}{dx} & 0\end{pmatrix}\begin{pmatrix}\phi_1\\ \phi_2\end{pmatrix} \qquad [5]$$

One of the positive energy solutions is obtained by taking: $\phi_2 = 0$ and therefore: $\chi_1 = 0$. From [4], the general solution for ϕ_1 is

$$\phi_1 = A_1\phi_1^{(1)} + B_1\phi_1^{(2)} = A_1 e^{ikx} + B_1 e^{-ikx} \qquad [6]$$

where A_1, 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.

$$\phi_1^{(1)}\frac{d\phi_1^{(2)}}{dx} - \phi_1^{(2)}\frac{d\phi_1^{(1)}}{dx} \neq 0 \qquad [7]$$

From [5] one gets

$$\chi_2 = \frac{-i\hbar c}{E+mc^2}\left(A_1\frac{d\phi_1^{(1)}}{dx} + B_1\frac{d\phi_1^{(2)}}{dx}\right) =$$

$$\frac{\hbar ck}{E+mc^2}\left(A_1 e^{ikx} - B_1 e^{-ikx}\right) \qquad [8]$$

If $\phi(0) = \begin{pmatrix}\phi_1(0)\\ 0\end{pmatrix} = 0$ and $\chi(0) = \begin{pmatrix}0\\ \chi_2(0)\end{pmatrix} = 0$

one obtains the homogeneous system

$$A_1\phi_1^{(1)}\Big|_{x=0} + B_1\phi_1^{(2)}\Big|_{x=0} = 0 \qquad [9]$$

$$A_1\frac{d\phi_1^{(1)}}{dx}\Big|_{x=0} + B_1\frac{d\phi_1^{(2)}}{dx}\Big|_{x=0} = 0 \qquad [10]$$

whose determinant cannot be zero due to [7]. 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 [5], it can be seen that the vanishing of the small component χ_2 at $x = 0$ is equivalent to $\frac{d\phi_1}{dx}\Big|_{x=0} = 0$. The non existence of non trivial solutions for the given boundary condition is certainly a consequence of the fact that [4] 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 wave function at the beginning of an impenetrable barrier is not admissible. Though in non-relativistic quantum mechanics a vanishing wave function 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 has not this boundary condition as one of its self-adjoint extensions. However, taking as zero only the large component is a physically acceptable boundary condition, because this condition is a self-adjoint extension of H_0 (6).

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

$$\phi_1(0) = \phi_1(L) = 0 \qquad [11]$$

one obtains inside the interval Ω

$$\psi = 2A_1\begin{pmatrix} i\sin(kx)\\ 0\\ 0\\ \frac{\hbar ck}{E+mc^2}\cos(kx)\end{pmatrix} \qquad [12]$$

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

By using the appendix, it can be seen that condition [11] corresponds, in the non relativistic limit, to the familiar condition of vanishing the wavefunction at the walls of the box, that is: $\phi_1^{(NR)}(0) = \phi_1^{(NR)}(L) = 0$. Likewise, and according to the Schrödinger-Pauli problem, the small components of [12] are of the order $\frac{v^{(NR)}}{c}$ and $k \to k^{(NR)} = \frac{(2mE^{(NR)})^{\frac{1}{2}}}{\hbar}$, from which one obtains the energy $E^{(NR)} = \left(\frac{\hbar^2}{2m}\right)\left(\frac{N\pi}{L}\right)^2$.

The Dirac probability density and current are given by

$$\rho = \overline{\phi}_1\phi_1 + \overline{\chi}_2\chi_2 \qquad [13]$$

$$j = ec\psi^{\dagger}\alpha_x\psi = ec(\overline{\phi}_1\chi_2 + \overline{\chi}_2\phi_1) \qquad [14]$$

where $\psi^{\dagger}$ is the hermitian conjugate spinor and $\bar{\phi}$ is the complex conjugate of ϕ. With the boundary condition [11], these quantities verify

$$\rho(0) = \rho(L) \qquad [15]$$

$$j(0) = j(L) = 0 \qquad [16]$$

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

There is a variety of other ways of satisfying [16]; even though the four components of the Dirac's spinor cannot be equal to zero simultaneously. In fact, in addition to [11], 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 $\pm(-i)\beta\alpha_x\psi = \psi$ where the minus sign corresponds to $x = 0$ and the plus sign to $x = L$. This boundary condition in the Dirac representation is precisely: $\frac{\chi_2(L)}{\phi_1(L)} = -\frac{\chi_2(0)}{\phi_1(0)} = i$. All these conditions, which can be used if we consider the walls of the box as impenetrable barriers, are self-adjoint extensions for the "free" Dirac Hamiltonian (6).

It may be 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 $\rho(0) \neq \rho(L)$; so that these boundary conditions are not symmetric and consequently the corresponding wave functions exhibit a set of eigenvalues, $k = \frac{\left(N - \frac{1}{2}\right)\pi}{L}$ with $N = 1, 2, 3, \ldots$, which are different from those of the wave function [12]. In the non-relativistic limit these conditions correspond to a vanishing of $\phi_1^{(NR)}$ at $x = 0$ $(x = L)$ and a vanishing of $\frac{d\phi_1^{(NR)}}{dx}$ in $x = L$ $(x = 0)$.

On the other hand, the boundary condition

$$\chi_2(0) = \chi_2(L) = 0 \qquad [17]$$

yields the eigenfunction in Ω

$$\psi = 2A_1\begin{pmatrix} \cos(kx) \\ 0 \\ 0 \\ \frac{\hbar ck}{E + mc^2}\sin(kx) \end{pmatrix} \qquad [18]$$

which has the same eigenvalues as the wave function [12] and satisfies the same relations [15] and [16]. In the non-relativistic limit this state corresponds to a vanishing of $\frac{d\phi_1^{(NR)}}{dx}$ at $x = 0$ and $x = L$. The spinor [18] describes a positive energy electron, however, one may consider the charge conjugate of this spinor which has a vanishing large component, and which may be regarded as describing a negative energy positron.

It is important to emphasize that by taking only into account the physical symmetry [15], the requirement of impenetrability [16] and the corresponding energy spectrum, one cannot distinguish between the boundary conditions [11] and [17], that is: $\phi_1(0)=\phi_1(L)=0$ and $\chi_2(0)=\chi_2(L)=0$. Hence, the wave functions [12] and [18] should be regarded as equivalent; though not trivially equivalent, inasmuch as they cannot be taken one into the other by means of a symmetry operation which commute with the Hamiltonian. Indeed, we consider that it is not possible to distinguish physically between these two solutions, in spite of 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 the uncertainty relation $\Delta x \Delta p \geq \frac{\hbar}{2}$, 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 wave length, because otherwise the electron energy would be sufficient for pair production. Clearly, L must be much bigger than the Compton wave length.

Finally, the boundary condition

$$\frac{\chi_2(L)}{\phi_1(L)}=\frac{\chi_2(0)}{\phi_1(0)}=i \qquad [19]$$

yields the following eigenfunction in Ω

$$\psi=2A_1 e^{i\frac{\delta}{2}}\begin{pmatrix}\cos\left(kx-\frac{\delta}{2}\right)\\ 0\\ 0\\ \frac{i\hbar ck}{E+mc^2}\sin\left(kx-\frac{\delta}{2}\right)\end{pmatrix} \qquad [20]$$

where: $\delta=\arctan\left(-\frac{\hbar k}{mc}\right)$. In this case the eigenvalues are obtained from the transcendental equation: $\tan(kL)+\left(\frac{\hbar k}{mc}\right)=0$.

It is worth to point 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 walls of the box. Our results coincide with those given in (14) when they tend to infinite the particle mass in the external region of the box, where a scalar potential is being used. However, we just impose adequate boundary conditions, such that the Hamiltonian be self-adjoint.

Taking the non-relativistic limit of [19], as is done in the appendix, we obtain:

$$\lambda\left(\frac{d\phi_1^{(NR)}}{dx}\right)(L)=(\phi_1^{(NR)})(L) \text{ and}$$

$$\lambda\left(\frac{d\phi_1^{(NR)}}{dx}\right)(0)=(\phi_1^{(NR)})(0).$$

The non-relativistic energy eigenvalues are obtained from: $\tan(k^{(NR)}L)+\left(\frac{\hbar k^{(NR)}}{mc}\right)=0$. Obviously, by eliminating the term of order $\frac{v^{(NR)}}{c}$ and causing that the size of the box grow, we obtain that the spectrum, the wave function and the boundary condition go to their 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 (6):

$$\psi(0)=\pm\psi(L) \qquad [21]$$

The corresponding plane wave eigenfunctions have the form:

$$\psi = C_1 \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dfrac{\hbar ck}{E+mc^2} \end{pmatrix} e^{ikx} \qquad [22]$$

and the energy eigenvalues are obtained from: $k = \dfrac{2n\pi}{L}$ with $n = 0, \pm1, \pm2, \ldots$ for the periodic condition, and from $k = \dfrac{(2n-1)\pi}{L}$, for the anti-periodic one. On the other hand, taking the non-relativistic limit of these boundary conditions, we obtain: $\phi_1^{(NR)}(0) = \pm\phi_1^{(NR)}(L)$, $\left(\dfrac{d\phi_1^{(NR)}}{dx}\right)(0) = \pm\left(\dfrac{d\phi_1^{(NR)}}{dx}\right)(L)$, 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.

Conclusions

As distinguished from the non-relativistic problem, the relativistic wave function at the boundaries of a not permitted region cannot vanish thoroughly. A necessary and sufficient condition in order to find non-trivial solutions is to impose on the wave function boundary conditions that makes 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 impenetrable barrier. By taking the non-relativistic limit of the boundary conditions that we have considered, some results already known are recovered. We believe that the subject of this note 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.

Appendix

By considering $\phi = \begin{pmatrix} \phi_1(x) \\ 0 \end{pmatrix}$ and $\chi = \begin{pmatrix} 0 \\ \chi_2(x) \end{pmatrix}$ equations [1] and [2] lead to the system

$$-i\hbar c\frac{d}{dx}\phi_1 = (E+mc^2)\chi_2$$

$$-i\hbar c\frac{d}{dx}\chi_2 = (E-mc^2)\phi_1 \qquad [A1]$$

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 eqns. [A1] with $c \to -c$; consequently we may write the following expansions in c for $\phi_1(x,c)$ and $\chi_2(x,c)$ (9):

$$\phi_1 = \phi_1^{(NR)} + \frac{1}{c^2}\phi_{1(1)} + \frac{1}{c^4}\phi_{1(2)} + \ldots$$

$$\chi_2 = \frac{1}{c}\chi_2^{(NR)} + \frac{1}{c^3}\chi_{2(1)} + \frac{1}{c^5}\chi_{2(2)} + \ldots \qquad [A2]$$

and for the energy

$$E = mc^2 + E^{(NR)} + \frac{1}{c^2}E_{(1)} + \frac{1}{c^4}E_{(2)} + \ldots \qquad [A3]$$

Substituting relations [A2] and [A3] in [A1] and comparing the terms of lower order, we obtain the following system:

$$i\frac{d}{dx}\phi_1^{(NR)} + \frac{2m}{\hbar}\chi_2^{(NR)} = 0$$

$$i\frac{d}{dx}\chi_2^{(NR)} + \frac{E^{(NR)}}{\hbar}\phi_1^{(NR)} = 0 \qquad [A4]$$

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

$$\left[\frac{d^2}{dx^2}+(k^{(NR)})^2\right]\phi_1^{(NR)}=0 \qquad \text{[A5]}$$

where: $(k^{(NR)})^2=\dfrac{2mE^{(NR)}}{\hbar^2}$.

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: $\phi_1^{(NR)}$, is obtained keeping only the first term of the expansions [A2], and using the first equation of [A4], that is:

$$\phi_1 \to \phi_1^{(NR)}$$

$$\chi_2 \to -\lambda_i \frac{d}{dx}\phi_1^{(NR)} \qquad \text{[A6]}$$

where: $\lambda=\dfrac{\hbar}{2mc}$.

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

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