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Ehrenfest-Type Theorems for a One-Dimensional Dirac Particle

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Abstract

The time evolution of the mean values of the standard position, velocity and momentum operators, for a relativistic Dirac particle in a one-dimensional box, as well as for a free Dirac particle on a line with a hole, are studied. By considering the cases of "free" particle, confined particle and particle with a delta function interaction, it is shown that the Ehrenfest-type theorems for these operators are not always valid.

1. Introduction

In non-relativistic quantum mechanics the Ehrenfest theorem [1] gives the law of motion of the mean values $\langle X\rangle = (\Psi, X\Psi)$ and $\langle P\rangle = (\Psi, P\Psi)$ of a quantum system. In fact, these equations of motion are formally identical to the Hamilton equations of classical mechanics, except that the quantities which occur on both sides of the classical equations must be replaced by their corresponding operator mean values. Certainly, if there exists a potential energy, the mean values $\langle X\rangle$ and $\langle P\rangle$ follow the laws of classical mechanics; but this holds rigorously only when $U(x)$ is a polynomial of at most second degree in x, for example, with $U(x) \sim x^2$ (harmonic oscillator), $U(x) \sim x$ (charged particle in a constant electric field) and when $U(x) = 0$ (free particle). Otherwise $U(x)$ must vary sufficiently slowly over a distance of the order of the extension of the wavepacket, in which case the time derivative of the mean value of the momentum operator is almost equal to the mean value of a local "force".

In non-relativistic model problems, for example, in the infinite potential well, the Ehrenfest theorem has been studied [2], however, some important aspects were not properly considered. The usual requirement that the wavefunction vanish at the two walls (Dirichlet boundary condition) is not the most general boundary condition. In fact, there is a four-parameter family of boundary conditions (or, equivalently, different self-adjoint extensions of the free Hamiltonian) each of which leads to unitary time evolution [3]. It has been shown that the Ehrenfest theorem does not hold as is usually written in the literature for some of the above mentioned self-adjoint extensions of H [4], in particular, for the operators X and P we have $(\mathrm{d}/\mathrm{d}t)\langle X\rangle \neq (\mathrm{i}/\hbar)\langle[H, X]\rangle$ and $(\mathrm{d}/\mathrm{d}t)\langle P\rangle \neq (\mathrm{i}/\hbar)\langle[H, P]\rangle$. For example, for a "free" particle in a box, that is, for a non-vanishing probability current density at the walls (periodic boundary condition), the Ehrenfest theorem does not hold because $X\Psi \notin \mathrm{Dom}(H)$, so the commutator $[H, X]$ cannot be defined. On the other hand, since $H = (P \cdot P/2m)$ is a function of P, they commute [4]. For a confined particle in a box, i.e., with vanishing probability current density at the walls (for example, with the Dirichlet boundary condition), the commutator $[H, P]$ cannot be defined because $P\Psi \notin \mathrm{Dom}(H)$, moreover, the operator P^2 in the Hamiltonian is not really defined as $P \cdot P$ [4,5]. However, the time evolution of the mean values of the operators X and P, in a box, may be easily obtained just by being careful with the involved operators domains.

Another non-relativistic model problem where the potential may become infinite in some region or points is that of the point interaction potential. These potentials may be used to approximate, in a simple way, more structured and more complex, short-ranged potentials. Calculations involving point interaction potentials, usually represented as delta-function potentials, are greatly simplified. The general point interaction in one dimension is obtained by considering the self-adjoint extensions of the Hamiltonian of a free particle moving on a line with the origin excluded. It is found that there is a four-parameter family of self-adjoint Hamiltonians that can be characterized by a four-parameter family of boundary conditions imposed on the wavefunction [6]. One of these point interactions corresponds to the familiar delta-function potential.

In the framework of one-particle relativistic quantum mechanics, the observables are associated with operators which do not mix positive and negative energy states. Such operators are called even operators [7]. In that case, at least in three-dimensional problems with potentials which are bounded at infinity, the relativistic quantum mechanical operator equations and the corresponding relativistic classical equations should be similar. This means that the mean value of any operator complies with the classical equations (Ehrenfest's theorem).

In this paper we study the time evolution of the mean values of the operators representing position (which we may call "coordinate operator"), velocity, and momentum, in the Dirac representation, for a free Dirac particle in a one-dimensional box, as well as for a free Dirac particle on a line with a hole. As we shall see below, the domains of the operators in the equations of motion, in the Schrödinger picture, must be treated with care. Clearly, in none of these cases can we obtain the relativistic classical relations for the mean values, because we are not restricted to the even part of each operator.

We consider the standard position operator X because of its simplicity, but this operator mixes up positive and negative energy states. As is well known, this effect is the origin of the Zitterbewegung. By choosing the even part of the X operator, which leaves invariant the positive and negative energy subspaces, we would obtain the quantum analog of the classical relativistic relation between energy and velocity without Zitterbewegung (with well-defined domains

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of the involved operators). However, in three dimensions there is a difficulty with the even part of the position operator because its components do not commute, so for this operator the notion of localization in a finite region has no clear meaning (see [8] and references therein). As is well known, there is another position operator without these problems. This is the so-called Newton Wigner position operator (which is just multiplication by x in the Foldy-Wouthuysen representation), but then we will have an acausal propagation of initially localized particles. This problem remains with all position operators commuting with the sign of energy [8]. Thus there are several possible choices for position operators, each having attractive features but also disadvantages. In conclusion, all this indicates that for particles with positive energy we have no relativistic notion of position analogous to the non-relativistic one and satisfying the causality requirements of a relativistic theory.

In Section 2, we present in the Schrödinger picture the time evolution equations of the mean values of the coordinate, standard velocity and momentum operators. The results take into account the involved operators domains. In Section 3, we consider a "free" particle in a box, i.e., with probability current density $j(x,t) = \Psi^{+}\alpha\Psi$ not zero at the walls: $j(0,t) = j(L,t) \neq 0$. In Section 4, we study an example of boundary conditions that describes a confined particle, i.e., with vanishing current at the walls: $j(0,t) = j(L,t) = 0$. In Section 5 we consider a particle on the x-axis with a hole at the origin, which simulates a delta relativistic point interaction potential. A summary is given in Section 6.

2. The evolution of the mean values

In the Schrödinger picture, the time derivative of the mean value of a time independent self-adjoint operator A in the normalized state $\Psi = \Psi(x,t)$ is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{d}}{\mathrm{d}t}(\Psi, A\Psi) = \left(\frac{\partial\Psi}{\partial t}, A\Psi\right) + \left(\Psi, A\frac{\partial\Psi}{\partial t}\right).$$

Taking into account the Dirac evolution equation, $\mathrm{i}\hbar(\partial\Psi/\partial t) = H\Psi$, one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{i}}{\hbar}(H\Psi, A\Psi) - \frac{\mathrm{i}}{\hbar}(\Psi, AH\Psi) \tag{1}$$

where for all t we must have $\Psi \in \mathrm{Dom}(A) \cap \mathrm{Dom}(H)$ and $H\Psi \in \mathrm{Dom}(A)$.

Since the operator A is self-adjoint: $(\Psi, AH\Psi) = (A\Psi, H\Psi)$, and we write

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{i}}{\hbar}(H\Psi, A\Psi) - \frac{\mathrm{i}}{\hbar}(A\Psi, H\Psi) \equiv -\frac{2}{\hbar}\mathrm{Im}(H\Psi, A\Psi). \tag{2}$$

With the above requirements on $\Psi(x,t)$, this equation is always true and may be used to calculate the time derivative of $\langle A\rangle$. One might have $\mathrm{Ran}(A) \cap \mathrm{Dom}(H) = \emptyset$, where $\mathrm{Ran}(A)$ is the range of A, in which case HA and $[H, A]$ are meaningless.

However, if $A\Psi \in \mathrm{Dom}(H)$, the commutator $[H, A]$ may be introduced, and Eq. (1) written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{i}}{\hbar}(H\Psi, A\Psi) - \frac{\mathrm{i}}{\hbar}(\Psi, HA\Psi) + \left(\Psi, \frac{\mathrm{i}}{\hbar}[H, A]\Psi\right). \tag{3}$$

The Hamiltonian operator is self-adjoint, so $(H\Psi, A\Psi) = (\Psi, HA\Psi)$, and hence

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{i}}{\hbar}\langle[H, A]\rangle. \tag{4}$$

It is worth pointing out that equation (4) makes sense only in those cases where $A\Psi \in \mathrm{Dom}(H)$. In particular, for the operators X, v and P we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = \frac{\mathrm{i}}{\hbar}\langle[H, X]\rangle = \langle v\rangle, \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle = \frac{\mathrm{i}}{\hbar}\langle[H, v]\rangle,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = \frac{\mathrm{i}}{\hbar}\langle[H, P]\rangle \tag{5}$$

where we have assumed that $X\Psi, v\Psi$ and $P\Psi$ belong to $\mathrm{Dom}(H)$. These three equations constitute the usual equations of motion for the mean values $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$ (see Appendix I).

On the other hand, if $X\Psi, v\Psi$ and $P\Psi$ do not belong to $\mathrm{Dom}(H)$, the time derivative of the mean value of the coordinate, standard velocity and momentum operators must be written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = -\frac{2}{\hbar}\mathrm{Im}(H\Psi, X\Psi),$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle = -\frac{2}{\hbar}\mathrm{Im}(H\Psi, v\Psi), \tag{6}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = -\frac{2}{\hbar}\mathrm{Im}(H\Psi, P\Psi).$$

In the following sections, this theorem is considered in the cases of a "free" particle and a particle confined in a box, as well as for a relativistic particle with a delta function interaction. The commutator $[H, A]$ will be introduced wherever possible.

3. "Free" particle in a box

Let us consider a relativistic particle in a one-dimensional box on the interval $\Omega = [0, L]$. The Hilbert space of the system is $\mathsf{H} = \mathsf{L}^2(\Omega) \oplus \mathsf{L}^2(\Omega)$, with scalar product denoted by $(\Psi_1, \Psi_2) = \int_0^L \Psi_1^{+}\Psi_2 \mathrm{d}x$, where Ψ^{+} is the adjoint of Ψ. Using the Dirac representation we write

$$\Psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix},$$

which denotes a two-component spinor depending upon $x \in \Omega$ and upon time. ϕ and χ are respectively the so-called large and small components of the Dirac spinor.

A necessary condition in order to have a relativistic "free" particle in Ω is that the probability current density be non zero at the walls: $j(0) = j(L) \neq 0$. The relativistic physical momentum operator P in Ω, defined by $P\Psi(x,t) = (-\mathrm{i}\hbar(\partial/\partial x))\Psi(x,t)$, has the domain [9],

$$\mathrm{Dom}(P) = \left\{\Psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix} \middle| \Psi \in \mathsf{H}, \text{a.c. on } \Omega,\ P\Psi \in \mathsf{H}, \right.$$
$$\left. \Psi \text{ fulfils } \Psi(L) = \Psi(0) \neq 0 \right\} \tag{7}$$

where hereafter a.c. means absolutely continuous functions.

The Hamiltonian operator for a "free" particle, $H \equiv H_{\mathrm{F}}$, is a function of P in the interval Ω, and is given by

$$H_{\mathrm{F}}(P) = c\alpha P + mc^2\beta. \tag{8}$$

The domain of H_F is essentially induced by that of P. If Ψ belongs to Dom(P), then Ψ belongs to Dom(H_F) if $P\Psi \in$ Dom(α) and $\Psi \in$ Dom(β). Since the domain of the matrices $\alpha = \sigma_x$ and $\beta = \sigma_z$ is the whole space, all these conditions are satisfied. So, if $\Psi \in$ Dom(P) then $\Psi \in$ Dom ($H_F(P)$). Therefore the domain of H_F is [9]

$$\mathrm{Dom}(H_F) = \left\{ \Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \Psi \in \mathsf{H}, \text{a.c. on } \Omega, H_F\Psi \in \mathsf{H}, \right. \\ \left. \Psi \text{ fulfils } \Psi(L) = \Psi(0) \neq 0 \right\} \tag{9}$$

which is one of the self-adjoint extensions of the Hamiltonian operator: periodic boundary condition [9,10].

The operator X (multiplication by x) is the standard position operator (or coordinate operator): $X\Psi(x,t) = x\Psi(x,t)$; its domain is the whole space, that is

$$\mathrm{Dom}(X) = \{\Psi | \Psi \in \mathsf{H}, X\Psi \in \mathsf{H}\} = \mathsf{H}. \tag{10}$$

The standard velocity operator of a Dirac particle is defined by $v\Psi(x,t) \equiv c\alpha\Psi(x,t)$. $c\alpha$ is a bounded operator. In fact, this matrix has the eigenvalues $+c$, $-c$. So its domain is also the whole space.

The equations (6) are satisfied by requiring, for all t

$$\Psi(L) = \Psi(0) \neq 0, \quad (H_F\Psi)(L) = (H_F\Psi)(0) \neq 0. \tag{11}$$

Since $X\Psi$ does not satisfy the periodicity condition in (9), then $X\Psi \notin \mathrm{Dom}(H_F)$. On the other hand $(v\Psi)(L,t) = (v\Psi)(0,t) \neq 0$; therefore $v\Psi \in \mathrm{Dom}(H_F)$. Likewise, since $H_F\Psi \in \mathrm{Dom}(H_F)$. and $(\beta\Psi)(L,t) = (\beta\Psi)(0,t) \neq 0$, it follows that $(\alpha P\Psi)(L,t) = (\alpha P\Psi)(0,t) \neq 0$,, and therefore $P\Psi \in \mathrm{Dom}(H_F)$. So, the evolution equations for the mean values $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$ are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_F\Psi, X\Psi), \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_F\Psi, v\Psi) = \frac{\mathrm{i}}{\hbar}\langle[H_F, v]\rangle, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_F\Psi, P\Psi) = -\frac{\mathrm{i}}{\hbar}\langle[H_F, P]\rangle, \end{aligned} \tag{12}$$

where

$$\frac{\mathrm{i}}{\hbar}\langle[H_F, v]\rangle = \frac{2\mathrm{i}c^2}{\hbar}\langle P\rangle - \frac{2\mathrm{i}}{\hbar}\langle vH_F\rangle,$$

since $\Psi \in \mathrm{Dom}(P)$, and $(\mathrm{i}/\hbar)\langle[H_F, P]\rangle = 0$, since in this case H_F commutes with P. thus, the three equations (5) cannot be applied, only two of them are valid.

Let us consider, without loss of generality, an example where the wavefunction $\Psi(x,t)$ is a linear combination of four stationary states: two of them are positive energy solutions and the other two are negative ones. This wavefunction satisfies the periodic boundary condition: $\Psi(L,t) = \Psi(0,t) \neq 0$, i.e.,

$$\Psi(x,t) = \tfrac{1}{2}\left[u_1(x)\mathrm{e}^{-\mathrm{i}\frac{|E_1|}{\hbar}t} + u_2(x)\mathrm{e}^{-\mathrm{i}\frac{|E_2|}{\hbar}t} \right. \\ \left. + w_1(x)\mathrm{e}^{\mathrm{i}\frac{|E_1|}{\hbar}t} + w_2(x)\mathrm{e}^{\mathrm{i}\frac{|E_2|}{\hbar}t}\right]$$

where the common orthonormal eigenfunctions of H_F and P are

$$u_n(x) = \frac{1}{\sqrt{L}}\sqrt{\frac{|E_n| + mc^2}{2|E_n|}}\begin{pmatrix} 1 \\ \dfrac{\hbar c k_n}{|E_n| + mc^2}\end{pmatrix}\mathrm{e}^{\mathrm{i}k_n x}$$

for

$$E_n = |E_n| = \sqrt{\hbar^2c^2k_n^2 + m^2c^4} > 0,$$

with

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

and

$$w_n(x) = \frac{1}{\sqrt{L}}\sqrt{\frac{|E_n| + mc^2}{2|E_n|}}\begin{pmatrix} \dfrac{-\hbar c k_n}{|E_n| + mc^2} \\ 1 \end{pmatrix}\mathrm{e}^{\mathrm{i}k_n x}$$

for $E_n = -|E_n| < 0$,

Let us evaluate the mean values $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$ for the Dirac wavepacket $\Psi(x,t)$. They are given by

$$\begin{aligned} \langle X\rangle &= \frac{L}{2} - \frac{L}{4\pi}\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}} \\ &\quad \times \left(\frac{\hbar c k_2}{|E_2| + mc^2} - \frac{\hbar c k_1}{|E_1| + mc^2}\right)\sin\left[\frac{(|E_2| + |E_1|)}{\hbar}t\right], \\ \langle v\rangle &= 0, \\ \langle P\rangle &= \frac{3\pi\hbar}{L}. \end{aligned}$$

In this example, the time dependent term in $\langle X\rangle$ is due to interference between the positive and negative energy components in the wavepacket.

This function describes the Zitterbewegung. In contrast, the mean values $\langle P\rangle$ and $\langle v\rangle$ do not oscillate in the box. The time derivatives of $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$, which coincide with the right hand side of equations (12), are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{(|E_2| + |E_1|)L}{4\pi\hbar}\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}} \\ &\quad \times \left(\frac{\hbar c k_2}{|E_2| + mc^2} - \frac{\hbar c k_1}{|E_1| + mc^2}\right)\cos\left[\frac{(|E_2| + |E_1|)}{\hbar}t\right], \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle &= \frac{2\mathrm{i}c^2}{\hbar}\langle P\rangle - \frac{2\mathrm{i}}{\hbar}\langle vH_F\rangle = 0, \quad \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = 0 \end{aligned}$$

where $\langle vH_F\rangle = (3\pi\hbar c^2/L)$. Clearly, $(\mathrm{d}/\mathrm{d}t)\langle X\rangle \neq \langle v\rangle$, so, the time derivative of the mean coordinate is not given by equation (4) with $A = X$. It is worth mentioning that in this case the mean value $\langle v\rangle$ is always constant (in our example $\langle v\rangle = 0$), therefore $(\mathrm{d}/\mathrm{d}t)\langle v\rangle = (\mathrm{i}/\hbar)\langle[H_F, v]\rangle = 0$, in spite of the fact that the operators H_F and v do not commute.

4. Confined particle in a box

A necessary condition in order to have a relativistic confined particle on Ω is $j(0) = j(L) = 0$. Thus, let $H \equiv H_D = -\mathrm{i}\hbar c\alpha(\partial/\partial x) + mc^2\beta$ be the Hamiltonian operator with the Dirichlet boundary condition for the large component. This boundary condition is one of the self-adjoint extensions of the Hamiltonian operator for a Dirac particle in a one-dimensional box [9,10]. The domain of H_D is given by

$$\mathrm{Dom}(H_D) = \left\{ \Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \Psi \in \mathsf{H}, \text{a.c. on } \Omega, H_D\Psi \in \mathsf{H}, \; \Psi \text{ fulfils } \phi(L) = \phi(0) \neq 0 \right\}. \quad (13)$$

On the other hand, the standard velocity operator is given by $v = c\alpha$ with domain the whole space. Likewise, the operator X is defined for every $\Psi \in \mathsf{H}$. The domain of the momentum operator P can be written as [9],

$$\mathrm{Dom}(P) = \left\{ \Psi = \begin{pmatrix} \phi \\ \chi \end{pmatrix} \middle| \Psi \in \mathsf{H}, \text{a.c. on } \Omega, P\Psi \in \mathsf{H}, \; \Psi \text{ fulfils } \Psi(L) = \Psi(0) \right\}. \quad (14)$$

Note that in this case H_D is not a function of P, so the domain of H_D is not induced by that of P.

Since H_D acts on a spinor $\Psi(x, t)$ for which the upper component satisfies $\phi(L, t) = \phi(0, t) = 0$, it can easily be checked that $(x\phi)(0, t) = (x\phi)(L, t) = 0$, so, on this $\Psi(x, t)$ the operators $H_D X$ and $[H_D, X]$ make sense. On the other hand, if $v\Psi \in \mathrm{Dom}(H_D)$, the spinor $\Psi(x, t)$ must additionally satisfy $\chi(L, t) = \chi(0, t) = 0$, for all t, then $\Psi(L, t) = \Psi(0, t) = 0$, which is too restrictive for the solutions of the Dirac equation [11]. Thus, in this case the commutator $[H_D, v]$ is formally meaningless. Likewise, the equation $(\mathrm{d}/\mathrm{d}t)\langle P\rangle = -(2/\hbar)\mathrm{Im}(H_D\Psi, P\Psi)$ is satisfied by requiring, for all t, the boundary conditions: $\phi(L, t) = \phi(0, t) = 0$, $\Psi(L, t) = \Psi(0, t)$ and $(H_D\Psi)(L) = (H_D\Psi)(0)$. This last relation implies that: $((\partial/\partial x)\Psi)(0) = ((\partial/\partial x)\Psi)(L)$. If $P\Psi \in \mathrm{Dom}(H_D)$, then $\phi(x, t)$ must additionally satisfy $((\partial/\partial x)\phi)(0) = ((\partial/\partial x)\phi)(L) = 0$. but this is not compatible with the other requirements on $\Psi(x, t)$. So we write the time derivatives of $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$ as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_D\Psi, X\Psi) = \frac{\mathrm{i}}{\hbar}\langle [H_D, X]\rangle = \langle v\rangle, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_D\Psi, v\Psi), \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_D\Psi, P\Psi). \end{aligned} \quad (15)$$

Let us consider, without loss of generality, a wavepacket $\Psi(x, t)$ consisting of a linear combination of positive and negative energy stationary states

$$\Psi(x, t) = \tfrac{1}{2}\left[f_1(x)\mathrm{e}^{-\mathrm{i}\frac{|E_1|}{\hbar}t} + f_2(x)\mathrm{e}^{-\mathrm{i}\frac{|E_2|}{\hbar}t} + g_1(x)\mathrm{e}^{\mathrm{i}\frac{|E_1|}{\hbar}t} + g_2(x)\mathrm{e}^{\mathrm{i}\frac{|E_2|}{\hbar}t} \right]$$

where the normalized H_D-eigenfunctions are

$$f_N(x) = \sqrt{\frac{2}{L}}\sqrt{\frac{|E_N| + mc^2}{2|E_N|}} \begin{pmatrix} \sin(k_N x) \\ \dfrac{-\mathrm{i}\hbar c k_N}{|E_N| + mc^2}\cos(k_N x) \end{pmatrix}$$

for

$$E_N = |E_N| = \sqrt{\hbar^2 c^2 k_N^2 + m^2 c^4} > 0,$$

with

$$k_N = \frac{N\pi}{L}, \quad N = 1, 2, \ldots,$$

and

$$g_N(x) = \sqrt{\frac{2}{L}}\sqrt{\frac{|E_N| + mc^2}{2|E_N|}} \begin{pmatrix} \dfrac{-\mathrm{i}\hbar c k_N}{|E_N| + mc^2}\sin(k_N x) \\ \cos(k_N x) \end{pmatrix}$$

for $E_N = -|E_N| < 0$. Note that $\Psi(x, t) \in \mathrm{Dom}(v) \cap \mathrm{Dom}(H_D)$. In fact, $\phi(L, t) = \phi(0, t) = 0$. Moreover, $H_D\Psi(x, t) \in \mathrm{Dom}(v)$. Since for any eigenfunction of H_D it is easy to see that $\chi_N(L) = (-1)^N \chi_N(0)$, it follows that $\Psi(x, t) \notin \mathrm{Dom}(P)$. The mean values of X and v are

$$\begin{aligned} \langle X\rangle = \frac{L}{2} - \frac{L}{\pi^2}&\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}} \\ &\times \left(1 + \frac{\hbar c k_2}{(|E_2| + mc^2)}\,\frac{\hbar c k_1}{(|E_2| + mc^2)}\right) \\ &\times \cos\left[\frac{(|E_2| - |E_1|)}{\hbar}t\right] \\ &+ \frac{L}{9\pi^2}\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}} \\ &\times \left(\frac{\hbar c k_2}{|E_2| + mc^2} + \frac{\hbar c k_1}{|E_1| + mc^2}\right)\sin\left[\frac{(|E_2| + |E_1|)}{\hbar}t\right] \end{aligned}$$

$$\begin{aligned} \langle v\rangle = \frac{c}{\pi}&\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}} \\ &\times \left(\frac{\hbar c k_2}{(|E_2| + mc^2)} + \frac{\hbar c k_1}{(|E_1| + mc^2)}\right)\sin\left[\frac{(|E_2| + |E_1|)}{\hbar}t\right] \\ &+ \frac{c}{3\pi}\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}} \\ &\times \left(1 + \frac{\hbar c k_2}{|E_2| + mc^2}\,\frac{\hbar c k_1}{|E_1| + mc^2}\right)\cos\left[\frac{(|E_2| + |E_1|)}{\hbar}t\right]. \end{aligned}$$

From (15), the times derivatives of the mean values are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= \langle v\rangle, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle &= \frac{3c^2}{L}\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}}\left(\frac{|E_2| - |E_1|}{|E_2| + |E_1|}\right) \\ &\quad\times \left(1 + \frac{\hbar c k_2}{(|E_2| + mc^2)}\,\frac{\hbar c k_1}{(|E_1| + mc^2)}\right) \\ &\quad\times \cos\left[\frac{(|E_2| - |E_1|)}{\hbar}t\right] \\ &\quad- \frac{c^2}{3L}\sqrt{\frac{(|E_2| + mc^2)(|E_1| + mc^2)}{|E_2||E_1|}}\left(\frac{|E_2| + |E_1|}{|E_2| - |E_1|}\right) \\ &\quad\times \left(\frac{\hbar c k_2}{|E_2| + mc^2} + \frac{\hbar c k_1}{|E_1| + mc^2}\right)\sin\left[\frac{(|E_2| + |E_1|)}{\hbar}t\right]. \end{aligned}$$

Note that the time dependent terms in the mean values obtained above consist of two parts, one varies in times more rapidly than the other does. The rapidly varying part is caused by the interference between positive and negative energy states. This term is due to Zitterbewegung.

Another linear combination of positive and negative energy stationary states is

$$\Psi(x,t)=\tfrac{1}{2}\Big[f_2(x)e^{-i\frac{|E_2|}{\hbar}t}+f_4(x)e^{-i\frac{|E_4|}{\hbar}t}+g_2(x)e^{i\frac{|E_2|}{\hbar}t}+g_4(x)e^{i\frac{|E_4|}{\hbar}t}\Big].$$

Note that in this case, $\Psi(x,t)\in \mathrm{Dom}(P)\cap\mathrm{Dom}(H_D)$. In fact $\phi(L,t)=\phi(0,t)=0$ and $\Psi(L,t)=\Psi(0,t)$; moreover $H_D\Psi(x,t)\in\mathrm{Dom}(P)$. So the mean values of X, v and P are

$$\langle X\rangle=\frac{L}{2},\qquad \langle v\rangle=0,\qquad \langle P\rangle=0.$$

And from (15), the time derivatives of these mean values are

$$\frac{d}{dt}\langle X\rangle=\langle v\rangle,\qquad \frac{d}{dt}\langle v\rangle=\frac{d}{dt}\langle P\rangle=0.$$

Let us point out that in spite of having a vanishing probability current density at the walls, the mean value of the "quantum force" $(d/dt)\langle P\rangle$ vanishes. However, the evolution of the probability density shows that the particle "interacts" with each wall of the box.

5. Particle on a line with a hole: delta relativistic interaction

Let us consider a relativistic particle on the real line with the origin excluded, $\Re-\{0\}$. The Hilbert space of this system is $\mathsf{H}=\mathsf{L}^2(\Re-\{0\})\oplus\mathsf{L}^2(\Re-\{0\})$, with scalar product denoted by $(\Psi_1,\Psi_2)=\int_{-\infty}^{0-}\Psi_1^+\Psi_2dx+\int_{0+}^{+\infty}\Psi_1^+\Psi_2dx$, where Ψ^+ is the adjoint of

$$\Psi=\begin{pmatrix}\phi\\ \chi\end{pmatrix}.$$

Let $H\equiv H_\delta=-i\hbar c\alpha(\partial/\partial x)+mc^2\beta$ be the Hamiltonian operator with relativistic point interaction (δ-type relativistic potential). The domain of H_δ is given by

$$\mathrm{Dom}(H_\delta)=\left\{\Psi=\begin{pmatrix}\phi\\ \chi\end{pmatrix}\Big|\Psi\in\mathsf{H},\ \text{a.c. in }\Re-\{0\},\ H_\delta\Psi\in\mathsf{H},\ \Psi\text{ fulfils}\ \begin{pmatrix}\phi(0+)\\ \chi(0+)\end{pmatrix}=\begin{pmatrix}\cos\mu & i\sin\mu\\ i\sin\mu & \cos\mu\end{pmatrix}\begin{pmatrix}\phi(0-)\\ \chi(0-)\end{pmatrix}\right\}\tag{16}$$

with

$$\mu\equiv-2\tan^{-1}\left(\frac{g}{2\hbar c}\right),$$

where $-\infty<g<0$ with $0<\mu<\pi$, and $0<g<+\infty$ with $\pi<\mu<2\pi$ The boundary condition in (16) corresponds to the so-called δ relativistic interaction with potential energy $U(x)=g\delta(x)$. This boundary condition is obtained by directly integrating the Dirac equation [12], making use of the relation: $\int_{0-}^{0+}\Psi(x)\delta(x)dx=\frac{1}{2}[\Psi(0+)+\Psi(0-)]$[13]. This relation has been used because the relativistic wavefunction is not continuous at $x=0$, in contrast with the non-relativistic case. However, this last relation cannot be imposed in general [13,14].

In the limit $((g/2\hbar c))^2\ll 1$, we obtain $\mu\sim-(g/\hbar c)$, if $g<0$, and $\mu\sim 2\pi-(g/\hbar c)$ if $g>0$. In both cases the boundary condition in (16) may be rewritten as

$$\begin{pmatrix}\phi(0+)\\ \chi(0+)\end{pmatrix}=\begin{pmatrix}\cos\left(\frac{g}{\hbar c}\right) & -i\sin\left(\frac{g}{\hbar c}\right)\\ -i\sin\left(\frac{g}{\hbar c}\right) & \cos\left(\frac{g}{\hbar c}\right)\end{pmatrix}\begin{pmatrix}\phi(0-)\\ \chi(0-)\end{pmatrix}\tag{17}$$

and corresponds again to the potential energy $U(x)=g(x)$, but comes from solving the Dirac equation for a general sharply peaked potential and then taking the δ-function limit of the potential [13,15]. This boundary condition seems to be the correct jump condition in the one-dimensional Dirac equation with a local δ-potential. Moreover, it is worth noting that the sign of the strength g, positive for repulsive potentials and negative for attractive ones, is not important as far as the existence of bound states is concerned, in accordance with general results for bound states of the one-dimensional Dirac equation [16]. In any case, both boundary conditions, (16) and (17), are self-adjoint extensions of H_δ [17].

For very small potential strength, these relativistic boundary conditions have the same non-relativistic limit, in fact, one obtains (see appendix II),

$$\phi_{NR}(0+)\cong\phi_{NR}(0-)-\frac{g}{2mc^2}\phi'_{NR}(0-)\cong\phi_{NR}(0-)\equiv\phi_{NR}(0),$$

$$\phi'_{NR}(0+)-\phi'_{NR}(0-)\cong\frac{2mg}{\hbar^2}\phi_{NR}(0).$$

So the δ relativistic point interaction (17), as well as (16), reduces to the well know non-relativistic δ interaction. For instance, for the "relativistic one-dimensional hydrogen atom" [18] $g=-Ze^2$ and we obtain $\mu\equiv 2\tan^{-1}((Z\alpha_{fsc}/2))$ where $\alpha_{fsc}\cong(1/137)$ is the fine structure constant. For $Z\sim 1$ we can write $\mu\sim\alpha_{fsc}$. The results given by the two relativistic deltas, in this last case, become identical.

On the other hand, the standard velocity operator is $v=c\alpha$, with domain the whole space. In this case, the domain of the coordinate operator, which is again defined by $X\Psi(x,t)=x\Psi(x,t)$, is not the whole Hilbert space, in fact, X is an unbounded self-adjoint operator with domain

$$\mathrm{Dom}(X)=\{\Psi|\Psi\in\mathsf{H},\ X\Psi\in\mathsf{H}\}.\tag{18}$$

In analogy with the problem of the confined particle in a box, the relativistic momentum operator P in $\Re-\{0\}$, defined by $P\Psi(x,t)=(-i\hbar(\partial/\partial x))\Psi(x,t)$, has the domain [9],

$$\mathrm{Dom}(P)=\left\{\Psi=\begin{pmatrix}\phi\\ \chi\end{pmatrix}\Big|\Psi\in\mathsf{H},\ \text{a.c. on }\Re-\{0\},\ P\Psi\in\mathsf{H},\ \Psi\text{ fulfils }\Psi(0+)=\Psi(0-)\right\}.\tag{19}$$

It is worth noting that, in the quantum system consisting of a relativistic free particle in a one-dimensional box of length L, we can imagine bringing the extremities of the interval close to each other, making it look like a circle with a hole. So the result of [9], with respect to (19), applies to this system as well.

The Hamiltonian operator H_δ acts upon the spinors $\Psi(x,t)$ for which

$$\Psi(0+,t)=\begin{pmatrix}\cos\mu & i\sin\mu\\ i\sin\mu & \cos\mu\end{pmatrix}\Psi(0-,t)$$

is satisfied, with $\mu=-(g/\hbar c)$, if $g<0$, and $\mu=2\pi-(g/\hbar c)$ if

$g > 0$, i.e., the boundary condition (17). It can be easily checked that

$$(X\Psi)(0+, t) = \begin{pmatrix} \cos\mu & \mathrm{i}\sin\mu \\ \mathrm{i}\sin\mu & \cos\mu \end{pmatrix} (X\Psi)(0-, t),$$

which is trivially satisfied. On this $\Psi(x, t)$, therefore, the operators $H_\delta X$ and $[H_\delta, X]$ make sense.

On the other hand, if $v\Psi \in \mathrm{Dom}(H_\delta)$, the spinor $\Psi(x, t)$ must satisfy for all t:

$$(v\Psi)(0+, t) = \begin{pmatrix} \cos\mu & \mathrm{i}\sin\mu \\ \mathrm{i}\sin\mu & \cos\mu \end{pmatrix} (v\Psi)(0-, t),$$

which implies the boundary condition (16). Likewise, the equation $(\mathrm{d}/\mathrm{d}t)\langle P\rangle = -(2/\hbar)Im(H_\delta\Psi, P\Psi)$ is satisfied by requiring, for all t, the boundary conditions (16), $\Psi(0+) = \Psi(0-)$ and $(H_\delta\Psi)(0+) = (H_\delta\Psi)(0-)$, which implies $((\partial/\partial x)\Psi)(0+) = ((\partial/\partial x)\Psi)(0-)$. All these relations are very restrictive and are satisfied only if $\mu \to 0, \pi$, in which case $(\mathrm{d}/\mathrm{d}t)\langle P\rangle = (i/\hbar)\langle[H_\delta, P]\rangle$, owing to $P\Psi \in \mathrm{Dom}(H_\delta)$. Then the evolution equations for the mean values $\langle X\rangle$, $\langle v\rangle$, and $\langle P\rangle$ are

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_\delta\Psi, X\Psi) = \frac{\mathrm{i}}{\hbar}\langle[H_\delta, X]\rangle = \langle v\rangle, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle &= -\frac{2}{\hbar}\mathrm{Im}(H_\delta\Psi, v\Psi) = \frac{\mathrm{i}}{\hbar}\langle[H_\delta, v]\rangle, \\ \frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle &= -\frac{\mathrm{i}}{\hbar}\langle[H_\delta, P]\rangle, \end{aligned} \tag{20}$$

where $\frac{\mathrm{i}}{\hbar}\langle[H_\delta, v]\rangle = \frac{2\mathrm{i}c^2}{\hbar}\langle P\rangle - \frac{2\mathrm{i}}{\hbar}\langle vH_\delta\rangle$, since $\Psi \in \mathrm{Dom}(P)$. Thus, the three equations (5) can be applied.

As an example, let us consider the normalized wavepacket $\Psi(x, t)$, which is a linear combination of the two bound states, one of positive energy and the other with negative energy:

$$\Psi(x, t) = \tfrac{1}{\sqrt{2}}\left[f_+(x)\mathrm{e}^{-\mathrm{i}\frac{|E|}{\hbar}t} + f_-(x)\mathrm{e}^{\mathrm{i}\frac{|E|}{\hbar}t}\right]$$

where the orthonomal H_δ bound state wavefunctions are

$$f_+(x) = \sqrt{\kappa}\sqrt{\frac{|E| + mc^2}{2mc^2}} \begin{pmatrix} 1 \\ \dfrac{\pm\mathrm{i}\hbar c\kappa}{|E| + mc^2} \end{pmatrix} \mathrm{e}^{-\kappa|x|}$$

for $E = |E| = \sqrt{m^2c^4 - \hbar^2c^2\kappa^2} > 0$, with $\kappa > 0$, and

$$f_-(x) = \sqrt{\kappa}\sqrt{\frac{|E| + mc^2}{2mc^2}} \begin{pmatrix} \dfrac{\mp\mathrm{i}\hbar c\kappa}{|E| + mc^2} \\ 1 \end{pmatrix} \mathrm{e}^{-\kappa|x|}$$

for $E = -|E| < 0$ with $\kappa > 0$. The upper sign refers to $x \geq 0+$ and the lower sign refers to $x \leq 0-$. The magnitude of the energy is

$$|E| = \left[\frac{1 - \tan^2\left(\frac{\mu}{2}\right)}{1 + \tan^2\left(\frac{\mu}{2}\right)}\right] mc^2.$$

Note that if $\Psi(x, t) \in \mathrm{Dom}(H_\delta)$, then $\mu \to 0, \pi$ and $|E| \to mc^2$. As in the boundary condition (17), $\mu \sim -(g/\hbar c)$, if $g < 0$, in the limit $(g/2\hbar c)^2 \ll 1$, then when $\mu \to 0$ the mean values $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$ for the Dirac wavepacket $\Psi(x, t)$ are given by

$$\langle X\rangle = \frac{\hbar}{2mc}\sin\left(\frac{2|E|}{\hbar}t\right), \qquad \langle v\rangle = \frac{|E|}{mc}\cos\left(\frac{2|E|}{\hbar}t\right),$$
$$\langle P\rangle = 0.$$

From (20), the time derivatives of the mean values are

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = \langle v\rangle, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle = -\frac{2|E|^2}{mc\hbar}\sin\left(\frac{2|E|}{\hbar}t\right),$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = 0.$$

6. Summary and discussion

We have found some restrictions on the circumstances in which the time evolution of the mean values $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$ hold, as they are usually written in the literature, for a free Dirac particle in a box, as well as for a free Dirac particle on a line with a hole. A common feature of the self-adjoint extensions of the Hamiltonian operators of the former cases is such that, in general, $(\mathrm{d}/\mathrm{d}t)\langle A\rangle \neq (\mathrm{i}/\hbar)\langle[H, A]\rangle$ when $A = X$, v or P.

For a "free" particle in a box (that is, for a non-vanishing probability current density at the walls), equations (5) do not all hold because $X\Psi \notin \mathrm{Dom}(H_\mathrm{F})$; nevertheless, the time derivatives of $\langle X\rangle$, $\langle v\rangle$ and $\langle P\rangle$ can always be calculated using (6). By considering an example of a Hamiltonian for a confined particle in a box, i.e., with vanishing probability current density at the walls, the laws of motion of the mean values of X, v and P were obtained, and it was pointed out that these mean values do not satisfy equations (5). However, in the problem of a Dirac particle with a delta relativistic interaction, which is simulated by means of boundary conditions, the three equations (5) can be applied. In conclusion, the usual time evolution for an operator, which is proportional to the mean value of the commutator between the Hamiltonian and the corresponding operator, is not always valid.

In this paper we have chosen the usual Dirac representation. As is well known, in the Foldy-Wouthuysen representation [19] the positive and negative energy states are completely separated; therefore, this representation is more appropriate in order to take the classical limit [20]. Moreover, in the Foldy-Wouthuysen representation the wavepackets behave much more like a classical particle than in the Dirac one. Recently, this was confirmed by examining the behaviour of wavepackets for the one-dimensional version of the Dirac oscillator [21]. In a forthcoming note, the Ehrenfest theorem in the Foldy-Wouthuysen representation for a one-dimensional Dirac particle in a box, will be considered.

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Appendix I

Let us consider a particle in the interval $\Omega = [0, L]$. If the formal steps that yield to the Eq. (3) for the operator X

are written out explicitly in coordinate representation, one has

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle X\rangle = -c(x\Psi^{+}\alpha\Psi)\Big|_{0}^{L} + \frac{\mathrm{i}}{\hbar}\langle[H, X]\rangle \tag{21}$$

where $\Psi \in \mathrm{Dom}([H, X])$ for all t. For a particle on the real line with the origin excluded, it is enough to replace the integration limits: $0 \to 0-$ and $L \to 0+$ If in addition $\Psi \in \mathrm{Dom}(v)$, then $(\mathrm{i}/\hbar)\langle[H, X]\rangle = \langle v\rangle$. Since the corresponding Hamiltonian operator is self-adjoint, the boundary term in (2l) is automatically null and we obtain the Eq. (4) for X. Likewise, we can write Eq. (3) for the operator v.

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle v\rangle = -c^2(\Psi^{+}\Psi)\Big|_{0}^{L} + \frac{\mathrm{i}}{\hbar}\langle[H, v]\rangle \tag{22}$$

where $\Psi \in \mathrm{Dom}([H, v])$ for all t. If additionally $\Psi \in \mathrm{Dom}(P)$, then $(\mathrm{i}/\hbar)\langle[H, v]\rangle = (2\mathrm{i}c^2/\hbar)\langle P\rangle - (2\mathrm{i}/\hbar)\langle vH\rangle$. As the corresponding Hamiltonian operator is self-adjoint, the boundary term in (22) is null and we obtain Eq. (4) for v.

In the same way, Eq. (3) for the operator P is

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle P\rangle = \mathrm{i}\hbar c\left(\Psi^{+}\alpha\frac{\partial\Psi}{\partial x}\right)\Big|_{0}^{L} + \frac{\mathrm{i}}{\hbar}\langle[H, P]\rangle \tag{23}$$

where $\Psi \in \mathrm{Dom}([H, P])$ for all t. This last condition is very restrictive owing to the fact that Ψ and $(\partial\Psi/\partial x)$ must both belong to $\mathrm{Dom}(H)$, moreover $\Psi(L, t) = \Psi(0, t)$ and $((\partial/\partial x)\Psi)(0, t) = ((\partial/\partial x)\Psi)(L, t)$ since $\Psi \in \mathrm{Dom}(P)$ and $H\Psi \in \mathrm{Dom}(P)$.

Finally, as the corresponding Hamiltonian operator is self-adjoint, the boundary term in (23) is null and we obtain Eq. (4) for P.

When it is possible to write Eqs (21), (22) or (23) then, the boundary terms are automatically null. In fact, for the dynamics studied in sections 3, 4 and 5 we can verify this.

Appendix II

The free Dirac equation for stationary states is given by

$$H\Psi(x) = \left(-\mathrm{i}\hbar c\alpha\frac{\mathrm{d}}{\mathrm{d}x} + mc^2\beta\right)\Psi(x) = E\Psi(x). \tag{24}$$

In the Dirac representation we write

$$\Psi = \begin{pmatrix}\phi\\ \chi\end{pmatrix},$$

where ϕ and χ are respectively the spatial parts of the so-called large and small components of the Dirac spinor.

Assuming that the components satisfy $\phi(x, c) = \phi(x, -c)$, $\chi(x, c) = -\chi(x, -c)$ and $E(c) = E(-c)$, the functions $\phi(x, -c)$, and $\chi(x, -c)$ satisfy equation (24) with $c \to -c$; consequently, we may write the following expansions in c for $\phi(x, c)$ and $\chi(x, c)$

$$\phi = \phi_{\mathrm{NR}} + \frac{1}{c^2}\phi_1 + \frac{1}{c^4}\phi_2 + \dots,$$
$$\chi = \frac{1}{c}\chi_{\mathrm{NR}} + \frac{1}{c^3}\chi_1 + \frac{1}{c^4}\chi_2 + \dots$$

and for the energy

$$E = mc^2 + E_{\mathrm{NR}} + \frac{1}{c^2}E_1 + \frac{1}{c^4}E_2 + \dots$$

Substituting these expansions in (24) and comparing the terms of the lower order, the following system is obtained

$$\mathrm{i}\phi'_{\mathrm{NR}} + \frac{2m}{\hbar}\chi_{\mathrm{NR}} = 0, \qquad \mathrm{i}\chi'_{\mathrm{NR}} + \frac{E_{\mathrm{NR}}}{\hbar}\phi_{\mathrm{NR}} = 0$$

where the primes denote differentiation with respect to x. The connection between the components ϕ and χ of the Dirac spinor and the Schrödinger eigenfunction ϕ_{NR} is obtained by keeping only the first term of the expansions, that is

$$\phi \to \phi_{\mathrm{NR}}, \qquad \chi \to -\lambda\mathrm{i}\phi'_{\mathrm{NR}}$$

where

$$\lambda = \frac{\hbar}{2mc}.$$

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