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OPERATORS AND BILINEAR DENSITIES IN THE DIRAC FORMAL 1D EHRENFEST THEOREM

Salvatore De Vincenzo
Escuela de Física, Facultad de Ciencias, Universidad Central de Venezuela,
A.P. 47145, Caracas 1041-A, Venezuela, e-mail:salvatore.devincenzo@ucv.ve
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We calculate formal time derivatives of the mean values of the standard position, velocity, and mechanical momentum operators, i. e., the Ehrenfest theorem for a one-dimensional Dirac particle in the coordinate representation. We show that these derivatives contain boundary terms that essentially depend on the values taken there by characteristic bilinear densities. We do not automatically take the boundary terms to vanish (as is usually done); nevertheless, we relate the boundary terms to similar terms that must be zero if one requires the hermiticity of certain specific unbounded operators. Throughout the article, we thoroughly discuss and illustrate all these aspects, which include the relations to certain boundary conditions. To clarify, we call our approach formal because all operations involving operators (for example, some operators products) are performed without respecting the restrictions imposed by the sets of functions on which the self-adjoint operators can act. Moreover, the Dirac Hamiltonian that we consider in our calculations contains a potential that is the time component of a Lorentz two-vector; nevertheless, we also obtain and concisely discuss the Ehrenfest theorem for a Hamiltonian with the most general Lorentz potential in (1+1) dimensions.
Key words: relativistic quantum mechanics, Dirac equation, Ehrenfest theorem, bilinear densities, relativistic Dirac operators.

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I. INTRODUCTION

As is well known, if the time derivatives of the mean values of the standard position, velocity, and mechanical momentum operators (i. e., the Ehrenfest theorem), are determined in a standard way for a three-dimensional Dirac particle in an external electromagnetic field (i. e., $\boldsymbol{E} = -\nabla\varphi - \partial\boldsymbol{A}/\partial(ct)$ and $\boldsymbol{B} = \nabla\times\boldsymbol{A}$), in the coordinate representation, the result is as follows (see, for example, Refs. [1–4]):

$$\frac{d}{dt}\langle\hat{\boldsymbol{x}}\rangle_\psi = \langle\hat{\boldsymbol{v}}\rangle_\psi, \tag{1}$$

$$\frac{d}{dt}\langle\hat{\boldsymbol{v}}\rangle_\psi = \frac{2ic^2}{\hbar}\langle\hat{\boldsymbol{p}}\rangle_\psi + \frac{2i}{\hbar}\langle\varphi\hat{\boldsymbol{v}}\rangle_\psi - \frac{2i}{\hbar}\langle\hat{\boldsymbol{v}}\hat{\boldsymbol{H}}\rangle_\psi$$

$$= -\frac{2c^2}{\hbar}\langle\hat{\boldsymbol{\Sigma}}\times\hat{\boldsymbol{p}}\rangle_\psi + \frac{2imc^2}{\hbar}\langle\beta\hat{\boldsymbol{v}}\rangle_\psi, \tag{2}$$

$$\frac{d}{dt}\langle\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\rangle_\psi = e\langle\boldsymbol{E}\rangle_\psi + \frac{e}{c}\langle\hat{\boldsymbol{v}}\times\boldsymbol{B}\rangle_\psi. \tag{3}$$

Clearly, these derivatives do not exactly satisfy the classical equations of motion. This is because the velocity operator in equations (1)-(3) is $\hat{\boldsymbol{v}} = c\hat{\boldsymbol{\alpha}}$, instead of being, for example, the operator $c^2\hat{\boldsymbol{p}}/\sqrt{c^2\hat{\boldsymbol{p}}^2 + m^2c^4}$, which is the classical velocity operator for positive energies. The standard textbooks demostration of results (1)-(3) in three dimensions (and therefore in one dimension) in the Heisenberg picture [4] appears to have no problems. However, in a formal demonstration of these results in the coordinate representation under the Schrödinger picture, one observes the presence of certain boundary terms that are not necessarily zero [5] (the one-dimensional case was precisely treated in Ref. [5], but the treatment placed emphasis on certain aspects that are related to the domains of the operators). Each boundary term can be obtained by evaluating a characteristic bilinear density (or, as is sometimes called, a "local observable") at the ends of the region in which the particle lies and then subtracting these two results.

In the present article, we carefully examine the usual formal approach to obtaining the relativistic (or Dirac) Ehrenfest theorem in one dimension in the coordinate representation. We call this approach formal because in our calculations, all operations involving operators (for example, some operators products) are performed without respecting the (excessively demanding) restrictions imposed by the involved domains (i. e., the sets of functions on which the self-adjoint operators can act, which include the boundary conditions). Moreover, we essentially use the concept of the hermiticity of an operator instead of the self-adjointness, which is known to be more restrictive. We believe that a formal study of this problem is valuable and pertinent. Let us also mention that, as far as we know, no rigorous mathematical derivation of Ehrenfest's equations for a one-dimensional Dirac particle has previously been made. The non-relativistic (or Schrödinger) Ehrenfest theorem (in one dimension) was recently treated in Ref. [6] in a similar manner to that used in the present article.

We begin this section by introducing the operators and the bilinear densities. The latter are real-valued quantities that can be properly integrated in the region of interest, and each of these integrals is essentially the mean value of some operator or some field quantity (these are space-time functions, so they may be considered to be local quantities; however, they are, in fact, dependent of the quantum state in question, so in this sense, they may be considered to be non-local quantities). In addition, each bilinear density is related (in a certain form) to the hermiticity of a specific unbounded operator. All these issues are also discussed in this section. In Section II, we formally calculate the time derivatives of the mean values of the operators and introduce other results that are relevant to our study. A potential that is the time component of a Lorentz two-vector was exclusively considered. We do not automatically take the boundary terms that are presents in these derivatives to vanish (as is usually done); nevertheless, we connect these boundary terms to similar (but not necessarily equal) terms that must be zero if one requires the hermiticity of certain unbounded operators. We also extensively discuss and illustrate these aspects (which include the relations to certain boundary conditions) in Section II. The conclusions are presented in Section III. Finally, in the appendix we obtain and concisely discuss the Ehrenfest theorem for a Dirac Hamiltonian with a general Lorentz potential (i. e., a linear combination of a scalar, a two-vector, and a pseudoscalar potential).

We have a one-dimensional relativistic Dirac particle moving in the (finite or infinite) region $x \in \Omega = [a, b]$. The standard position operator is $\hat{x} = x$, the velocity operator is $\hat{v} = c\hat{\alpha}$ (where $\hat{\alpha}$ is one of the 2×2 Dirac matrices), and $\hat{p} = -i\hbar\partial/\partial x$ is the momentum operator. The scalar product of the two-component column vectors (Dirac wave functions) $\psi = \psi(t,x) = (\psi_1(t,x)\ \psi_2(t,x))^{\mathsf{T}}$ and $\phi = \phi(t,x) = (\phi_1(t,x)\ \phi_2(t,x))^{\mathsf{T}}$ (where the symbol T represents the transpose of a matrix), which belong to the Hilbert space $\mathcal{H} = \mathcal{L}^2(\Omega) \oplus \mathcal{L}^2(\Omega)$, is $\langle \psi, \phi \rangle = \int_\Omega dx\, \psi^\dagger \phi$ (the symbol $\dagger$ denotes the adjoint of a matrix). Let $\hat{L}$ be a time-independent operator (such as $\hat{x}$, $\hat{v}$ or $\hat{p}$). The time derivative of its mean value $\langle \hat{L} \rangle_\psi = \langle \psi, \hat{L}\psi \rangle$ in the normalized state $\psi = \psi(t,x)$ ($\Rightarrow \psi \in \mathcal{H}$) can be calculated as follows:

$$\begin{aligned}\frac{d}{dt}\langle \hat{L} \rangle_\psi &= \left\langle \frac{\partial \psi}{\partial t}, \hat{L}\psi \right\rangle + \left\langle \psi, \hat{L}\frac{\partial \psi}{\partial t} \right\rangle \\ &= \frac{i}{\hbar}\langle \hat{H}\psi, \hat{L}\psi \rangle - \frac{i}{\hbar}\langle \psi, \hat{L}\hat{H}\psi \rangle \\ &= \frac{i}{\hbar}\Big(\langle \hat{H}\psi, \hat{L}\psi \rangle - \langle \psi, \hat{H}\hat{L}\psi \rangle\Big) + \frac{i}{\hbar}\langle \psi, [\hat{H}, \hat{L}]\psi \rangle,\end{aligned} \tag{4}$$

where $[\hat{H}, \hat{L}] = \hat{H}\hat{L} - \hat{L}\hat{H}$, as usual. The state ψ evolves in time according to the Dirac equation $\partial\psi/\partial t = -i\hat{H}\psi/\hbar$; the Hamiltonian operator is

$$\begin{aligned}\hat{H} = c\hat{\alpha}\hat{p} + mc^2\hat{\beta} + U(x) = -i\hbar c\hat{\alpha}\frac{\partial}{\partial x} \\ + mc^2\hat{\beta} + U(x),\end{aligned} \tag{5}$$

where $\hat{\beta}$ is the other 2×2 Dirac matrix and $U(x) = e\varphi(x)$ is the potential energy function, or simply the external potential. In fact, φ is a Lorentz vector type potential, i. e., it is the time component of a Lorentz two-vector.

The corresponding mean values of the operators $\hat{x}$, $\hat{v}$ and $\hat{p}$ in the complex normalized state $\psi = \psi(t,x)$ ($\|\psi\|^2 \equiv \langle \psi, \psi \rangle = 1$) are as follows:

$$\langle \hat{x} \rangle_\psi = \langle \psi, \hat{x}\psi \rangle = \int_\Omega dx\, x\psi^\dagger\psi = \int_\Omega dx\, x\varrho, \tag{6}$$

whree $\varrho = \varrho(t,x) = \psi^\dagger\psi$ is the probability density. The operator $\hat{x}$ is hermitian because it automatically satisfies the following relation:

$$\langle \psi, \hat{x}\phi \rangle - \langle \hat{x}\psi, \phi \rangle = 0, \tag{7}$$

where ψ and ϕ are functions belonging to $\mathcal{H}$. Clearly, we can also write the following relation: $\langle \psi, \hat{x}\psi \rangle = \langle \hat{x}\psi, \psi \rangle = \overline{\langle \psi, \hat{x}\psi \rangle}$ (where the bar represents complex conjugation); therefore, $\mathrm{Im}\langle \psi, \hat{x}\psi \rangle = 0$, i. e., $\langle \hat{x} \rangle_\psi \in \mathbb{R}$, as is expected for a hermitian operator. Note that because $\langle \hat{L} \rangle_\psi = \int_\Omega dx\, \psi^\dagger \hat{L}\psi$, we can also write $\overline{\langle \hat{L} \rangle_\psi} = \int_\Omega dx\, \overline{\psi^\dagger \hat{L}\psi} = \int_\Omega dx\, (\psi^\dagger \hat{L}\psi)^\dagger$. Likewise,

$$\langle \hat{v} \rangle_\psi = \langle \psi, \hat{v}\psi \rangle = c\int_\Omega dx\, \psi^\dagger\hat{\alpha}\psi = \int_\Omega dx\, j, \tag{8}$$

where $j = j(t,x) = c\psi^\dagger\hat{\alpha}\psi$ is the probability current density. The probability density and the probability current density satisfy the continuity equation $\partial\varrho/\partial t + \partial j/\partial x = 0$. The operator $\hat{v}$ is a hermitian matrix because $\hat{\alpha} = \hat{\alpha}^\dagger$; therefore, it satisfies the following relation:

$$\langle \psi, \hat{v}\phi \rangle - \langle \hat{v}\psi, \phi \rangle = 0, \tag{9}$$

where ψ and ϕ are functions belonging to $\mathcal{H}$. As expected, we can also write the result $\langle \psi, \hat{v}\psi \rangle = \langle \hat{v}\psi, \psi \rangle = \overline{\langle \psi, \hat{v}\psi \rangle}$; therefore $\mathrm{Im}\langle \psi, \hat{v}\psi \rangle = 0$, i. e., $\langle \hat{v} \rangle_\psi \in \mathbb{R}$. Note that a velocity field defined as $V = V(t,x) = j/\varrho$ has the same mean value as the operator $\hat{v}$, i. e., $\langle V \rangle_\psi = \langle \hat{v} \rangle_\psi$ (this is so because $\langle V \rangle_\psi = \int_\Omega dx\, V\varrho$). Similarly,

$$\langle \hat{p} \rangle_\psi = \langle \psi, \hat{p}\psi \rangle = \int_\Omega dx\, \psi^\dagger \frac{\hbar}{i}\frac{\partial}{\partial x}\psi. \tag{10}$$

The operator $\hat{p}$ satisfies the following relation:

$$\langle \psi, \hat{p}\phi \rangle - \langle \hat{p}\psi, \phi \rangle = -i\hbar \left[\psi^\dagger\phi\right]\Big|_a^b, \tag{11}$$

where we introduce the notation $[\,f\,]\big|_a^b = f(t,b) - f(t,a)$, and ψ and ϕ are vectors in $\mathcal{H}$. If the boundary conditions imposed on ψ and ϕ lead to the cancellation of the term evaluated at the endpoints of the interval Ω, we can write relation (11) as $\langle \psi, \hat{p}\phi \rangle = \langle \hat{p}\psi, \phi \rangle$. In this case, $\hat{p}$ is a hermitian operator. If we impose $\psi = \phi$ in this last relation and in Eq. (11), we obtain the following condition:

$$\left[\psi^\dagger\psi\right]\Big|_a^b = [\,\varrho\,]\Big|_a^b = 0. \tag{12}$$

What is more, $\langle \psi, \hat{p}\psi \rangle = \langle \hat{p}\psi, \psi \rangle = \overline{\langle \psi, \hat{p}\psi \rangle}$; therefore, $\mathrm{Im}\langle \psi, \hat{p}\psi \rangle = 0$, i. e., $\langle \hat{p} \rangle_\psi \in \mathbb{R}$.

The results that are relevant to the Hamiltonian operator $\hat{H}$ are the following. The way this operator acts was given in (5), where also $\hat{\beta} = \hat{\beta}^\dagger$ and $U(x) \in \mathbb{R}$. The mean value of $\hat{H}$ in the state $\psi = \psi(t, x) \in \mathcal{H}$ is the expression

$$\langle \hat{H} \rangle_\psi = \langle \psi, \hat{H}\psi \rangle = c \int_\Omega dx\, \psi^\dagger \hat{\alpha} \frac{\hbar}{i} \frac{\partial}{\partial x} \psi + mc^2 \int_\Omega dx\, \psi^\dagger \hat{\beta} \psi + \int_\Omega dx\, U \psi^\dagger \psi \tag{13}$$

and it satisfies the following relation:

$$\langle \psi, \hat{H}\phi \rangle - \langle \hat{H}\psi, \phi \rangle = -i\hbar c \left[\psi^\dagger \hat{\alpha} \phi \right]\Big|_a^b, \tag{14}$$

where ψ and ϕ are vectors in $\mathcal{H}$. If the boundary conditions imposed on ψ and ϕ lead to the cancellation of the term evaluated at the endpoints of the interval Ω, we can write relation (14) as $\langle \psi, \hat{H}\phi \rangle = \langle \hat{H}\psi, \phi \rangle$. In this case, $\hat{H}$ is a hermitian operator. If we impose $\psi = \phi$ in this last relation and in Eq. (14), we obtain the following condition:

$$c \left[\psi^\dagger \hat{\alpha} \psi \right]\Big|_a^b = [\, j\,]|_a^b = 0. \tag{15}$$

In addition, $\langle \psi, \hat{H}\psi \rangle = \langle \hat{H}\psi, \psi \rangle = \overline{\langle \psi, \hat{H}\psi \rangle}$; therefore, $\mathrm{Im}\langle \psi, \hat{H}\psi \rangle = 0$, i. e., $\langle \hat{H} \rangle_\psi \in \mathbb{R}$.

We would also like to introduce the following family of operators:

$$\hat{h}_A = c\hat{\Gamma}_A\, \hat{p}, \tag{16}$$

where the four 2×2 hermitian matrices $\hat{\Gamma}_A$ $(A = 1, 2, 3, 4)$ are

$$\hat{\Gamma}_1 = \hat{1}, \quad \hat{\Gamma}_2 = \hat{\alpha}, \quad \hat{\Gamma}_3 = \hat{\beta}, \quad \hat{\Gamma}_4 = i\hat{\beta}\hat{\alpha}. \tag{17}$$

We know that the following relations must be satisfied: $\hat{\alpha}\hat{\beta} + \hat{\beta}\hat{\alpha} = 0$ and $\hat{\alpha}^2 = \hat{\beta}^2 = \hat{1}$. Therefore, the matrices $\hat{\Gamma}_A$ have the following properties: (i) $\hat{\Gamma}_A^2 = \hat{1}$; (ii) $\hat{\Gamma}_B \hat{\Gamma}_A \hat{\Gamma}_B = -\hat{\Gamma}_A$ for $A \neq B$ and $A, B = 2, 3, 4$; therefore, (iii) $\mathrm{tr}(\hat{\Gamma}_A) = 0$ (where tr denotes the trace of a matrix); (iv) they are all linearly independent, and therefore, any 2×2 matrix can be expanded in terms of the $\hat{\Gamma}_A$. In other words, we can write an arbitrary 2×2 matrix, say $\hat{C}$, as $\hat{C} = \sum_{A=1}^4 C_A \hat{\Gamma}_A$, where $C_A = \mathrm{tr}(\hat{\Gamma}_A \hat{C})/2$. Naturally, the algebra generated by the $\hat{\Gamma}_A$ is a Clifford algebra. It is worth noting that if the arbitrary matrix $\hat{C}$ is hermitian, then $C_A \in \mathbb{R}$ (this is because $\hat{\Gamma}_A = \hat{\Gamma}_A^\dagger$). Let the following be the four real-valued quantities C_A:

$$C_A = c\psi^\dagger \hat{\Gamma}_A \psi. \tag{18}$$

These functions are usually known as bilinear densities, but they are also called bilinear covariants because they have definite transformation properties under the Lorentz transformations (in 1+1 dimensions). Specifically, $C_1 = c\varrho$ (the time component of a Lorentz divector) and $C_2 = j$ (the spatial component of a divector); furthermore, $C_3 \equiv cs = c\psi^\dagger \hat{\beta} \psi$ (a scalar) and $C_4 \equiv cw = c\psi^\dagger i\hat{\beta}\hat{\alpha}\psi$ (a pseudoscalar) [7]. In this article, we do not assign a specific name to the densities s and w. It is worth noting that the matrix $\hat{C}$ can be written as $\hat{C} = 2c\psi\psi^\dagger$. In effect, $C_A = \mathrm{tr}(\hat{\Gamma}_A 2c\psi\psi^\dagger)/2 = \mathrm{tr}(c\hat{\Gamma}_A \psi\psi^\dagger) = \mathrm{tr}(c\psi^\dagger \hat{\Gamma}_A \psi) = c\psi^\dagger \hat{\Gamma}_A \psi$. Moreover, the following properties of $\hat{C}$ can be verified: (i) $(\hat{C}/2c\varrho)^\dagger = \hat{C}/2c\varrho$. (ii) $(\hat{C}/2c\varrho)^2 = \hat{C}/2c\varrho$, and (iii) $\mathrm{tr}(\hat{C}/2c\varrho)^2 = 1$. Hence, $\hat{C}/2c\varrho$ is a density matrix and also a projector; therefore, it can represent the quantum state of the system, as well [8]. It is worth noting that property (ii) implies that $(c\varrho)^2 = (cs)^2 + j^2 + (cw)^2$, i. e., only three of the bilinear densities are independent [7].

The results that are relevant to the operators $\hat{h}_A = c\hat{\Gamma}_A\, \hat{p}$ are the following. We have $\hat{h}_1 = c\hat{p}$, so the results that are valid for $\hat{p}$ are obviously also valid for $\hat{h}_1$(Eqs. (11) and (12)). Similarly, the so-called Dirac operator, $\hat{h}_2 = c\hat{\alpha}\hat{p}$, also satisfies relations (14) and (15) as does the Hamiltonian operator ($\hat{H} = \hat{h}_2 + mc^2\hat{\beta} + U(x)$). In contrast, the operator $\hat{h}_3 = c\hat{\beta}\hat{p} = -i\hbar c\hat{\beta}\, \partial/\partial x$ satisfies the following relation:

$$\langle \psi, \hat{h}_3\phi \rangle - \langle \hat{h}_3\psi, \phi \rangle = -i\hbar c \left[\psi^\dagger \hat{\beta} \phi \right]\Big|_a^b, \tag{19}$$

where ψ and ϕ are vectors in $\mathcal{H}$. If the boundary conditions imposed on ψ and ϕ lead to the cancellation of the term evaluated at the endpoints of the interval Ω, we can write relation (19) as $\langle \psi, \hat{h}_3\phi \rangle = \langle \hat{h}_3\psi, \phi \rangle$. In this case, $\hat{h}_3$ is a hermitian operator. If we impose $\psi = \phi$ in this last relation and in Eq. (19), we obtain the following condition:

$$\left[\psi^\dagger \hat{\beta} \psi \right]\Big|_a^b = [\, s\,]|_a^b = 0. \tag{20}$$

In addition, $\langle \psi, \hat{h}_3\psi \rangle = \langle \hat{h}_3\psi, \psi \rangle = \overline{\langle \psi, \hat{h}_3\psi \rangle}$; therefore, $\mathrm{Im}\langle \psi, \hat{h}_3\psi \rangle = 0$, i. e., $\langle \hat{h}_3 \rangle_\psi \in \mathbb{R}$. In the same way, the operator $\hat{h}_4 = ci\hat{\beta}\hat{\alpha}\hat{p} = +\hbar c\hat{\beta}\hat{\alpha}\, \partial/\partial x$ satisfies the following relation:

$$\langle \psi, \hat{h}_4\phi \rangle - \langle \hat{h}_4\psi, \phi \rangle = -i\hbar c \left[\psi^\dagger i\hat{\beta}\hat{\alpha} \phi \right]\Big|_a^b, \tag{21}$$

where ψ and ϕ are functions in $\mathcal{H}$. Again, if the boundary conditions imposed on ψ and ϕ lead to the cancellation of the term evaluated at the endpoints of the interval Ω, we can write relation (21) as $\langle \psi, \hat{h}_4\phi \rangle = \langle \hat{h}_4\psi, \phi \rangle$. In this situation, $\hat{h}_4$ is a hermitian operator. By imposing $\psi = \phi$ in this last relation and in Eq. (21), we obtain the following condition:

$$\left[\psi^\dagger i\hat{\beta}\hat{\alpha} \psi \right]\Big|_a^b = [\, w\,]|_a^b = 0. \tag{22}$$

Additionally, $\langle \psi, \hat{h}_4\psi \rangle = \langle \hat{h}_4\psi, \psi \rangle = \overline{\langle \psi, \hat{h}_4\psi \rangle}$; therefore, $\mathrm{Im}\langle \psi, \hat{h}_4\psi \rangle = 0$, i. e., $\langle \hat{h}_4 \rangle_\psi \in \mathbb{R}$.

II. TIME DERIVATIVES FOR $\langle \hat{x} \rangle$, $\langle \hat{v} \rangle$, AND $\langle \hat{p} \rangle$

From formula (4) with $\hat{L} = \hat{x}$, we can write:

$$\frac{d}{dt}\langle \hat{x} \rangle_\psi = \frac{i}{\hbar}\left(\langle \hat{H}\psi, \hat{x}\psi \rangle - \langle \hat{H}\hat{x} \rangle_\psi \right) + \frac{i}{\hbar}\langle [\hat{H}, \hat{x}] \rangle_\psi. \tag{23}$$

We now compute the following scalar products:

$$\langle\hat{H}\psi,\hat{x}\psi\rangle = i\hbar c\int_\Omega dx\, x\frac{\partial\psi^\dagger}{\partial x}\hat{\alpha}\psi + mc^2\int_\Omega dx\, x\psi^\dagger\hat{\beta}\psi + \int_\Omega dx\, xU\psi^\dagger\psi,$$

$$\langle\hat{H}\hat{x}\rangle_\psi = -i\hbar c\int_\Omega dx\,\psi^\dagger\hat{\alpha}\frac{\partial}{\partial x}(x\psi) + mc^2\int_\Omega dx\, x\psi^\dagger\hat{\beta}\psi + \int_\Omega dx\, xU\psi^\dagger\psi.$$

By integrating by parts the first integral in $\langle\hat{H}\psi,\hat{x}\psi\rangle$ and then substracting these two expressions, we obtain

$$\langle\hat{H}\psi,\hat{x}\psi\rangle - \langle\hat{H}\hat{x}\rangle_\psi = +i\hbar\left[x\, c\psi^\dagger\hat{\alpha}\psi\right]\Big|_a^b = +i\hbar\left[\, xj\,\right]\Big|_a^b \tag{24}$$

(this result can also be obtained by imposing $\phi = \hat{x}\psi$ in relation (14)). Moreover, the mean value $\langle[\hat{H},\hat{x}]\rangle_\psi$ in Eq. (23) can be explicitly computed by using $\langle\hat{H}\hat{x}\rangle_\psi$ and calculating $\langle\hat{x}\hat{H}\rangle_\psi$; in effect,

$$\langle[\hat{H},\hat{x}]\rangle_\psi = \langle\hat{H}\hat{x}\rangle_\psi + i\hbar c\int_\Omega dx\, x\psi^\dagger\hat{\alpha}\frac{\partial\psi}{\partial x} - mc^2\int_\Omega dx\, x\psi^\dagger\hat{\beta}\psi - \int_\Omega dx\, xU\psi^\dagger\psi.$$

By developing this expression and simplifying, we obtain the result

$$\langle[\hat{H},\hat{x}]\rangle_\psi = -i\hbar c\int_\Omega dx\,\psi^\dagger\hat{\alpha}\psi = -i\hbar\int_\Omega dx\, j = -i\hbar\langle\hat{v}\rangle_\psi \tag{25}$$

where we have also used formula (8). Finally, Eq. (23) can be written as follows:

$$\frac{d}{dt}\langle\hat{x}\rangle_\psi = -\left[\, xj\,\right]\Big|_a^b + \langle\hat{v}\rangle_\psi. \tag{26}$$

The boundary term evaluated at the ends of the interval Ω does not vanish just because $\hat{H}$ and/or $\hat{h}_2$ are/is hermitian, i. e., in formula (26), condition (15) ($j(t,b) = j(t,a)$) is not sufficient to eliminate that boundary term. From the latter condition, we can write the formula $d\langle\hat{x}\rangle_\psi/dt = -(b-a)j(t,a) + \langle\hat{v}\rangle_\psi$; therefore, only a boundary condition that leads to the vanishing of the probability current density at $x = a$ ($\Rightarrow$ at $x = b$) gives the equation $d\langle\hat{x}\rangle_\psi/dt = \langle\hat{v}\rangle_\psi$ (see Eq. (1)). Let us specifically consider the Dirac representation, in which the Dirac matrices are $\hat{\alpha} = \hat{\sigma}_x$ and $\hat{\beta} = \hat{\sigma}_z$ (where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are two of the Pauli matrices) and the wavefunction is written as $\psi = \psi(t,x) \equiv (\phi(t,x)\;\chi(t,x))^\intercal$ (where ϕ is the so-called large component of ψ, and χ is the small component). In this representation, the probability current density is $j = c\psi^\dagger\hat{\sigma}_x\psi = c(\bar{\phi}\chi + \bar{\chi}\phi)$. For example, with the boundary condition $\phi(t,a) = \phi(t,b) = 0$, the operator $\hat{H}$ is hermitian [9]; therefore, the probability current density is zero at $x = a$ and $x = b$, but the boundary term in Eq. (26) also vanishes at the ends of Ω. However, with the periodic boundary condition $\psi(t,a) = \psi(t,b)$ ($\Rightarrow \phi(t,a) = \phi(t,b)$ and $\chi(t,a) = \chi(t,b)$), $\hat{H}$ is hermitian [9] and, therefore, Eq. (15) is satisfied, but the boundary term in Eq. (26) is not zero. It is worth noting that boundary terms arising from the term $\langle\hat{H}\psi,\hat{L}\psi\rangle - \langle\psi,\hat{H}\hat{L}\psi\rangle$ (see Eq. (4)) usually cancel because the particle lies inside the (open) interval $\Omega = (-\infty,+\infty)$, and the wavefunction and its successive derivatives tend to zero when $x\to\pm\infty$. Clearly, one cannot automatically assume that these terms are zero if the interval is, for example, finite. However, the boundary term in Eq. (26) always vanishes if the following operator, sometimes called the center-of-energy operator (see Ref. [2], pag. 8), is hermitian:

$$\hat{N} = \frac{1}{2}(\hat{H}\hat{x}+\hat{x}\hat{H}) = -i\hbar c\,\hat{\alpha}\left(x\frac{\partial}{\partial x}+\frac{1}{2}\right)+mc^2x\hat{\beta}+xU(x).$$

In fact, this operator satisfies the following relation:

$$\langle\psi,\hat{N}\phi\rangle - \langle\hat{N}\psi,\phi\rangle = -i\hbar c\left[x\psi^\dagger\hat{\alpha}\phi\right]\Big|_a^b.$$

By assuming that $\hat{N}$ is hermitian, the latter boundary term vanishes, i. e., we find that $\left[x\, c\psi^\dagger\hat{\alpha}\psi\right]\Big|_a^b = \left[\, xj\,\right]\Big|_a^b = 0$.

It is worth mentioning that the probability density that corresponds to the energy-eigenstate solutions to the Dirac equation in one dimension, for a constant (or uniform) external potential, is different to zero almost everywhere [10, 11] (in fact, this is not necessarily true at infinite), i. e., the entire eigensolution does not vanish at a boundary. What is more, the Hamiltonian operator with a (bounded-from-below) potential in a closed interval is not self-adjoint for the Dirichlet boundary condition [9, 12], but it is a hermitian operator. In any case, there are many boundary conditions for which the Hamiltonian is self-adjoint and therefore hermitian. Some examples are (*i*) $\phi(t,a) = \phi(t,b) = 0$, (*ii*) $\chi(t,a) = \chi(t,b) = 0$, (*iii*) $\phi(t,a) = \chi(t,b) = 0$, (*iv*) $\chi(t,a) = \phi(t,b) = 0$, and (*v*) $\psi(t,a) = \psi(t,b)$ (Ref. [9] contains more examples of self-adjoint boundary conditions).

Returning to Eq. (23), it is clear that by developing (and simplifying) that result, we can write

$$\frac{d}{dt}\langle\hat{x}\rangle_\psi = \frac{i}{\hbar}\langle\hat{H}\psi,\hat{x}\psi\rangle - \frac{i}{\hbar}\langle\psi,\hat{x}\hat{H}\psi\rangle.$$

Now, as we know that $\langle\psi,\hat{x}\hat{H}\psi\rangle = \langle\hat{x}\psi,\hat{H}\psi\rangle$ (from Eq. (7) with $\phi = \hat{H}\psi$), we can write the following result:

$$\frac{d}{dt}\langle\hat{x}\rangle_{\psi} = \frac{i}{\hbar}\langle\hat{H}\psi,\hat{x}\psi\rangle - \frac{i}{\hbar}\overline{\langle\hat{H}\psi,\hat{x}\psi\rangle} = -\frac{2}{\hbar}\mathrm{Im}\langle\hat{H}\psi,\hat{x}\psi\rangle. \qquad (27)$$

Clearly, this (real-valued) expression is equivalent to Eq. (23). To be precise, formula (26) was also obtained in Ref. [5], but there the emphasis was on the validity of Eq. (27) each time that $\hat{x}$ is hermitian.

Similarly, from the formula (4) with $\hat{L} = \hat{v}$, we can write

$$\frac{d}{dt}\langle\hat{v}\rangle_{\psi} = \frac{i}{\hbar}\left(\langle\hat{H}\psi,\hat{v}\psi\rangle - \langle\hat{H}\hat{v}\rangle_{\psi}\right) + \frac{i}{\hbar}\langle[\hat{H},\hat{v}]\rangle_{\psi}. \qquad (28)$$

We now compute the following scalar products:

$$\langle\hat{H}\psi,\hat{v}\psi\rangle = i\hbar c^2\int_{\Omega}dx\,\frac{\partial\psi^{\dagger}}{\partial x}\psi + mc^2\int_{\Omega}dx\,\psi^{\dagger}\hat{\beta}\hat{v}\psi + \int_{\Omega}dx\,U\psi^{\dagger}\hat{v}\psi,$$

$$\langle\hat{H}\hat{v}\rangle_{\psi} = -i\hbar c\int_{\Omega}dx\,\psi^{\dagger}\frac{\partial\psi}{\partial x} + mc^2\int_{\Omega}dx\,\psi^{\dagger}\hat{\beta}\hat{v}\psi + \int_{\Omega}dx\,U\psi^{\dagger}\hat{v}\psi.$$

By integrating by parts the first integral in $\langle\hat{H}\psi,\hat{v}\psi\rangle$ and then substracting these two expressions, we obtain

$$\langle\hat{H}\psi,\hat{v}\psi\rangle - \langle\hat{H}\hat{v}\rangle_{\psi} = +i\hbar c^2\left[\psi^{\dagger}\psi\right]\Big|_a^b = +i\hbar c^2\left[\,\varrho\,\right]\Big|_a^b \qquad (29)$$

(this result can also be obtained by imposing $\phi = \hat{v}\psi$ in relation (14)). Additionally, the mean value $\langle[\hat{H},\hat{v}]\rangle_{\psi}$ in Eq. (28) can be explicitly computed using $\langle\hat{H}\hat{v}\rangle_{\psi}$ and calculating $\langle\hat{v}\hat{H}\rangle_{\psi}$; in effect,

$$\langle[\hat{H},\hat{v}]\rangle_{\psi} = \langle\hat{H}\hat{v}\rangle_{\psi} + i\hbar c^2\int_{\Omega}dx\,\psi^{\dagger}\frac{\partial\psi}{\partial x} - mc^2\int_{\Omega}dx\,\psi^{\dagger}\hat{v}\hat{\beta}\psi - \int_{\Omega}dx\,U\psi^{\dagger}\hat{v}\psi.$$

By developing this expression and simplifying, we obtain the following result:

$$\langle[\hat{H},\hat{v}]\rangle_{\psi} = mc^2\int_{\Omega}dx\,\psi^{\dagger}[\hat{\beta},\hat{v}]\psi = 2mc^2\int_{\Omega}dx\,\psi^{\dagger}\hat{\beta}\hat{v}\psi = \frac{\hbar}{i}\langle\hat{a}\rangle_{\psi}, \qquad (30)$$

where we have also made use of the relation $\hat{v}\hat{\beta}+\hat{\beta}\hat{v}=0$. The acceleration operator, $\hat{a} = 2mc^2 i\hat{\beta}\hat{v}/\hbar$, is a hermitian matrix because $\hat{v} = c\hat{\alpha}$ and $\hat{\beta}$ are hermitian; as a result, it satisfies the following relation:

$$\langle\psi,\hat{a}\phi\rangle - \langle\hat{a}\psi,\phi\rangle = 0, \qquad (31)$$

where ψ and ϕ are functions belonging to $\mathcal{H}$. As expected, we can also write the result $\langle\psi,\hat{a}\psi\rangle = \langle\hat{a}\psi,\psi\rangle = \overline{\langle\psi,\hat{a}\psi\rangle}$; therefore, $\mathrm{Im}\langle\psi,\hat{a}\psi\rangle = 0$, i. e., $\langle\hat{a}\rangle_{\psi}\in\mathbb{R}$. Note that an acceleration field defined as $A = A(t,x) = 2mc^3 w/\hbar\varrho$ has the same mean value as the operator $\hat{a}$, i. e., $\langle A\rangle_{\psi} = \langle\hat{a}\rangle_{\psi}$ (this is so because $\langle A\rangle_{\psi} = \int_{\Omega}dx\,A\varrho$). Finally, Eq. (28) can be written as follows:

$$\frac{d}{dt}\langle\hat{v}\rangle_{\psi} = -c^2\left[\,\varrho\,\right]\Big|_a^b + \langle\hat{a}\rangle_{\psi}. \qquad (32)$$

Returning to results (28) and (29), we can simply write

$$\frac{d}{dt}\langle\hat{v}\rangle_{\psi} = -c^2\left[\,\varrho\,\right]\Big|_a^b + \frac{i}{\hbar}\langle[\hat{H},\hat{v}]\rangle_{\psi},$$

where the commutator can be written as $[\hat{H},\hat{v}] = \hat{H}\hat{v} + \hat{v}\hat{H} - 2\hat{v}\hat{H}$. By substituting the Hamiltonian operator (Eq.(5)) into this commutator, developing this quantity and simplifying, we obtain the following result: $[\hat{H},\hat{v}] = 2c^2\hat{p} + 2U(x)\,\hat{v} - 2\hat{v}\hat{H}$. Therefore,

$$\langle[\hat{H},\hat{v}]\rangle_{\psi} = 2c^2\langle\hat{p}\rangle_{\psi} + 2\langle U\hat{v}\rangle_{\psi} - 2\langle\hat{v}\hat{H}\rangle_{\psi}. \qquad (33)$$

Consequently, result (32) can also be written as

$$\frac{d}{dt}\langle\hat{v}\rangle_{\psi} = -c^2\left[\,\varrho\,\right]\Big|_a^b + \frac{2ic^2}{\hbar}\langle\hat{p}\rangle_{\psi} + \frac{2i}{\hbar}\langle U\hat{v}\rangle_{\psi} - \frac{2i}{\hbar}\langle\hat{v}\hat{H}\rangle_{\psi}. \qquad (34)$$

Once again, the boundary term in (32) and/or (34) does not necessarily vanish because condition (15) is satisfied (or because $\hat{H}$ and/or $\hat{h}_2$ are/is hermitian). An example of this situation is provided by the boundary condition $\phi(t,a) = \phi(t,b) = 0$. Certainly, with this boundary condition, $\hat{H}$ is hermitian [9], but the boundary term in (32) and/or (34) is not necessarily zero. However, for the periodic boundary condition, $\phi(t,a) = \phi(t,b)$ and $\chi(t,a) = \chi(t,b)$, the boundary term in (32) and/or (34) does vanish. Therefore, only a boundary condition that leads to the same value of the probability density ($\varrho = \psi^{\dagger}\psi = \bar{\phi}\phi + \bar{\chi}\chi$) at both ends of the interval Ω (i. e., $\varrho(t,a) = \varrho(t,b)$) yields the equation $d\langle\hat{v}\rangle_{\psi}/dt =$

$\langle \hat{a} \rangle_\psi = 2i(c^2 \langle \hat{p} \rangle_\psi + \langle U \hat{v} \rangle_\psi - \langle \hat{v} \hat{H} \rangle_\psi)/\hbar$. Note the agreement of these results with those given in Eq. (2). To be precise, in Eq. (2), $\hat{\mathbf{\Sigma}}$ is the spin operator in units of $\hbar/2$ for the Dirac particle in three dimensions; nevertheless, for a Dirac particle in one dimension, there is no orbital angular momentum and therefore no need for an intrinsic angular momentum. Let us also add that boundary conditions for which the momentum operator is a hermitian operator always lead to the cancellation of the boundary term in (32) and/or (34) (see the discussion that precedes Eq. (12)).

Returning to Eq. (28), it is clear that by developing (and simplifying) that result, we can write

$$\frac{d}{dt} \langle \hat{v} \rangle_\psi = \frac{i}{\hbar} \langle \hat{H}\psi, \hat{v}\psi \rangle - \frac{i}{\hbar} \langle \psi, \hat{v}\hat{H}\psi \rangle.$$

Now, as we know that $\langle \psi, \hat{v}\hat{H}\psi \rangle = \langle \hat{v}\psi, \hat{H}\psi \rangle$ (from Eq. (9) with $\phi = \hat{H}\psi$), we can write the following result:

$$\frac{d}{dt} \langle \hat{v} \rangle_\psi = \frac{i}{\hbar} \langle \hat{H}\psi, \hat{v}\psi \rangle - \frac{i}{\hbar} \overline{\langle \hat{H}\psi, \hat{v}\psi \rangle} = -\frac{2}{\hbar} \mathrm{Im} \langle \hat{H}\psi, \hat{v}\psi \rangle. \tag{35}$$

Clearly, this expression is always equivalent to Eq. (28) [5].

By the same token, from formula (4) with $\hat{L} = \hat{p}$, we can write

$$\frac{d}{dt} \langle \hat{p} \rangle_\psi = \frac{i}{\hbar} \left(\langle \hat{H}\psi, \hat{p}\psi \rangle - \langle \hat{H}\hat{p} \rangle_\psi \right) + \frac{i}{\hbar} \langle [\hat{H}, \hat{p}] \rangle_\psi. \tag{36}$$

We now compute the following scalar products:

$$\langle \hat{H}\psi, \hat{p}\psi \rangle = \hbar^2 c \int_\Omega dx \, \frac{\partial \psi^\dagger}{\partial x} \hat{\alpha} \frac{\partial \psi}{\partial x} - i\hbar m c^2 \int_\Omega dx \, \psi^\dagger \hat{\beta} \frac{\partial \psi}{\partial x} - i\hbar \int_\Omega dx \, U \psi^\dagger \frac{\partial \psi}{\partial x},$$

$$\langle \hat{H}\hat{p} \rangle_\psi = -\hbar^2 c \int_\Omega dx \, \psi^\dagger \hat{\alpha} \frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial x} \right) - i\hbar m c^2 \int_\Omega dx \, \psi^\dagger \hat{\beta} \frac{\partial \psi}{\partial x} - i\hbar \int_\Omega dx \, U \psi^\dagger \frac{\partial \psi}{\partial x}.$$

By integrating by parts the first integral in $\langle \hat{H}\psi, \hat{p}\psi \rangle$ and then substracting these two expressions, we obtain

$$\langle \hat{H}\psi, \hat{p}\psi \rangle - \langle \hat{H}\hat{p} \rangle_\psi = +\hbar^2 c \left[\psi^\dagger \hat{\alpha} \frac{\partial \psi}{\partial x} \right] \Big|_a^b = +i\hbar \left[\psi^\dagger c \hat{\alpha} \hat{p} \psi \right] \Big|_a^b$$

$$= -i\hbar \left[-\psi^\dagger \hat{H} \psi + mc^2 s + U \varrho \right] \Big|_a^b \tag{37}$$

(this result can also be obtained by imposing $\phi = \hat{p}\psi$ in relation (14)). Similarly, the mean value $\langle [\hat{H}, \hat{p}] \rangle_\psi$ in Eq. (36) can be explicitly computed using $\langle \hat{H}\hat{p} \rangle_\psi$ and calculating $\langle \hat{p}\hat{H} \rangle_\psi$; in effect,

$$\langle [\hat{H}, \hat{p}] \rangle_\psi = \langle \hat{H}\hat{p} \rangle_\psi + \hbar^2 c \int_\Omega dx \, \psi^\dagger \hat{\alpha} \frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial x} \right) + i\hbar m c^2 \int_\Omega dx \, \psi^\dagger \hat{\beta} \frac{\partial \psi}{\partial x}$$

$$+ i\hbar \int_\Omega dx \, \psi^\dagger \frac{\partial}{\partial x} (U\psi).$$

By developing this expression and simplifying, we obtain the following result:

$$\langle [\hat{H}, \hat{p}] \rangle_\psi = -\frac{\hbar}{i} \int dx \, \psi^\dagger \frac{dU}{dx} \psi = \frac{\hbar}{i} \langle \hat{f} \rangle_\psi, \tag{38}$$

where $\hat{f} = f(x) = -dU/dx$ is the external classical force operator. Finally, Eq. (36) can be written as follows:

$$\frac{d}{dt} \langle \hat{p} \rangle_\psi = -\left[\psi^\dagger c \hat{\alpha} \hat{p} \psi \right] \Big|_a^b + \langle \hat{f} \rangle_\psi \tag{39}$$
$$= -i\hbar \left[\psi^\dagger \frac{\partial \psi}{\partial t} \right] \Big|_a^b + \left[mc^2 s + U \varrho \right] \Big|_a^b + \langle \hat{f} \rangle_\psi,$$

where we have used the formula $\hat{H} = i\hbar \partial/\partial t$.

Returning to Eq. (36), it is clear that this formula can also be written as follows:

$$\frac{d}{dt} \langle \hat{p} \rangle_\psi = \frac{i}{\hbar} \langle \hat{H}\psi, \hat{p}\psi \rangle - \frac{i}{\hbar} \langle \psi, \hat{p}\hat{H}\psi \rangle.$$

Now, by using Eq. (11) with $\phi = \hat{H}\psi = i\hbar \partial\psi/\partial t$, we can write the following result:

$$\langle \psi, \hat{p}\hat{H}\psi \rangle = \langle \hat{p}\psi, \hat{H}\psi \rangle + \hbar^2 \left[\psi^\dagger \frac{\partial \psi}{\partial t} \right] \Big|_a^b, \tag{40}$$

and by substituting for $\langle\psi, \hat{p}\hat{H}\psi\rangle$ in the previous relation, the following formula is obtained:

$$\frac{d}{dt}\langle\hat{p}\rangle_\psi = -\frac{2}{\hbar}\mathrm{Im}\langle\hat{H}\psi, \hat{p}\psi\rangle - i\hbar\left[\psi^\dagger\frac{\partial\psi}{\partial t}\right]\Big|_a^b. \tag{41}$$

Indeed, formulas (39) and (41) are equivalent. Note that if the boundary conditions imposed on ψ lead to the cancellation of the boundary term in the latter equation (and in Eq. (40)), the operator $\hat{p}$ will be hermitian, i.e., Eq. (12) is satisfied (the spatial part of the boundary term in Eq. (40) is not affected by the presence of the time derivative). For instance, the operator $\hat{p}$ (in an interval) is self-adjoint (and therefore hermitian) when $\psi(t,b) = \hat{M}\psi(t,a)$ (where the matrix $\hat{M}$ is unitary). Then, we also have $\dot{\psi}(t,b) = \hat{M}\dot{\psi}(t,a)$ (where the dot represents a time derivative), and therefore the boundary term in Eq. (40) vanishes. Note that as an immediate consequence of Eq. (12) (provided that $U|_a^b = 0$), Eq. (39) takes the form $d\langle\hat{p}\rangle_\psi/dt = mc^2\,[\,s\,]|_a^b + \langle\hat{f}\rangle_\psi$, i.e., we could have a nonzero boundary term. However, some boundary conditions that satisfy Eq. (12) could also satisfy $[\,s\,]|_a^b = 0$ (Eq. (20)). In fact, the latter condition is satisfied if, in addition, we have $\hat{\beta} = \hat{M}^{-1}\hat{\beta}\hat{M}$. Lastly, it is worthwhile to note that the boundary term $[\,s\,]|_a^b$ can be written as the mean value of the following force field (or boundary quantum force): $F = F(t,x) = mc^2\varrho^{-1}\partial s/\partial x$ (this is so because $\langle F\rangle_\psi = \int_\Omega dx\, F\varrho$). Hence, we can write the following nice expression: $d\langle\hat{p}\rangle_\psi/dt = \langle F\rangle_\psi + \langle\hat{f}\rangle_\psi$.

As a final illustration of formula (39), let us consider the problem of a Dirac particle in a finite step potential: $U(x) = V_0\Theta(x)$ ($x \in \Omega = (a,b) = (-\infty, +\infty)$), where $\Theta(x)$ is the Heaviside step function. We consider a normalizable wavefunction $\psi = \psi(t,x)$, i.e., $\psi(t, x \to \pm\infty) = 0$. We can then conclude (from Eq. (39)) that

$$\frac{d}{dt}\langle\hat{p}\rangle_\psi = \langle\hat{f}\rangle_\psi, \tag{42}$$

where the external classical force operator is $\hat{f} = -dU/dx = -V_0\delta(x)$, and $\delta(x) = d\Theta(x)/dx$ is the Dirac delta function. Clearly, the mean value of $\hat{f}$ in the state ψ can be immediately obtained as follows:

$$\langle\hat{f}\rangle_\psi = \langle\psi, \hat{f}\psi\rangle = -V_0\int_{-\infty}^{+\infty} dx\,\delta(x)\psi^\dagger(t,x)\psi(t,x) \\ = -V_0\,\varrho(t,0). \tag{43}$$

This result can alternatively be obtained as follows: (a) multiply (properly) the (time-dependent) Dirac equation for ψ by $\partial\psi^\dagger/\partial x$ and the equation for $\psi^\dagger$ by $\partial\psi/\partial x$, and then sum the two resulting equations; (b) integrate each term of the result obtained in (a) around $x = 0$. We finally obtain

$$-\int_{0-}^{0+} dx\,\frac{dU(x)}{dx}\psi^\dagger(t,x)\psi(t,x) \\ = -\int_{-\infty}^{+\infty} dx\,\frac{dU(x)}{dx}\psi^\dagger(t,x)\psi(t,x) \tag{44} \\ = \langle\hat{f}\rangle_\psi = -mc^2\,[\,s\,]|_{0-}^{0+} - [\,U\varrho\,]|_{0-}^{0+},$$

where we use the notation $0\pm = \lim_{\epsilon\to 0}(0\pm\epsilon)$. In this problem, because we have $s(t,0+) = s(t,0-) \equiv s(t,0)$ and $\varrho(t,0+) = \varrho(t,0-) \equiv \varrho(t,0)$ as well as $U(0+) = V_0$ and $U(0-) = 0$, we obtain result (43), as expected.

Let us suppose that the particle with positive energy is approaching the potential step such that $E - V_0 < 0$, or more specifically, $E - V_0 < -mc^2$ ($\Rightarrow V_0 > E + mc^2$), and momentum $\hbar k > 0$ (this interesting energy range is associated with the so-called Klein energy zone). The physical eigensolutions of the (time-independent) Dirac equation $\hat{H}\psi = E\psi$ in the Dirac representation (see the Hamiltonian operator in Eq. (5)) must be written as follows:

$$\psi(x) = \Theta(-x)\,[\psi_{\mathrm{i}}(x) + \psi_{\mathrm{r}}(x)] + \Theta(x)\psi_{\mathrm{t}}(x), \tag{45}$$

where the incoming and reflected solutions are given by

$$\psi_{\mathrm{i}}(x \le 0) = \begin{pmatrix} 1 \\ a \end{pmatrix} e^{ikx}, \\ \psi_{\mathrm{r}}(x \le 0) = \left(\frac{a+b}{a-b}\right)\begin{pmatrix} 1 \\ -a \end{pmatrix} e^{-ikx}, \tag{46}$$

respectively, whereas the transmitted solution is given by

$$\psi_{\mathrm{t}}(x \ge 0) = \frac{2a}{a-b}\begin{pmatrix} 1 \\ -b \end{pmatrix} e^{-i\kappa x} \tag{47}$$

(in addition, these solutions satisfy the boundary condition $\psi_{\mathrm{i}}(0) + \psi_{\mathrm{r}}(0) = \psi_{\mathrm{t}}(0)$). The (real-valued) quantities a and b are given below:

$$a = \frac{c\,\hbar k}{E + mc^2} > 0\,, \quad b = \frac{c\,\hbar\kappa}{E - V_0 + mc^2} < 0, \tag{48}$$

where

$$c\,\hbar k = \sqrt{E^2 - (mc^2)^2} > 0, \\ c\,\hbar\kappa = \sqrt{(E - V_0)^2 - (mc^2)^2} > 0. \tag{49}$$

It is noteworthy that both $E - V_0 + mc^2$ and $E - V_0 - mc^2$ are negative. Likewise, the reflection and transmission coefficients are

$$R = \frac{|\,j_{\mathrm{r}}(x)|}{|\,j_{\mathrm{i}}(x)|} = \left(\frac{a+b}{a-b}\right)^2, \quad T = \frac{|\,j_{\mathrm{t}}(x)|}{|\,j_{\mathrm{i}}(x)|} = \frac{4a\,|b|}{(a-b)^2}, \tag{50}$$

where the incident ($j_{\mathrm{i}}(x)$), reflected ($j_{\mathrm{r}}(x)$) and transmitted ($j_{\mathrm{t}}(x)$) probability current densities are calculated for the solutions $\psi_{\mathrm{i}}(x)$, $\psi_{\mathrm{r}}(x)$ and $\psi_{\mathrm{t}}(x)$, respectively (in the Dirac representation, i.e., $j_{\mathrm{i}} = c\psi_{\mathrm{i}}^\dagger\hat{\sigma}_x\psi_{\mathrm{i}}$, etc). It can be easily shown that $R + T = 1$ (in fact, we have $R < 1$, and particularly $R \to 1$ when $V_0 \to E + mc^2$, because $b \to -\infty$), and there is no paradox. Notice that we have only used solutions of the single-particle Dirac equation. In this regard, our results are mathematically similar to those reported, for example, in Ref. [13].

The momentum values associated with the transmitted wave are the eigenvalues of $\hat{p} = -i\hbar\partial/\partial x$ that correspond to $\psi_{\rm t}(x)$; therefore (from Eq. (47)), these values satisfy $-\hbar\kappa < 0$. However, the transmitted velocity field (constant) is given by

$$V_{\rm t}(x) = \frac{j_{\rm t}(x)}{\varrho_{\rm t}(x)} = \frac{-2cb}{1+b^2} = \frac{-c^2\hbar\kappa}{E-V_0} = c\sqrt{1-\left(\frac{mc^2}{E-V_0}\right)^2} > 0, \qquad (51)$$

i. e., it is positive, as expected. Likewise, the mean value of $\hat{f}$ in the eigenstate ψ given by Eq. (45) can be obtained from the following formula (see Eq. (43)):

$$\langle \hat{f}\rangle_\psi = -V_0\varrho_{\rm t}(0) = -V_0\frac{4a^2(1+b^2)}{(a-b)^2}. \qquad (52)$$

As is well known, when $V_0 \to \infty$ (a very strong field), the finite step potential becomes an infinite step potential. However, the latter potential is not an impenetrable barrier, unlike in the non-relativistic case. Let us expand $\langle \hat{f}\rangle_\psi$ into a series that involves positive powers of $\varepsilon \equiv mc^2/(V_0-E)$:

$$\langle \hat{f}\rangle_\psi = -V_0\frac{8a^2}{\left(a+\sqrt{\frac{1+\varepsilon}{1-\varepsilon}}\right)^2(1-\varepsilon)}$$

$$= -V_0\frac{8a^2}{(a+1)^2}\varepsilon^0 - V_0\frac{8a^2}{(a+1)^2}\frac{(a-1)}{(a+1)}\varepsilon^1 - V_0\,O(\varepsilon^2). \qquad (53)$$

Clearly, in the limit of $V_0 \to \infty$, we obtain the following result:

$$\langle \hat{f}\rangle_\psi = -\infty - mc^2\frac{8a^2(a-1)}{(a+1)^3} + 0 = -\infty. \qquad (54)$$

That is to say, only the second term in the expansion given in Eq. (53) is a finite constant and independent of V_0 when $V_0 \to \infty$; this is the same as in the non-relativistic case for solutions of the Schrödinger equation [14]. Naturally, in the non-relativistic case for $V_0 \gg E$, no solution as that given in Eq. (45) is obtained.

III. CONCLUSIONS

In summary, we have calculated in detail formal time derivatives of $\langle\hat{x}\rangle$, $\langle\hat{v}\rangle$ and $\langle\hat{p}\rangle$ for a one-dimensional Dirac particle. As we have seen, these quantities contain boundary terms that will not necessarily be simultaneously equal to zero, and these boundary terms can be (essentially) obtained by simply evaluating a bilinear density at both ends of the interval and then subtracting the two results. Similar (but not necessarily equal) terms to these must be zero if one claims the hermiticity of certain specific unbounded operators. For example, it is not sufficient that $\hat{H}$ be a hermitian operator to satisfy the relation $d\langle\hat{x}\rangle_\psi/dt = \langle\hat{v}\rangle_\psi$. This is because the relation $[\,j\,]|_a^b = 0$ does not imply that $[\,xj\,]|_a^b = 0$ (see Eqs. (15) and (26)). On the other hand, if $\hat{p}$ is a hermitian operator ($\Rightarrow [\,\varrho\,]|_a^b = 0$), then $d\langle\hat{v}\rangle_\psi/dt = \langle\hat{a}\rangle_\psi$, but $d\langle\hat{p}\rangle_\psi/dt = mc^2\,[\,s\,]|_a^b + \langle\hat{f}\rangle_\psi$, provided that $U|_a^b = 0$. Likewise, the condition $[\,j\,]|_a^b = 0$ is clearly not a sufficient condition to ensure that the boundary terms in the latter two time derivatives are zero (see Eqs. (12), (32) and (39)). Moreover, $\langle\hat{v}\rangle_\psi$ is the same as $\langle V\rangle_\psi$, where $V = j/\varrho$ is the velocity field; also, $\langle\hat{a}\rangle_\psi$ is equal to $\langle A\rangle_\psi$, where $A = 2mc^3w/\hbar\varrho$ is the acceleration field. In addition, we can write the expression $mc^2\,[\,s\,]|_a^b = \langle F\rangle_\psi$, where $F = mc^2\varrho^{-1}\partial s/\partial x$ is a type of force field.

As we have seen, a relationship generally exists between an unbounded hermitian operator and a bilinear density (via a vanishing boundary term). For example, in addition to the relation between $\hat{H}$ (and $\hat{h}_2 = c\hat{\alpha}\hat{p}$) and $[\,j\,]|_a^b = 0$ as well as that between $\hat{p}$ (and $\hat{h}_1 = c\hat{p}$) and $[\,\varrho\,]|_a^b = 0$, the hermiticity of $\hat{h}_3 = c\hat{\beta}\hat{p}$ is also connected to $[\,s\,]|_a^b = 0$, and in like manner, $\hat{h}_4 = ci\hat{\beta}\hat{\alpha}\hat{p}$ is related to $[\,w\,]|_a^b = 0$. Furthermore, there exists a relation that connects the bilinear densities of interest (j, ϱ, s and w). We have recently studied more of these matters, as well as certain connections among self-adjoint general boundary conditions for each of the four operators $\hat{h}_A = c\hat{\Gamma}_A\,\hat{p}$ [15]. We believe that various aspects of our study may be attractive to all who are interested in the fundamentals of quantum mechanics.

IV. APPENDIX

The free Dirac equation in covariant form is

$$(i\hbar\hat{\gamma}^\mu\partial_\mu - mc)\psi = 0. \qquad (A1)$$

Here, $\hat{\gamma}^\mu$, with $\mu = 0, 1.$, are the Dirac gamma matrices (remember that we are in (1+1) dimensions). Specifically, we have $\hat{\gamma}^0 = \hat{\beta}$, $\hat{\gamma}^1 = \hat{\beta}\hat{\alpha}$, and therefore $(\hat{\gamma}^0)^2 = -(\hat{\gamma}^1)^2 = \hat{1}$; and also $(\hat{\gamma}^\mu)^\dagger = \hat{\gamma}^0\hat{\gamma}^\mu\hat{\gamma}^0$. The standard minimal substitution, $\partial_\mu \to \partial_\mu + \frac{ie}{\hbar c}A_\mu$, where $A^\mu = (\varphi, \mathcal{A})$, can be introduced into Eq. (A1), but we could also introduce into Eq. (A1) a covariant potential of the form $\varphi_{\rm sc\oplus ps} = \frac{1}{c}S\hat{1} + \frac{1}{c}W\hat{\gamma}^5$, where S is a scalar potential, W is a pseudoscalar potential (under the Lorentz transformation), and $\hat{\gamma}^5 \equiv i\hat{\gamma}^0\hat{\gamma}^1 = i\hat{\alpha} = -(\hat{\gamma}^5)^\dagger$. By making these substitutions, the Dirac equation (A1) takes the form

$$\left[i\hbar\hat{\gamma}^\mu(\partial_\mu + \tfrac{ie}{\hbar c}A_\mu) - \varphi_{\mathrm{sc}\oplus\mathrm{ps}} - mc\right]\psi = (i\hbar\hat{\gamma}^\mu\partial_\mu - U_{\mathrm{cov}} - mc)\psi = 0, \tag{A2}$$

where

$$U_{\mathrm{cov}} = \tfrac{e}{c}A_\mu\hat{\gamma}^\mu + \varphi_{\mathrm{sc}\oplus\mathrm{ps}} = \tfrac{1}{c}S\hat{1} + \tfrac{e}{c}A_\mu\hat{\gamma}^\mu + \tfrac{1}{c}W\hat{\gamma}^5 \tag{A3}$$

is a general covariant potential (in fact, this is the most general Lorentz potential in (1+1) dimensions).

The latter equation can be easily rewritten as follows (by multiplying (A2) from the left with $c\hat{\beta}$):

$$i\hbar\,\partial_t\psi = \hat{H}\psi, \tag{A4}$$

where the Hamiltonian operator is

$$\hat{H} = c\hat{\alpha}(\hat{p} - \tfrac{e}{c}\mathcal{A}) + mc^2\hat{\beta} + U + S\hat{\beta} + Wi\hat{\beta}\hat{\alpha}. \tag{A5}$$

This operator is hermitian because the potentials, $\varphi = U/e$ (the time component of the two-vector A^μ), $\mathcal{A}$ (the spatial component of A^μ), S, and W, are real-valued functions. Moreover, $i\hat{\beta}\hat{\alpha}$ is a hermitian matrix because $\hat{\alpha}$ and $\hat{\beta}$ are also hermitian; thus, these matrices verify the following relations:

$$\langle\psi, i\hat{\beta}\hat{\alpha}\phi\rangle - \langle i\hat{\beta}\hat{\alpha}\psi, \phi\rangle = 0, \tag{A6}$$

$$\langle\psi, \hat{\alpha}\phi\rangle - \langle\hat{\alpha}\psi, \phi\rangle = 0, \tag{A7}$$

$$\langle\psi, \hat{\beta}\phi\rangle - \langle\hat{\beta}\psi, \phi\rangle = 0, \tag{A8}$$

where ψ and ϕ are functions belonging to $\mathcal{H}$.

As we know, the formal time derivative of the mean value of an operator depends of the Hamiltonian operator (see Eq. (4)); thus, we expect to obtain new terms in the Ehrenfest theorem when we use the Hamiltonian (A5). Although the first Ehrenfest equation, say, does not change,

$$\frac{d}{dt}\langle\hat{x}\rangle_\psi = -\left[\,xj\,\right]\Big|_a^b + \langle\hat{v}\rangle_\psi, \tag{A9}$$

i.e., this is just the Eq. (26). Again, because the operator (A5) is hermitian, then $[\,j\,]\big|_a^b = 0$ (see Eq. (15)). However, the second Ehrenfest equation is

$$\frac{d}{dt}\langle\hat{v}\rangle_\psi = -c^2\left[\,\varrho\,\right]\Big|_a^b + \langle\hat{a}\rangle_\psi + \langle\hat{a}_{\mathrm{S}}\rangle_\psi + \langle\hat{a}_{\mathrm{W}}\rangle_\psi, \tag{A10}$$

where, as before, $\hat{a} = 2mc^2 i\hat{\beta}\hat{v}/\hbar$ is the acceleration operator (see Eq. (32)). Moreover, $\hat{a}_{\mathrm{S}} = 2Si\hat{\beta}\hat{v}/\hbar$ is an acceleration operator linked to the scalar potential S, and $\hat{a}_{\mathrm{W}} = -2cW\hat{\beta}/\hbar$ is an acceleration operator linked to the pseudoscalar potential W. All these operators are hermitian because relations (A6) and (A8) are verified. Incidentally, as $\langle\hat{a}\rangle_\psi = \langle A\rangle_\psi$, where $A = 2mc^3w/\hbar\varrho$ is an acceleration field, we have that $\langle\hat{a}_{\mathrm{S}}\rangle_\psi = \langle A_{\mathrm{S}}\rangle_\psi$ and $\langle\hat{a}_{\mathrm{W}}\rangle_\psi = \langle A_{\mathrm{W}}\rangle_\psi$, where $A_{\mathrm{S}} = 2cwS/\hbar\varrho$ and $A_{\mathrm{W}} = -2csW/\hbar\varrho$ are acceleration fields associated to S and W, respectively (remember that $w \equiv \psi^\dagger i\hat{\beta}\hat{\alpha}\psi$ and $s \equiv \psi^\dagger\hat{\beta}\psi$). Likewise, the third Ehrenfest equation is

$$\frac{d}{dt}\langle\hat{p} - \tfrac{e}{c}\mathcal{A}\rangle_\psi = -\left[\psi^\dagger c\hat{\alpha}(\hat{p} - \tfrac{e}{c}\mathcal{A})\,\psi\right]\Big|_a^b + \langle\hat{f}\rangle_\psi + \langle\hat{f}_{\mathrm{S}}\rangle_\psi + \langle\hat{f}_{\mathrm{W}}\rangle_\psi, \tag{A11}$$

where, as before, $\hat{f} = -U'$ is the external classical force operator (see Eq. (39)). Furthermore, $\hat{f}_{\mathrm{S}} = -S'\hat{\beta}$ is a force operator linked to the scalar potential, and $\hat{f}_{\mathrm{W}} = -W'i\hat{\beta}\hat{\alpha}$ is a force operator linked to the pseudoscalar potential. Note that $\langle\hat{f}_{\mathrm{S}}\rangle_\psi = \langle F_{\mathrm{S}}\rangle_\psi$ and $\langle\hat{f}_{\mathrm{W}}\rangle_\psi = \langle F_{\mathrm{W}}\rangle_\psi$, where $F_{\mathrm{S}} = -sS'/\varrho$ and $F_{\mathrm{W}} = -wW'/\varrho$ are force fields linked to S and W, respectively. Incidentally, as far as we know, we have not seen in the literature an analysis similar to the one presented in this appendix.

The scalar and pseudoscalar potentials in one dimension have been considered in the literature. For example, a coherent state of the one-dimensional version of the so-called Dirac oscillator can be constructed. In this case the potential in the Dirac equation is a pseudoscalar potential for which we have that $W(x) \propto x$ [16]. Thus, the formal time derivatives of the expectation values of the operators $\hat{x}$, $\hat{v}$ and $\hat{p}$ are given by Eqs. (A9)-(A11) with $\mathcal{A} = U = S = 0$. On the other hand, one can construct a wave packet for which the Heisenberg uncertainty relation for $\hat{x}$ and $\hat{p}$ is exactly satisfied. This situation can be performed if the potential in the Dirac equation is only a scalar potential $S(x)$ (or if there is also a vector type potential $U(x)$, where $U(x) \propto S(x)$) [17]. In both cases, the writing of the Ehrenfest theorem is immediate. We hope to extend the results presented in this appendix in a forthcoming paper.

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ОПЕРАТОРИ І БІЛІНІЙНІ ГУСТИНИ У ФОРМАЛЬНІЙ ДІРАКІВСЬКІЙ ОДНОВИМІРНІЙ ТЕОРЕМІ ЕРЕНФЕСТА

Сальваторе де Вінченцо
Центральний університет Венесуели, Каракас, Венесуела

У статті розраховано формальні похідні за часом від середніх значень стандартних операторів координати, швидкості та механічного імпульсу, тобто отримано теорему Еренфеста для одновимірної діраківської частинки у координатному зображенні. Показано, що ці похідні містять граничні доданки, які суттєво залежать від значень відповідних характеристичних білінійних густин. На відміну від звичайних підходів, цими граничними доданками не нехтуємо. Водночас ми пов'язуємо їх із подібними доданками, які мусять дорівнювати нулеві з умови ермітовості певних необмежених операторів. У статті послідовно обговорено і проілюстровано всі ці аспекти, які включають зв'язок із певними граничними умовами. Використаний підхід названо формальним, оскільки всі процедури з використанням операторів (наприклад, деякі операторні добутки) зроблено без урахування обмежень, що накладаються множиною функцій, на які можуть діяти самоспряжені оператори. Окрім того, гамільтоніан Дірака, що фігурує в наших розрахунках, містить потенціал, який є часовою компонентною лоренцівського 2-вектора. Ми також отримуємо і послідовно аналізуємо теорему Еренфеста для гамільтоніана з найбільш загальним потенціалом Лоренца в $(1+1)$-вимірному просторі.