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**Abstract**

We reanalyze the problem of a 1D Dirac single particle colliding with the electrostatic potential step of height V_0 with a positive incoming energy that tends to the limit point of the so-called Klein energy zone, i.e. $E \rightarrow V_0 - mc^2$, for a given V_0 . In such a case, the particle is actually colliding with an impenetrable barrier. In fact, $V_0 \rightarrow E + mc^2$, for a given relativistic energy $E (< V_0)$, is the maximum value that the height of the step can reach and that ensures the perfect impenetrability of the barrier. Nevertheless, we note that, unlike the nonrelativistic case, the entire eigensolution does not completely vanish, either at the barrier or in the region under the step, but its upper component does satisfy the Dirichlet boundary condition at the barrier. More importantly, by calculating the mean value of the force exerted by the impenetrable wall on the particle in this eigenstate and taking its nonrelativistic limit, we recover the required result. We use two different approaches to obtain the latter two results. In one of these approaches, the corresponding force on the particle is a type of boundary quantum force. Throughout the article, various issues related to the Klein energy zone, the transmitted solutions to this problem, and impenetrable barriers related to boundary conditions are also discussed. In particular, if the negative-energy transmitted solution is used, the lower component of the scattering solution satisfies the Dirichlet boundary condition at the barrier, but the mean value of the external force when $V_0 \rightarrow E + mc^2$ does not seem to be compatible with the existence of the impenetrable barrier.

1. Introduction

Let us consider the problem of a (massive) 1D Dirac particle in the potential (energy) step of height V_0 :

$$\phi(x) = V_0 \Theta(x) \hat{1}, \quad (1)$$

where $x \in \mathbb{R}$, $\Theta(x)$ is the Heaviside step function ($\Theta(x < 0) = 0$ and $\Theta(x > 0) = 1$), and $\hat{1}$ is the 2×2 identity matrix. If the particle approaching the step potential from the left has positive momentum, $\hbar k > 0$, and positive energy $E (> mc^2)$ such that $E - V_0 < 0$, or more specifically, $E - V_0 < -mc^2$ ($\Rightarrow V_0 > E + mc^2$, for a given energy, but also, $V_0 > 2mc^2$ because $E > mc^2$), we say that the particle has energy in the so-called Klein energy zone. This is because Klein tunneling occurs in that range of energies (the latter physical phenomenon tells us that, among other things, high-energy Dirac particles can, in principle, pass an infinitely high barrier). Incidentally, this is what is currently called Klein's paradox [1–4]. In this paper, we are interested in the case in which the energy of the particle is just the limit point of this energy zone, i.e. $E - V_0 \rightarrow -mc^2$ ($\Rightarrow V_0 \rightarrow E + mc^2$, for a given positive energy). In such circumstances, the incident particle is actually colliding with an impenetrable barrier. This impenetrable barrier is the main subject of our work. We want to obtain the boundary condition that the 1D Dirac wavefunction must fulfill at the point where this impenetrable barrier is found (in this case, at $x = 0$). In nonrelativistic theory, the impenetrable barrier limit, i.e. the infinite-potential limit, leads to the Dirichlet boundary condition for the Schrödinger wavefunction. In the Dirac theory, and for high-energy particles, the latter limit does not lead to an impenetrability boundary condition for the Dirac wavefunction because the particle can penetrate through a very high potential barrier. We also want to know the average force

exerted by this impenetrable barrier on the 1D Dirac particle and to check its nonrelativistic limit. In our study of the problem, the situation where the reflection probability (or the reflection coefficient) is greater than one does not happen, and we consider the 1D Dirac theory as a one-particle theory with external fields.

We present the most important results corresponding to the Klein energy zone in the remainder of this section. Here, we also calculate the average force acting on the particle at $x = 0$. Then, in section 2, we impose on these results the limit that leads to results that are valid at the boundary of the Klein energy zone. Here, we also obtain the mean value of the force exerted by the hard wall and its nonrelativistic value using two different approaches. Additionally, we include in this section a discussion of impenetrable barriers related to boundary conditions. A final discussion of all these results is given in section 3. In the final part of this section, we also present results corresponding to two limiting cases that could arise within the Klein energy zone. Finally, some results that complement and clarify what has been stated throughout the article are exhibited in appendices A and B. Specifically, in appendix A, we present a discussion about the transmitted solutions that can be used in our approach to the problem. Then, we take one of these solutions and repeat the program followed in the Introduction to finally apply the impenetrable barrier limit $V_0 \rightarrow E + mc^2$ to these results. In appendix B, we present a specific discussion about the transmitted solutions that have commonly been used in the literature when dealing with the issue of Klein's paradox. In particular, we clearly establish the relation between our positive-energy transmitted solution and the sometimes included transmitted solution of negative energy. At the end of the appendix, we treat very briefly the problem of the 1D Dirac particle incident on the step potential, but we use the negative-energy transmitted solution.

The scattering eigensolution of the 1D Dirac Hamiltonian operator \hat{H} , i.e. the solution of the time-independent 1D Dirac equation,

$$\hat{H}\psi(x) = \left(-i\hbar c \hat{\alpha} \frac{d}{dx} + mc^2 \hat{\beta} + \phi \right) \psi(x) = E\psi(x), \quad (2)$$

in the Dirac representation, that is, $\hat{\alpha} = \hat{\sigma}_x$ and $\hat{\beta} = \hat{\sigma}_z$ ($\hat{\sigma}_x$ and $\hat{\sigma}_z$ are two of the Pauli matrices), and $\psi = [\varphi \ \chi]^T$ (the symbol T denotes the transpose of a matrix) can be written in a single expression as follows:

$$\psi(x) = (\psi_i(x) + \psi_r(x))\Theta(-x) + \psi_t(x)\Theta(x), \quad (3)$$

where the incoming and reflected plane-wave solutions are given by

$$\psi_i(x \leq 0) = \begin{bmatrix} 1 \\ a \end{bmatrix} e^{ikx}, \quad (4)$$

$$\psi_r(x \leq 0) = \begin{pmatrix} a+b \\ a-b \end{pmatrix} \begin{bmatrix} 1 \\ -a \end{bmatrix} e^{-ikx} \equiv r \begin{bmatrix} 1 \\ -a \end{bmatrix} e^{-ikx}, \quad (5)$$

and the transmitted solution is written (in a seemingly counterintuitive way) as follows:

$$\psi_t(x \geq 0) = \frac{2a}{a-b} \begin{bmatrix} 1 \\ -b \end{bmatrix} e^{-i\bar{k}x} \equiv t \begin{bmatrix} 1 \\ -b \end{bmatrix} e^{-i\bar{k}x}. \quad (6)$$

Naturally, the time-dependent scattering wavefunction corresponding to the solution $\psi(x)$ is given by

$$\Psi(x, t) = \psi(x) e^{-iEt/\hbar}. \quad (7)$$

The real quantities a and b are given by

$$a = \frac{c \hbar k}{E + mc^2} > 0, \quad b = \frac{c \hbar \bar{k}}{E - V_0 + mc^2} < 0, \quad (8)$$

where

$$c \hbar k = \sqrt{E^2 - (mc^2)^2} > 0, \quad c \hbar \bar{k} = \sqrt{(E - V_0)^2 - (mc^2)^2} > 0. \quad (9)$$

Particularly, $E - V_0 + mc^2$ and $E - V_0 - mc^2$ are negative when $E - V_0 < -mc^2$. Additionally, it should be noted that the solution given in equation (6) is essentially obtained by replacing $E \rightarrow E - V_0$ in the solution given by equation (5) (also \bar{k} is obtained from k by making this replacement). Furthermore, note that a and b can be written as follows:

$$a = \sqrt{\frac{E - mc^2}{E + mc^2}}, \quad b = -\sqrt{\frac{E - V_0 - mc^2}{E - V_0 + mc^2}}. \quad (10)$$

We are also introducing in equations (5) and (6) the quantities r and t that some authors call coefficient for reflection (to the left) and transmission (to the right). The solution $\psi(x)$ in equation (3) is a continuous function at $x = 0$, i.e.

$$\psi(0 -) = \psi(0 +) \equiv \psi(0) \quad (\Rightarrow \psi_i(0 -) + \psi_r(0 -) = \psi_t(0 +)) \quad (11)$$

(we use the notation $x \pm \equiv \lim_{\epsilon \rightarrow 0}(x \pm \epsilon)$, with $x = 0$). Thus, $\varrho(x) = \psi^\dagger(x)\psi(x) = |\varphi(x)|^2 + |\chi(x)|^2$, the probability density, and $j(x) = c\psi^\dagger(x)\hat{\sigma}_x\psi(x) = 2c \operatorname{Re}(\varphi^*(x)\chi(x))$, the probability current density, are also continuous functions at $x = 0$ (the symbol † represents the adjoint of a matrix and the symbol * denotes the complex conjugate, as usual), i.e.

$$\varrho(0^-) = \varrho(0^+) = \varrho_t(0^+) = \frac{4a^2(1+b^2)}{(a-b)^2} \quad (12)$$

and

$$j(0^-) = j(0^+) = j_t(0^+) = -\frac{8c a^2 b}{(a-b)^2} > 0. \quad (13)$$

Obviously, $\varrho_t(x)$ and $j_t(x)$ are calculated for the transmitted solution $\psi_t(x)$, and the result in equation (13) is what one would expect for a transmitted wave traveling to the right in the region $x > 0$. Additionally, the evaluation of $\varrho_t(x)$ and $j_t(x)$ at $x = 0$ made in equations (12) and (13) is not necessary because the solutions we are using are just plane-wave solutions, i.e. ϱ_t and j_t , and the other probability and current densities (ϱ_i, j_i , etc.) are constant quantities (obviously, this is not the case when we have a wave packet).

The reflection and transmission coefficients, or the reflection and transmission probabilities, are given by

$$R = \frac{|j_r|}{|j_i|} = \left(\frac{a+b}{a-b}\right)^2 = r^2 \left[\left(\frac{1 - \frac{|b|}{a}}{1 + \frac{|b|}{a}} \right)^2 \right] \quad (14)$$

and

$$T = \frac{|j_t|}{|j_i|} = \frac{4a|b|}{(a-b)^2} = \frac{|b|}{a} \left(\frac{2a}{a-b} \right)^2 = \frac{|b|}{a} t^2 \left[\frac{4 \frac{|b|}{a}}{\left(1 + \frac{|b|}{a}\right)^2} \right]. \quad (15)$$

Note that the latter two quantities verify $R + T = 1$, i.e. $r^2 + (|b|/a)t^2 = 1$, as is to be required by the conservation of the probability; equivalently but also more intuitively, $|j_r| + |j_t| = |j_i|$. Thus, a 1D Dirac particle with (positive) energies in the Klein energy zone can propagate on both sides of the step potential, but the original Klein paradox [5], i.e. the situation where R is greater than one, does not occur [4, 6–9]. In particular, when the infinite-potential limit is taken, i.e. $V_0 \rightarrow \infty$, we have that $b \rightarrow -1$, and the reflection and transmission coefficients go to $R \rightarrow ((a-1)/(a+1))^2$ and $T \rightarrow 4a/(a+1)^2$. Thus, the transmission coefficient does not vanish even when the height of the barrier is infinitely high. This specific tunneling (i.e. the case when $V_0 \rightarrow \infty$) is more noticeable when the particle has a high energy. In fact, when $E \gg mc^2$, we have that $a \rightarrow 1$, and therefore $T \rightarrow 1$. Certainly, it is not necessary for the potential jump to go to infinity for Klein tunneling to exist. Additionally, note that the eigenvalues of the momentum operator $\hat{p} = -i\hbar \hat{1} d/dx$ corresponding to the transmitted eigensolution are negative, that is, $\hat{p} \psi_t = -\hbar \bar{k} \psi_t$; however, the transmitted velocity field is positive, namely,

$$v_t \equiv \frac{j_t}{\varrho_t} = -\frac{2c b}{1+b^2} = -\frac{c^2 \hbar \bar{k}}{E - V_0} = c \sqrt{1 - \left(\frac{mc^2}{E - V_0} \right)^2} > 0. \quad (16)$$

The latter result confirms the use of a transmitted solution such as that given in equation (6).

The mean value of the external classical force operator

$$\hat{f} = -\frac{d}{dx}\phi(x) = -V_0 \delta(x) \hat{1} \quad (17)$$

($\delta(x) = d\Theta(x)/dx$ is the Dirac delta function), or the average force acting on the particle by the wall of potential at $x = 0$, in the scattering state ψ , is given by

$$\begin{aligned} \langle \hat{f} \rangle_\psi &= \langle \psi, \hat{f} \psi \rangle = -V_0 \int_{-\infty}^{+\infty} dx \delta(x) \psi^\dagger(x) \psi(x) = -V_0 \varrho(0) = -V_0 \varrho_t(0^+) \\ &= -V_0 \frac{4a^2(1+b^2)}{(a-b)^2}. \end{aligned} \quad (18)$$

That is, the result is dependent on V_0 , as expected (b is also a function of V_0).

2. The limit point of the Klein energy zone

When we take the precise limit $V_0 \rightarrow E + mc^2$, for a given energy, we reach the limit point of the Klein energy zone. More accurately, here, V_0 reaches the value $E + mc^2$ ‘from the right’, i.e. $V_0 \rightarrow (E + mc^2)^+$. Thus, from

equation (10), we obtain the result $b \rightarrow -\infty$, and therefore, $R \rightarrow 1$ and $T \rightarrow 0$ (see equations (14) and (15)). Consistently, the transmitted velocity field verifies that $v_t \rightarrow 0$ (see equation (16)). Additionally, \bar{k} tends to zero in this limit (see the second of the relations in equation (9)) and the solution of the Dirac equation in equation (3) takes the form

$$\psi(x) = \begin{bmatrix} 2i\sin(kx) \\ 2a \cos(kx) \end{bmatrix} \Theta(-x) + \begin{bmatrix} 0 \\ 2a \end{bmatrix} \Theta(x). \quad (19)$$

Now, note that the entire wavefunction is not zero in the region $x \geq 0$, only its upper component φ , i.e. only the so-called large component of the 1D Dirac wavefunction in the Dirac representation. Nevertheless, the particle does not penetrate into that region because the transmitted probability current density vanishes there (i.e. $j_t(x \geq 0) = 0$), i.e. because the probability current density is zero at $x = 0$ (i.e. $j(0^-) = j(0^+) \equiv j(0) = 0$), i.e. because the origin is an impenetrable barrier (see the result in equation (13)). The result in equation (19) confirms that, in general, the entire Dirac wavefunction does not disappear at a point where an impenetrable barrier exists [10]; in fact, ϱ is not zero at $x = 0$, and the barrier is still impenetrable (note that as the energy of the particle increases, the quantity a moves away from zero and approaches one); however, the wavefunction must satisfy some other impenetrability boundary condition. In effect, in this case, we have that $\psi(0^-) = \psi(0^+) \equiv \psi(0) \neq 0$, but the large component satisfies the Dirichlet boundary condition at $x = 0$, i.e.

$$\varphi(0^-) = \varphi(0^+) \equiv \varphi(0) = 0 \quad (20)$$

(see equation (19)), and the lower component of ψ , i.e. χ , remains continuous there. Thus, when the origin becomes an impenetrable barrier (i.e. after the limit $V_0 \rightarrow E + mc^2$ has been taken), the respective boundary condition emerges naturally. Certainly, the limit $V_0 \rightarrow E + mc^2$ can be considered the impenetrable barrier limit in 1D Dirac theory, and the boundary condition in equation (20) as the natural impenetrability boundary condition when the Dirac representation is used (at least for positive energies E). Instead, in Schrödinger nonrelativistic theory, the respective impenetrable barrier limit (i.e. $V_0 \rightarrow \infty$) leads to the Dirichlet boundary condition for the (one-component) wavefunction.

Incidentally, for positive energies, the energy eigensolutions of the time-independent 1D Dirac equation in the (momentum-dependent) Foldy-Wouthuysen representation [11, 12] (in the free case and in the case of a static external field) essentially have the form $\psi_{\text{FW}} = [\psi_1 \ 0]^T$, where ψ_1 and φ only differ by a constant factor (i.e. by a factor depending on the energy eigenvalue) [13–15]. Thus, the boundary condition in equation (20) would take the form $\psi_{\text{FW}}(0^-) = \psi_{\text{FW}}(0^+) \equiv \psi_{\text{FW}}(0) = 0$, i.e. the entire Foldy-Wouthuysen eigensolution would verify the Dirichlet boundary condition at $x = 0$. The latter boundary condition imposed on ψ_{FW} appears to be acceptable; in fact, the (free-particle) 1D Foldy-Wouthuysen Hamiltonian operator, for example, unlike the (free) 1D Dirac Hamiltonian operator, depends on $(c\hat{p})^2 + (mc^2)^2$ (although this quantity is under a square root) [13–15].

When the height of the potential V_0 reaches the value $E + mc^2$, for a given relativistic energy that is always less than V_0 , the potential reaches the maximum value that it can reach and that ensures the impenetrability of the barrier. In fact, as we explained before, if $V_0 > E + mc^2$, for a given relativistic energy (and then $E < V_0$) but also $V_0 \rightarrow \infty$, then we have that $R \neq 1$. In effect, in this situation, only if the energies are low or nonrelativistic, i.e. $E \cong mc^2$, would we have that $R \rightarrow 1$ (see the comment related to the limit $V_0 \rightarrow \infty$ in the paragraph following equation (15)) [9]. Finally, when V_0 is less than $E + mc^2$ and still greater than E , i.e. $E < V_0 < E + mc^2$, the reflection is still a total reflection, i.e. $R = 1$ [3, 16, 17]. The latter means that when the potential reaches the value $E + mc^2$ ‘from the left’, i.e. $V_0 \rightarrow (E + mc^2)^-$, we also have that $R \rightarrow 1$. In addition, as we know, when $V_0 \rightarrow (E + mc^2)^+$, $R \rightarrow 1$. Thus, the limit when $V_0 \rightarrow E + mc^2$ effectively leads to total reflection, and we can be sure of our conclusions by taking the limit $V_0 \rightarrow E + mc^2$ on results that are only valid in the Klein energy zone.

Actually, the boundary condition in equation (20) is just one of the physically (and mathematically) suitable boundary conditions that one could impose on the 1D Dirac wavefunction at a point such as $x = 0$ (where a kind of hard wall exists). In fact, there are an infinite number of impenetrability boundary conditions at our disposal, and for each of them, the Hamiltonian operator that describes a 1D Dirac particle moving on the real line with an impenetrable obstacle at the origin is self-adjoint (and consequently, the respective probability current density vanishes there). In the end, in all these cases, the particle could be in just one of the two half-spaces. In this regard, the subfamily of boundary conditions that ensures impenetrability at the origin is given by the two relations in equation (B6) in [18]. This (two-real-parameter) subfamily is obtained from the most general (four-real-parameter) family of boundary conditions given in equation (B1) in [18] by setting $\theta = 0$ (See [19], although the discussion of this topic was made for the similar problem of a 1D Dirac particle moving in the interval $[0, L]$). However, by substituting $0 \rightarrow 0^+$ and $L \rightarrow 0^-$ in the boundary conditions of this reference, the corresponding boundary conditions for the case in which the particle moves along the real line with an obstacle at the origin can be obtained). In particular, the boundary condition in equation (20) is obtained from equation (B6) in [18] by imposing $\mu = \tau = \pi/2, 3\pi/2$, and it certainly defines a relativistic point interaction at the point $x = 0$. Clearly, the Dirichlet boundary condition imposed on the entire (two-component) Dirac wavefunction at $x = 0$ is not

included in equation (B6) of [18], i.e. the corresponding (first-order) Dirac Hamiltonian operator with this boundary condition is not self-adjoint.

Additionally, in the impenetrable barrier limit $V_0 \rightarrow E + mc^2$, the mean value of the force exerted by the wall on the particle in equation (18) takes the form

$$\langle \hat{f} \rangle_\psi = -(E + mc^2)4a^2 = -4(E - mc^2). \tag{21}$$

To be more precise, the latter result should be written as $\langle \hat{f} \rangle_\psi = -4(E - mc^2)|A|^2$, where A is a complex-value (normalization) constant that multiplies the right-hand side of the scattering solution in equation (3). Thus, the average force on a 1D Dirac particle that is in a stationary state and hits an impenetrable wall at $x = 0$ is proportional to the relativistic kinetic energy of the particle.

The result in equation (21) can be obtained in an alternative way. In effect, due to the presence of an impenetrable barrier at $x = 0$, the problem can be reduced to that of a (free) 1D Dirac particle that can only be on the half-line $x \in (-\infty, 0]$. In this case, the force on the particle due to the wall at $x = 0$ is a type of boundary quantum force. In effect, the time derivative of the mean value of the momentum operator for a 1D Dirac particle on the half-line is given by

$$\frac{d}{dt} \langle \hat{p} \rangle_\Psi = [-i\hbar \Psi^\dagger \Psi_t + mc^2 \Psi^\dagger \hat{\sigma}_z \Psi] \Big|_{-\infty}^0, \tag{22}$$

where we use the notation $[g] \Big|_{-\infty}^0 \equiv g(0, t) - g(-\infty, t)$, and Ψ has the form given in equation (7) with ψ given in equation (19), also $\Psi_t \equiv \partial\Psi/\partial t$ (see equation (39) in [4]). If the function Ψ is a nonstationary state that goes to zero at $x = -\infty$, the right-hand side of equation (22) would simply be the function enclosed in square brackets in equation (22) evaluated at $x = 0$. That quantity can be written as the mean value of a boundary quantum force due to the impenetrable barrier at $x = 0$, namely,

$$\langle \hat{f}_B \rangle_\Psi = -i\hbar \Psi^\dagger(0, t)\Psi_t(0, t) + mc^2 \Psi^\dagger(0, t)\hat{\sigma}_z \Psi(0, t). \tag{23}$$

Certainly, because in our case the state Ψ is a stationary state, equation (22) would lead us to the relation $0 = 0 - 0$. Indeed, using the solution given in equation (19), it can be demonstrated that the function enclosed in square brackets in equation (22) has the same value at $x = 0$ and $x = -\infty$. In fact, the result that is finally obtained from equation (23) is given by

$$\langle \hat{f}_B \rangle_\Psi = -4a^2(E + mc^2) = -4(E - mc^2), \tag{24}$$

which is precisely the result given in equation (21).

In the nonrelativistic limit, we have that $E \rightarrow E^{(NR)} + mc^2 \cong mc^2 (E^{(NR)}$ is the nonrelativistic kinetic energy), and we obtain in this approximation the following result:

$$a \rightarrow \sqrt{\frac{E^{(NR)}}{2mc^2}} \cong 0 \tag{25}$$

(see the first of the relations in equation (10)). Likewise, the solution of the Dirac equation in equation (19) approaches

$$\psi(x) \rightarrow \begin{bmatrix} \psi^{(NR)}(x) \\ 0 \end{bmatrix} = \begin{bmatrix} 2i \sin(k^{(NR)}x) \\ 0 \end{bmatrix} \Theta(-x) + \begin{bmatrix} 0 \\ 0 \end{bmatrix} \Theta(x) \tag{26}$$

($k^{(NR)} = \sqrt{2mE^{(NR)}}/\hbar$), which is an expected result. Certainly, in this approximation, and when the energies are positive, the upper component of the Dirac wavefunction is essentially the Schrödinger wavefunction, and the lower component is practically zero, i.e. the Schrödinger eigensolution satisfies $\psi^{(NR)}(0 -) = \psi^{(NR)}(0 +) \equiv \psi^{(NR)}(0) = 0$. Additionally, in the nonrelativistic limit, the mean value of the operator \hat{f} in equation (21) takes the form

$$\langle \hat{f} \rangle_\psi \rightarrow -4 E^{(NR)}. \tag{27}$$

The latter is precisely the result obtained from the 1D Schrödinger theory by taking the limit $V_0 \rightarrow \infty$ on the mean value of \hat{f} calculated in the respective Schrödinger scattering eigenstate. To check this, see equation (10) in [20]. Additionally, because the particle is actually restricted to the semispace $x \leq 0$, we can also use the result given in equation (32) in [20] (with the operator \hat{o} used there being equal to the momentum operator for a 1D nonrelativistic particle on the half-line $\hat{p} = -i\hbar d/dx$), together with equations (36) and (37), also in [20], namely,

$$\frac{d}{dt} \langle \hat{p} \rangle_{\Psi^{(NR)}} = -\frac{\hbar^2}{2m} [(\Psi_x^{(NR)})^* \Psi_x^{(NR)} - (\Psi^{(NR)})^* \Psi_{xx}^{(NR)}] \Big|_{-\infty}^0, \tag{28}$$

where $\Psi^{(NR)}(x, t) = \psi^{(NR)}(x) \exp(-iE^{(NR)}t/\hbar)$, $\Psi_x^{(NR)} \equiv \partial\Psi^{(NR)}/\partial x$, and $\Psi_{xx}^{(NR)} \equiv \partial^2\Psi^{(NR)}/\partial x^2$. Again, if the function $\Psi^{(NR)}$ is a nonstationary state that tends to zero at $x = -\infty$, the right-hand side of equation (28) would simply be the function enclosed in square brackets in equation (28) evaluated at $x = 0$. That quantity is the mean

value of a boundary quantum force due to the hard wall at $x = 0$, namely,

$$\langle \hat{f}_B \rangle_{\Psi^{(NR)}} = -\frac{\hbar^2}{2m} |\Psi_x^{(NR)}(0, t)|^2 \quad (29)$$

(note that $\Psi^{(NR)}$ and $\Psi_{xx}^{(NR)}$ also vanish at $x = 0$). Obviously, because the state $\Psi^{(NR)}$ is a stationary state, equation (28) would lead us to the relation $0 = 0 - 0$. Using the solution given in equation (26), it can be demonstrated that the function enclosed in square brackets in equation (28) has the same value at $x = 0$ and $x = -\infty$. In that regard, the result that is obtained from equation (29) is given by

$$\langle \hat{f}_B \rangle_{\Psi^{(NR)}} = -4 E^{(NR)}, \quad (30)$$

which is the result given in equation (27), as expected.

3. Final discussion

In the 1D Schrödinger theory, the impenetrable barrier limit, that is, the infinite-potential limit, leads to the Dirichlet boundary condition for the respective (one-component) wavefunction (i.e. the latter satisfies this boundary condition at the barrier). On the other hand, in the 1D Dirac theory, and for particles with high energies, the infinite-potential limit does not lead to an impenetrability boundary condition for the respective (two-component) wavefunction (because the particle can perfectly penetrate into the potential step when the step goes to infinity). Most likely because of this, when one models an impenetrable barrier in the Dirac theory (let us call it a Dirac impenetrable barrier), the most common has always been just to select and then impose some impenetrability boundary condition on the Dirac wavefunction, but the Dirichlet boundary condition imposed on the entire (two-component) wavefunction at the point where the barrier is located is not acceptable. For example, in the problem of the 1D Dirac particle confined to a finite interval of the real line (a 1D box), different physically (and mathematically) suitable boundary conditions have been used (see, for example, Refs. [10, 21–24]). Again, the Dirichlet boundary condition imposed on the entire wavefunction at the ends of the box is not acceptable [10].

The results we have obtained confirm that the limit $V_0 \rightarrow E + mc^2$, for a given energy, can be considered the impenetrable barrier limit in 1D Dirac theory, i.e. by taking it in the problem of the particle incident on a step potential, the probability current density, calculated for the scattering eigensolution of the problem, disappears at the barrier. More importantly, in this limit, the impenetrability boundary condition for this positive-energy solution arises naturally, namely, only its upper or large component (in the Dirac representation) satisfies the Dirichlet boundary condition at the barrier. Certainly, we obtain the latter result before taking the nonrelativistic limit of the eigensolution. Furthermore, we calculated the mean value of the force exerted by the impenetrable barrier on the particle and showed that it tends to the required result when its nonrelativistic limit is calculated. The required result is none other than the result that is obtained when the infinite-potential limit is taken on the mean value of the force operator calculated in the Schrödinger eigenstate [20]. As we have seen, the latter two results can also be obtained by reducing the problem to that of a particle that has always lived on the half-line $x \in (-\infty, 0]$. In this case, the corresponding force on the particle at $x = 0$ is a type of boundary quantum force.

To summarize, we have obtained the boundary condition that the Dirac wavefunction must fulfill at a point where there is an impenetrable barrier only taking a limit on the potential, i.e. $V_0 \rightarrow E + mc^2$, for a given (positive) energy (in nonrelativistic theory, the impenetrability boundary condition is obtained by making $V_0 \rightarrow \infty$). Likewise, in the Dirac impenetrable barrier limit, we obtained the mean value of the force operator (calculated in the positive-energy scattering state of the problem), and by taking its nonrelativistic limit, we recovered the result obtained by calculating this quantity in the 1D Schrödinger theory. In fact, we used two different approaches to obtain the latter two results. Incidentally, these simple and specific results, obtained within the framework of a 1D relativistic quantum theory for a single particle in an external field, do not seem to have been considered before. Thus, we believe that our paper may be attractive to those interested in the fundamental and technical aspects of relativistic quantum mechanics.

In fact, the problem treated here, that is, that of a Dirac particle incident on a potential step, has been consistently attractive because of the Klein paradox. This paradox has been discussed in many textbooks and articles on relativistic quantum mechanics, and its interpretation is very varied. One of the problems is that a treatment made purely within the single-particle interpretation of the Dirac wavefunction often leads to paradoxical situations. We recently learned of [25], in which Klein's paradox was studied. Because we use an apparently counterintuitive transmitted solution (equation (6)), our results do not agree exactly with those obtained therein. Actually, the transmitted solution used in [25] is the charge conjugate of our positive-energy transmitted solution (see appendix B) and describes the state of the particle (not its antiparticle state) with negative energy in the sign-shifted potential (within the single-particle 1D Dirac theory). Thus, for example, in the case where $V_0 = 2E$ (and we are still within the Klein energy zone), we obtained the result $b = -1/a$, and

therefore, $R = ((a^2 - 1)/(a^2 + 1))^2$ and $T = 4a^2/(a^2 + 1)^2$, and $v_t = c^2 \hbar k/E$ (also, we have that $\bar{k} = k$). Thus, only when $E \gg mc^2$ one has that $a \rightarrow 1$, and therefore, $R \rightarrow 0$ and $T \rightarrow 1$, i.e. only when the particle has a high energy, there is a total transmission in this respect (see the paragraph that follows equation (2.12) in [25] and compare the results). Incidentally, when the mass of the particle disappears, i.e. $mc^2 = 0$ (and then we have that $E - V_0 < -mc^2 = 0$), we obtained the results $a = 1$ and $b = -1$ (see equation (10)), and again, we have that $R = 0$ and $T = 1$, and $v_t = c$ (see equations (14)–(16), as expected (see the first paragraph of subsection 3.3. in [25]). Instead of using a transmitted solution of negative energy, we used one of positive energy, which in the Klein energy zone would represent a particle traveling to the right in the region $x > 0$, i.e. the transmitted velocity field and probability current density are positive (see, for example, Refs. [6, 7]). On the other hand, we have noticed that if the negative-energy transmitted solution is used, the lower or small component of the scattering solution (in the Dirac representation) satisfies the Dirichlet boundary condition at the barrier; however, the average value of the external force operator in the Dirac impenetrable barrier limit does not seem to be compatible with the fact that all incident particles must be reflected by the barrier (see appendix B). In any case, the main goal of our paper has been to analyze the issue of the impenetrable barrier that arises at the limit point of the Klein energy range, i.e. when $V_0 \rightarrow E + mc^2$, for a given positive energy. As we have seen, this impenetrable barrier, which can also be characterized by means of a boundary condition, is only one of many impenetrable barriers that can exist in relativistic quantum mechanics; in fact, it is only one of many point interactions that can describe an impenetrable barrier at a point.

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Data availability statement

No data was used for the research described in the article.

Conflicts of interest

The author declares no conflicts of interest.

Appendix A

The transmitted solution given in equation (6) satisfies the equation $\hat{H}\psi_t(x \geq 0) = E\psi_t(x \geq 0)$, as expected. In the procedure to obtain this solution, one obtains the lower component of ψ_t from its upper component. If one decides to obtain the upper component from the lower component, one obtains the following transmitted solution:

$$\zeta_t(x \geq 0) = t' \begin{bmatrix} -b' \\ 1 \end{bmatrix} e^{-i\bar{k}x}, \quad (\text{A1})$$

where

$$b' = \frac{c \hbar \bar{k}}{E - V_0 - mc^2} = -\sqrt{\frac{E - V_0 + mc^2}{E - V_0 - mc^2}} = \frac{1}{b} < 0, \quad (\text{A2})$$

also, \bar{k} is given in equation (9) and $t' = 2a/(1 - ab')$ (certainly, t' is obtained after imposing the continuity of the corresponding scattering solution at $x = 0$). Obviously, this solution also satisfies $\hat{H}\zeta_t(x \geq 0) = E\zeta_t(x \geq 0)$.

Note that because in the Klein energy zone one has that $E - V_0 < -mc^2$ (i.e. $E - V_0 < 0$), the transmitted solution can also be explicitly written in terms of $|E - V_0|$, namely,

$$\zeta_t(x \geq 0) = t'' \begin{bmatrix} +b'' \\ 1 \end{bmatrix} e^{-i\bar{k}x}, \quad (\text{A3})$$

where

$$b'' = \frac{c \hbar \bar{k}}{|E - V_0| + mc^2} = \sqrt{\frac{|E - V_0| - mc^2}{|E - V_0| + mc^2}} = -b' > 0, \quad (\text{A4})$$

and the coefficient for transmission t'' can be obtained from t' making the replacement $b' \rightarrow -b''$. The transmitted solution given in equation (A3) is valid when $E - V_0 < -mc^2$ and is not a negative-energy solution

(it is just that $E - V_0 < 0$); in fact, it satisfies $\hat{H}\zeta_t = E\zeta_t$. Again, we take the solution that has the exponential function with a negative exponent (but we obtain the correct sign for the transmitted wave). The result in equation (A3) can also be essentially obtained by means of the charge-conjugation operation, namely,

$$\zeta_t(x \geq 0) = f_t^C(-\bar{k}; x \geq 0) = \hat{S}_C f_t^*(-\bar{k}; x \geq 0),$$

where

$$f_t(\bar{k}; x \geq 0) = \text{const} \times \left[\frac{1}{-c\hbar k} \right] e^{-ikx}$$

with the following replacements on the right-hand side, namely, $k \rightarrow \bar{k}$ and $E \rightarrow E - V_0$, and $\hat{S}_C = \hat{\sigma}_x$ (up to a phase factor) [16].

Indeed, we can use the transmitted solution given in equation (A3) to solve the problem. Naturally, the incoming and reflected plane-wave solutions are simply given by

$$\zeta_i(x \leq 0) = \begin{bmatrix} 1 \\ a \end{bmatrix} e^{ikx}, \quad \zeta_r(x \leq 0) = r'' \begin{bmatrix} 1 \\ -a \end{bmatrix} e^{-ikx}, \tag{A5}$$

which have the same form as equations (4) and (5), with a and k given in equations (8) and (9). Again, the solution $\zeta(x)$ of the problem can be written as the solution $\psi(x)$ in equation (3), and after imposing the continuity of $\zeta(x)$ at $x = 0$, i.e. $\zeta_i(0^-) + \zeta_r(0^-) = \zeta_t(0^+)$, we obtain the following results:

$$r'' = \frac{ab'' - 1}{ab'' + 1}, \quad t'' = \frac{2a}{1 + ab''}. \tag{A6}$$

Additionally, the reflection and transmission coefficients are given by

$$R'' = \frac{|J_r|}{|j_i|} = \left(\frac{ab'' - 1}{ab'' + 1} \right)^2 = (r'')^2, \quad T'' = \frac{|J_t|}{|j_i|} = \frac{4ab''}{(1 + ab'')^2} = \frac{b''}{a} \left(\frac{2a}{1 + ab''} \right)^2 = \frac{b''}{a} (t'')^2. \tag{A7}$$

These two quantities verify $R'' + T'' = 1$, and $j_i = J_i$, i.e. the incoming probability current density calculated for the incident solution ψ_i is equal to that calculated for ζ_i . Because b' is equal to $1/b$, and b'' is equal to $-b$, we have that $b'' = -1/b$; thus, from the latter relation, R'' and T'' can be obtained from R and T , and vice versa (in this case, r'' can also be obtained from r , but t'' cannot be obtained from t , and vice versa, as expected). The corresponding expressions for the probability density and probability current density evaluated at $x = 0$ can also be obtained by making the replacement $b \rightarrow -1/b''$ in equations (12) and (13). We obtain the following results:

$$\rho(0^-) = \rho(0^+) = \rho_t(0^+) = \frac{4a^2(1 + (b'')^2)}{(1 + ab'')^2} \tag{A8}$$

and

$$J(0^-) = J(0^+) = J_t(0^+) = \frac{8c a^2 b''}{(1 + ab'')^2} > 0. \tag{A9}$$

Similarly, the transmitted velocity field is given by

$$V_t \equiv \frac{J_t}{\rho_t} = \frac{2c b''}{(1 + (b'')^2)} = \frac{c^2 \hbar \bar{k}}{|E - V_0|} = c \sqrt{1 - \left(\frac{mc^2}{E - V_0} \right)^2} > 0, \tag{A10}$$

and the mean value of the external classical force operator in the scattering state ζ is given by

$$\langle \hat{f} \rangle_\zeta = -V_0 \rho_t(0^+) = -V_0 \frac{4a^2(1 + (b'')^2)}{(1 + ab'')^2}. \tag{A11}$$

Certainly, when the infinite-potential limit is taken, i.e. $V_0 \rightarrow \infty$, and therefore $b'' \rightarrow +1$, R'' and T'' go to the same results obtained before, i.e. $R'' \rightarrow ((a - 1)/(a + 1))^2$ and $T'' \rightarrow 4a/(a + 1)^2$. Likewise, when we take the impenetrable barrier limit $V_0 \rightarrow E + mc^2$, and therefore $b'' \rightarrow 0$ and $\bar{k} \rightarrow 0$, we again obtain $R'' \rightarrow 1$, $T'' \rightarrow 0$ and $V_t \rightarrow 0$, and $\langle \hat{f} \rangle_\zeta = -(E + mc^2)4a^2 = -4(E - mc^2)$. Certainly, the solution of the problem takes the form given in equation (19), namely,

$$\zeta(x) = \begin{bmatrix} \zeta_1 \\ \zeta_2 \end{bmatrix} = \begin{bmatrix} 2i \sin(kx) \\ 2a \cos(kx) \end{bmatrix} \Theta(-x) + \begin{bmatrix} 0 \\ 2a \end{bmatrix} \Theta(x). \tag{A12}$$

Again, we have that $\zeta(0^-) = \zeta(0^+) \equiv \zeta(0) \neq 0$, and the upper or large component of ζ satisfies the Dirichlet boundary condition at $x = 0$, i.e. $\zeta_1(0^-) = \zeta_1(0^+) \equiv \zeta_1(0) = 0$, and the lower or small component ζ_2 is continuous there. Certainly, from these results, we obtain the same nonrelativistic results as before.

Appendix B

Naturally, in the region below the potential step $x \geq 0$, one always has two transmitted solutions that are associated with opposite momenta. As discussed in section 1, one of these solutions is precisely the solution given in equation (6), namely,

$$\psi_t = \text{const} \begin{bmatrix} 1 \\ -c \hbar \bar{k} \\ E - V_0 + mc^2 \end{bmatrix} e^{-i\bar{k}x}, \quad (\text{B1})$$

that does not lead to the original Klein paradox, and the other solution is

$$\psi_t = \text{const} \begin{bmatrix} 1 \\ c \hbar \bar{k} \\ E - V_0 + mc^2 \end{bmatrix} e^{i\bar{k}x}. \quad (\text{B2})$$

The latter is the traditional solution in which Klein's paradox arises. For example, see the comment following equation (4) in [2] (although there, the solutions are four-component spinors). This is also the solution used in [25] to introduce the original Klein paradox. See equation (2.5) in that reference (and correct the typo $q \rightarrow p$).

On the other hand, another pair of transmitted solutions consists of the solution given in equation (A3), namely,

$$\psi_t = \text{const} \begin{bmatrix} c \hbar \bar{k} \\ |E - V_0| + mc^2 \\ 1 \end{bmatrix} e^{-i\bar{k}x}, \quad (\text{B3})$$

that does not lead to the original Klein paradox (see appendix A), and the solution given by

$$\psi_t = \text{const} \begin{bmatrix} -c \hbar \bar{k} \\ |E - V_0| + mc^2 \\ 1 \end{bmatrix} e^{i\bar{k}x}. \quad (\text{B4})$$

As demonstrated in [2], the latter solution also leads to the original Klein paradox, as expected (see the results given in equations (2), (3) and (4) of that reference). In [2], it is also mentioned that the solution given in equation (A3) (or equation (B3)) is the solution generally considered valid in the region $x \geq 0$. According to the authors of this reference, this solution should be discarded because it does not represent an antiparticle entering from the right (this conclusion would arise as a consequence of the physical interpretation of the results obtained by the authors using the transmitted solution in equation (B4)). Alternatively, our treatment of the problem leads to a situation in which the original Klein paradox does not arise, and we accomplish this without abandoning the 1D Dirac theory as a single-particle theory. Incidentally, in a rather old reference, it was already mentioned that a transmitted solution similar to the one we use in the present paper (equation (B1)) can avoid the original Klein paradox, but only in the case of fermions, i.e. in the case of 3D Dirac particles [26] (see the paragraph that follows equation (8) and the appendix in that reference). Additionally, a complete and plausible discussion of the Klein paradox within the framework of the 3D Dirac theory for a single particle can be found in two well-known books on relativistic quantum mechanics [6, 7]. In this regard, our results also indicate that the solution given in equation (B3) (or the solution given in equation (B1)) cannot be discarded because it leads to an impenetrable barrier whose nonrelativistic limit is the typical barrier of nonrelativistic theory (provided that the energies are positive).

The approach followed in [25] also leads to a situation in which the original paradox disappears. The author of that reference uses the following transmitted solution (and we will also name it ψ_{II}):

$$\psi_t = \text{const} \times \begin{bmatrix} -c \hbar \bar{k} \\ E - V_0 + mc^2 \\ 1 \end{bmatrix} e^{i\bar{k}x} \equiv \psi_{\text{II}} \quad (\text{B5})$$

(see equation (2.9) in [25]). This solution satisfies the following relation: $\hat{H}(\phi)\psi_{\text{II}} = (2V_0 - E)\psi_{\text{II}}$; thus, it is not an eigenfunction of the Hamiltonian given in equation (2) (here, we write \hat{H} as a function of the potential given in equation (1)). Actually, the solution in equation (B5) satisfies $\hat{H}(-\phi)\psi_{\text{II}} = -E\psi_{\text{II}}$; therefore, ψ_{II} is a negative-energy transmitted solution. Certainly, in the nonrelativistic limit, the upper component of ψ_{II} tends to zero; on the other hand, in the transmitted solution we used in section 1 (equation (B1)), it is the lower component that tends to zero in this approximation. These are expected results because ψ_{II} is a negative-energy solution, while ψ_t given in equation (B1) (or equation (6)) is a positive-energy solution.

Indeed, the transmitted solution ψ_{II} given in equation (B5) is none other than the charge-conjugate wavefunction of the solution ψ_t given in equation (B1). In fact,

$$\psi_{II} \propto \psi_t^C = \hat{S}_C \psi_t^* = \hat{\sigma}_x \begin{bmatrix} 1 \\ -c \hbar \bar{k} \\ E - V_0 + mc^2 \end{bmatrix} e^{+i\bar{k}x} = \begin{bmatrix} -c \hbar \bar{k} \\ E - V_0 + mc^2 \\ 1 \end{bmatrix} e^{+i\bar{k}x}. \quad (B6)$$

Thus, ψ_{II} must be an eigenfunction of $\hat{H}(-\phi)$ with eigenvalue $-E$. On the one hand, in a single-particle theory, we know that, if ψ_t describes a 1D Dirac particle's state with positive energy in the potential (energy) ϕ , then ψ_t^C describes a 1D Dirac particle's state (not a 1D Dirac antiparticle's state) with negative energy in the potential (energy) $-\phi$. Certainly, if the Dirac hole theory is invoked to obtain a physical picture of the negative-energy transmitted solution, then one would be abandoning 1D Dirac's theory as a single-particle theory. On the other hand, if ψ_t represents the motion of a 1D Dirac particle with a given charge in an external potential, ψ_t^C represents the motion of a 1D Dirac particle of opposite charge in the same external potential [27]. In this case, ψ_t and ψ_t^C clearly describe two different particles, as expected. The transmitted solution given in equation (B6) would admit either of the two interpretations presented above.

It is clear that our results cannot agree exactly with those of [25]. The reason for this discrepancy is that the transmitted solutions are not the same in the two works. As we have seen, when we reach the limit point of the Klein energy zone, i.e. $V_0 \rightarrow E + mc^2$, the potential step becomes an impenetrable barrier, and we obtain a solution describing a 1D Dirac particle that is restricted to the region $x < 0$. Then, a relativistic boundary condition naturally arises, and one has a precise value for the mean value of the force on the Dirac particle at $x = 0$. Taking the nonrelativistic limit of these results yields the expected results.

What happens if the solution given in [25] (equation (B5)) is used? We can answer this question here in a succinct manner. Naturally, the incoming and reflected plane-wave solutions have the same form as equations (4) and (5) with a and k given in equations (10) and (9). The negative-energy transmitted solution in equation (B6) can be written as follows:

$$\psi_{II} = \text{const} \times \begin{bmatrix} -b \\ 1 \end{bmatrix} e^{+i\bar{k}x}, \quad (B7)$$

where b and \bar{k} are given in equations (10) and (9). Assuming that the scattering solutions in the region $x < 0$ and in the region $x > 0$ can be joined at $x = 0$, the following result is obtained:

$$\psi(x) = \begin{bmatrix} \varphi \\ \chi \end{bmatrix} = \left(\begin{bmatrix} 1 \\ a \end{bmatrix} e^{ikx} + \left(\frac{ab+1}{ab-1} \right) \begin{bmatrix} 1 \\ -a \end{bmatrix} e^{-ikx} \right) \Theta(-x) + \frac{2a}{1-ab} \begin{bmatrix} -b \\ 1 \end{bmatrix} e^{i\bar{k}x} \Theta(x). \quad (B8)$$

Additionally, the reflection and transmission coefficients are given by

$$R = \left(\frac{ab+1}{ab-1} \right)^2, \quad T = \frac{4a|b|}{(1-ab)^2} = 1 - R, \quad (B9)$$

where $-ab$ is precisely β , which is given in equation (2.11) of [25]. Note that when $V_0 \rightarrow E + mc^2$ (for a given energy), i.e. when the limit point of the Klein energy zone is reached, the results $b \rightarrow -\infty$, $\bar{k} \rightarrow 0$, $R \rightarrow 1$ and $T \rightarrow 0$ are obtained. Likewise, the solution given in equation (B8) takes the form

$$\psi(x) = \begin{bmatrix} 2 \cos(kx) \\ 2i a \sin(kx) \end{bmatrix} \Theta(-x) + \begin{bmatrix} 2 \\ 0 \end{bmatrix} \Theta(x). \quad (B10)$$

Again, we have that $\psi(0-) = \psi(0+) \equiv \psi(0) \neq 0$, but the lower or small component of ψ (see equation (25)) satisfies the Dirichlet boundary condition at $x = 0$, i.e.

$$\chi(0-) = \chi(0+) \equiv \chi(0) = 0, \quad (B11)$$

and the upper or large component of ψ , i.e. φ , remains continuous there. Certainly, this boundary condition also defines a relativistic point interaction at $x = 0$. This boundary condition can be obtained from equation (B6) in [18] by imposing $\mu = \pi/2$ and $\tau = 3\pi/2$, or $\mu = 3\pi/2$ and $\tau = \pi/2$. In the nonrelativistic limit, the solution given by equation (B10) takes the form

$$\psi(x) \rightarrow \begin{bmatrix} \psi^{(NR)}(x) \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \cos(k^{(NR)}x) \\ 0 \end{bmatrix} \Theta(-x) + \begin{bmatrix} 2 \\ 0 \end{bmatrix} \Theta(x) \quad (B12)$$

($k^{(NR)} = \sqrt{2mE^{(NR)}}/\hbar$). Additionally, using the sifting property of the Dirac delta in its symbolic form and the fact that $\Theta_x(x) = \delta(x)$, one obtains the following result: $\psi_x^{(NR)}(x) = -2k^{(NR)} \sin(k^{(NR)}x) \Theta(-x) + 0 \Theta(x)$. Thus, in the nonrelativistic limit, the boundary condition given in equation (B11) leads to the Neumann boundary condition, i.e. the Schrödinger wavefunction satisfies $\psi_x^{(NR)}(0-) = \psi_x^{(NR)}(0+) \equiv \psi_x^{(NR)}(0) = 0$ [10, 19]. Certainly, the solution $\psi^{(NR)}(x)$ is not obtained by taking the infinite-potential limit (or the impenetrable barrier limit) in the 1D Schrödinger theory. Certainly, the Neumann boundary condition is not obtained in that limit either. Thus far, everything looks acceptable; however, if one calculates the mean value of the external classical force operator, in the state ψ given in equation (B8), one obtains the following result:

$$\langle \hat{f} \rangle_{\psi} = -V_0 \varrho_t(0) = -V_0 \frac{4a^2(1+b^2)}{(1-ab)^2}. \quad (\text{B13})$$

In the Dirac impenetrable barrier limit $V_0 \rightarrow E + mc^2$ (and therefore $b \rightarrow -\infty$), the result is as follows:

$$\langle \hat{f} \rangle_{\psi} = -4(E + mc^2). \quad (\text{B14})$$

Once the potential has reached the limit point of the Klein energy zone, the point $x = 0$ becomes an impenetrable barrier, and the 1D Dirac particle can only be on the half-line $x < 0$ (in fact, it is as if the particle has always been in that region); thus, we can resort to the procedure we followed in section II. Substituting Ψ from equation (7) (with ψ given in equation (B10)) into equation (23), we obtain the mean value of the (relativistic) boundary quantum force due to the impenetrable barrier at $x = 0$, namely,

$$\langle \hat{f}_B \rangle_{\Psi} = -i\hbar \Psi^\dagger(0, t) \Psi_t(0, t) + mc^2 \Psi^\dagger(0, t) \hat{\sigma}_z \Psi(0, t) = -4E + 4mc^2 = -4(E - mc^2). \quad (\text{B15})$$

Similarly, the average value of the (nonrelativistic) boundary quantum force due to the hard barrier at the origin can be obtained from equation (28) (with $\Psi^{(\text{NR})} = \psi^{(\text{NR})} \exp(-iE^{(\text{NR})}t/\hbar)$), from which the following result is obtained:

$$\langle \hat{f}_B \rangle_{\Psi^{(\text{NR})}} = +\frac{\hbar^2}{2m} (\Psi^{(\text{NR})})^*(0) \Psi_{xx}^{(\text{NR})}(0) = -4E^{(\text{NR})}. \quad (\text{B16})$$

Clearly, the result given in equation (B14) is not consistent with the result in equation (B15), i.e. it is not compatible with the fact that for $V_0 \rightarrow E + mc^2$, all 1D Dirac particles are reflected. In contrast, the nonrelativistic limit of the expression given in equation (B15) coincides with the result given in equation (B16). Presumably, some explanation of the result given in equation (B14) can be obtained by discarding the framework of the Dirac theory of a single particle and moving to the following scenario. This turns out to be most appropriate when the potentials are of the order of mc^2 . Specifically, it will always be attractive to consider particles in the region $x > 0$ as antiparticles (because in that region $E - V < 0$), and these antiparticles would have energy $-E$ above the potential (energy) $-V_0$. At the moment, we do not have a plausible explanation for the result in question. It is probably appropriate to leave that discussion for further research.

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