The Dirac impenetrable barrier in the limit point of the Klein energy zone

Salvatore De Vincenzo[1]

The Institute for Fundamental Study (IF),

Naresuan University, Phitsanulok 65000, Thailand

We reanalyze the problem of a 1D Dirac single-particle colliding with the electrostatic potential step of height V_0 with an incoming energy that tends to the limit point of the so-called Klein energy zone, i.e., $E \to V_0 - \mathrm{m}c^2$, for a given V_0. In this situation, the particle is actually colliding with an impenetrable barrier. In fact, $V_0 \to E + \mathrm{m}c^2$, 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 notice 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 wall on the particle in this eigenstate and taking its nonrelativistic limit, we recover the required result.

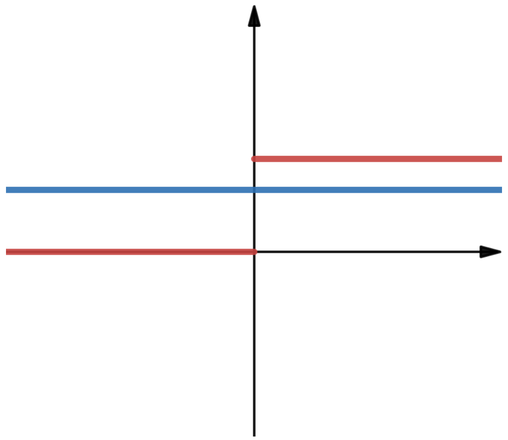
16:45 – 17:00, Thursday, 23$^{\text{th}}$ June 2022

[1] 0000-0002-5009-053X

1D Schrödinger theory

The potential step of height V_0 $(> E > 0)$

$$\phi(x) = \begin{cases} 0\,, & x < 0 \\ V_0\,, & x > 0 \end{cases}$$



- (a) The impenetrable barrier limit

  = The infinite-potential limit ($V_0 \to \infty$)

- (b) $\Rightarrow\ \psi^{(\mathrm{NR})}(0-) = \psi^{(\mathrm{NR})}(0+) \equiv \psi^{(\mathrm{NR})}(0) = 0$,

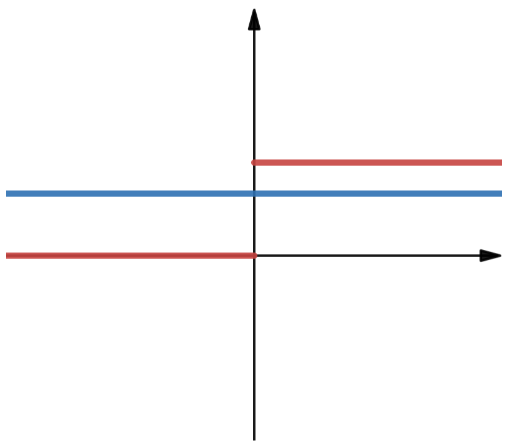
  i.e., the Dirichlet boundary condition

- (c) $\psi^{(\mathrm{NR})}$ has just one component

1D Dirac theory

The potential step of height V_0 $(> E > \mathrm{m}c^2)$

$$\phi(x) = \begin{cases} 0\,, & x < 0 \\ V_0\,, & x > 0 \end{cases}$$



(a) What is the impenetrable barrier limit?

(b) The infinite-potential limit $(V_0 \to \infty)$ $\Rightarrow$ Transmission!

$$T \to \frac{4a}{(a+1)^2}\,, \qquad a \equiv \sqrt{\frac{E - \mathrm{m}c^2}{E + \mathrm{m}c^2}}$$

T is the transmission coefficient

When $E \cong \mathrm{m}c^2$ (low energies): $a \to \sqrt{\frac{E^{(\mathrm{NR})}}{2\mathrm{m}c^2}} \cong 0 \;\Rightarrow\; T \cong 0$

When $E \gg \mathrm{m}c^2$ (high energies): $a \cong 1 \;\Rightarrow\; T \cong 1$

- Thus, this kind of tunneling is more noticeable when the particle has a high energy

- (c) The Dirichlet boundary condition is not acceptable!

$$\hat{H} = -\mathrm{i}\hbar c\,\hat{\alpha}\frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{m}c^2\hat{\beta} + \phi \quad \text{with} \quad D(\hat{H}) \;:\; \{\, \psi(0+) = \psi(0-) \equiv \psi(0) = 0 \,\}$$

is not self-adjoint! [1] [$x \in \mathbb{R} - \{0\}$, and $D(\hat{H})\,(\neq D(\hat{H}^\dagger))$ is the domain of $\hat{H}$]

- (d) ψ has two components

- (e) In fact, by imposing the Dirichlet boundary condition on the general solution of the 1D Dirac equation at a point like $x = 0$, the only solution is the trivial one. The problem is overdetermined!

[1] For example, use von Neumann's theory of self-adjoint extensions

The Klein energy zone

$$E - V_0 < -\mathrm{m}c^2 \qquad \Rightarrow \qquad V_0 > E + \mathrm{m}c^2 \quad (\text{for a given energy})$$

Thus, $V_0 > E$ (but we also know that $E = E_k + \mathrm{m}c^2 > \mathrm{m}c^2$, always)

(a) Tunneling occurs in this range of energies, it is the so-called Klein tunneling

$$T = \frac{4a\,|b|}{(a-b)^2}\,, \qquad a \equiv \sqrt{\frac{E - \mathrm{m}c^2}{E + \mathrm{m}c^2}}\,, \qquad b \equiv -\sqrt{\frac{E - V_0 - \mathrm{m}c^2}{E - V_0 + \mathrm{m}c^2}}$$

(when $V_0 \to \infty$, we have that $b \to -1$, and therefore $T \to 4a/(a+1)^2$)

The limit point of the Klein energy zone

$$V_0 \to E + \mathrm{m}c^2 \quad (\text{for a given energy})$$

(a) Tunneling disappears in this limit!

$$T \to 0$$

(In fact, when $V_0 \to E + \mathrm{m}c^2$, we have that $b \to -\infty$, and $T \to 0$)

- $V_0 \to E + \mathrm{m}c^2$ is the impenetrable barrier limit in the 1D Dirac theory!

  - (a) Thus, in this limit, the point $x = 0$ becomes an impenetrable barrier

  - (b) But, in this limit, what is the boundary condition that emerges? i.e., what is the boundary condition that the 1D Dirac wavefunction must satisfy at the impenetrable barrier?

- And now, the details

  - (a) In the Dirac representation, the time-independent 1D Dirac equation is given by

$$\hat{H}\psi(x) = \left(-\mathrm{i}\hbar c\,\hat{\sigma}_x \frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{m}c^2\hat{\sigma}_z + \phi\right)\psi(x) = E\psi(x)$$

where

$$\psi(x) = \begin{bmatrix} \varphi(x) \\ \chi(x) \end{bmatrix} = (\,\psi_{\mathrm{i}}(x) + \psi_{\mathrm{r}}(x)\,)\,\Theta(-x) + \psi_{\mathrm{t}}(x)\,\Theta(x)$$

is the scattering solution in compact form

(b) The incoming, reflected, and transmitted plane-wave solutions are given by

$$\psi_{\rm i}(x \le 0) \sim \begin{bmatrix} 1 \\ \frac{+c\hbar k}{E+{\rm m}c^2} \end{bmatrix} e^{+{\rm i}kx} \qquad \to \qquad \psi_{\rm i}(x \le 0) = \begin{bmatrix} 1 \\ a \end{bmatrix} e^{{\rm i}kx}$$

$$\psi_{\rm r}(x \le 0) \sim \begin{bmatrix} 1 \\ \frac{-c\hbar k}{E+{\rm m}c^2} \end{bmatrix} e^{-{\rm i}kx} \qquad \to \qquad \psi_{\rm r}(x \le 0) = \left(\frac{a+b}{a-b}\right) \begin{bmatrix} 1 \\ -a \end{bmatrix} e^{-{\rm i}kx}$$

$$\psi_{\rm t}(x \ge 0) \sim \begin{bmatrix} 1 \\ \frac{-c\hbar \bar{k}}{E-V_0+{\rm m}c^2} \end{bmatrix} e^{-{\rm i}\bar{k}x} \qquad \to \qquad \psi_{\rm t}(x \ge 0) = \frac{2a}{a-b} \begin{bmatrix} 1 \\ -b \end{bmatrix} e^{-{\rm i}\bar{k}x}$$

where

$$a \equiv \sqrt{\frac{E-{\rm m}c^2}{E+{\rm m}c^2}}\,, \qquad b \equiv -\sqrt{\frac{E-V_0-{\rm m}c^2}{E-V_0+{\rm m}c^2}}$$

$$k = \frac{\sqrt{E^2-({\rm m}c^2)^2}}{\hbar c}\,, \qquad \bar{k} = \frac{\sqrt{(E-V_0)^2-({\rm m}c^2)^2}}{\hbar c}$$

(c) ψ is a continuous function at $x = 0$

$$\psi(0-) = \psi(0+) \equiv \psi(0) \qquad \Rightarrow \qquad \psi_{\rm i}(0) + \psi_{\rm r}(0) = \psi_{\rm t}(0)$$

($x\pm \equiv \lim_{\epsilon\to 0}(x \pm \epsilon)$, with $x = 0$)

(d) The probability density and the probability current density, namely,

$$\varrho(x) = \psi^\dagger(x)\psi(x) = |\varphi(x)|^2 + |\chi(x)|^2 \ ,$$

$$j(x) = c\psi^\dagger(x)\hat{\sigma}_x\psi(x) = 2c\,{\rm Re}\,(\varphi^*(x)\chi(x))$$

are also continuous functions at $x = 0$, i.e.,

$$\varrho(0-) = \varrho(0+) = \varrho_{\rm t}(0) = \frac{4a^2(1+b^2)}{(a-b)^2} \ ,$$

$$j(0-) = j(0+) = j_{\rm t}(0) = -\frac{8c\,a^2 b}{(a-b)^2} > 0$$

($\varrho_{\rm t}(x)$ and $j_{\rm t}(x)$ are calculated for the solution $\psi_{\rm t}(x)$, etc)

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

$$R = \frac{|j_\mathrm{r}|}{|j_\mathrm{i}|} = \left(\frac{a+b}{a-b}\right)^2 ,$$

$$T = \frac{|j_\mathrm{t}|}{|j_\mathrm{i}|} = \frac{4a\,|b|}{(a-b)^2}$$

where $R + T = 1$ (No Klein paradox occurs, i.e., the situation where $R > 1$, just Klein tunneling)

(f) Note that

$$\hat{\mathrm{p}}\,\psi_\mathrm{t} = -\mathrm{i}\hbar\hat{1}_2\frac{\mathrm{d}}{\mathrm{d}x}\,\psi_\mathrm{t} = -\hbar\bar{k}\,\psi_\mathrm{t}$$

but

$$v_\mathrm{t} \equiv \frac{j_\mathrm{t}}{\varrho_\mathrm{t}} = -\frac{2c\,b}{1+b^2} = -\frac{c^2\hbar\bar{k}}{E-V_0} = c\sqrt{1-\left(\frac{\mathrm{m}c^2}{E-V_0}\right)^2} > 0$$

i.e., the transmitted velocity field is positive

(g) The mean value of the external classical force operator

$$\hat{f} = -\frac{\mathrm{d}}{\mathrm{d}x}\phi(x) = -V_0\,\delta(x)$$

i.e., the average force acting on the particle by the wall of potential at $x = 0$, in the scattering state ψ, is given by

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

$$= -V_0 \frac{4a^2(1+b^2)}{(a-b)^2}$$

The limit $V_0 \to E + \mathrm{m}c^2$

(a) It implies $b \to -\infty$, and therefore $R \to 1$ and $T \to 0$ (also $v_\mathrm{t} \to 0$)

(b) And the scattering solution of the Dirac equation,

$$\psi(x) = \left(\begin{bmatrix} 1 \\ a \end{bmatrix} e^{\mathrm{i}kx} + \left(\frac{a+b}{a-b}\right) \begin{bmatrix} 1 \\ -a \end{bmatrix} e^{-\mathrm{i}kx} \right) \Theta(-x) + \frac{2a}{a-b} \begin{bmatrix} 1 \\ -b \end{bmatrix} e^{-\mathrm{i}\bar{k}x}\,\Theta(x)\,,$$

takes the form

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

(c) Thus,

$$\psi(0-) = \psi(0+) \equiv \psi(0) \neq 0$$

i.e., the entire Dirac wavefunction is not zero where an impenetrable barrier exists

(d) But

$$\varphi(0-) = \varphi(0+) \equiv \varphi(0) = 0$$

This is the boundary condition that emerges when one imposes the impenetrable barrier limit in the 1D Dirac theory (in the Dirac representation, and for positive energies)

(e) Also note that

$$\varrho(0-) = \varrho(0+) \equiv \varrho(0) = 4a^2 \neq 0\,, \qquad j(0-) = j(0+) \equiv j(0) = 0$$

(f) Also, the mean value of the force exerted by the wall on the particle takes the form

$$\langle \hat{f} \rangle_\psi = -(E + \mathrm{m}c^2)\, 4a^2 = -4\,(E - \mathrm{m}c^2)$$

(g) In the nonrelativistic limit, i.e., $E \to E^{(\mathrm{NR})} + \mathrm{m}c^2 \cong \mathrm{m}c^2$ ($\Rightarrow a \to 0$), we obtain the results

$$\psi(x) \to \begin{bmatrix} 2\mathrm{i}\sin(k^{(\mathrm{NR})}x) \\ 0 \end{bmatrix} \Theta(-x)\,, \qquad \langle \hat{f} \rangle_\psi \to -4\, E^{(\mathrm{NR})}$$

($k^{(\mathrm{NR})} = \sqrt{2\mathrm{m}E^{(\mathrm{NR})}}/\hbar$). These are the required results!

Other impenetrability boundary conditions

(a) The Dirac Hamiltonian operator

$$\hat{H} = -\mathrm{i}\hbar c\, \hat{\sigma}_x \frac{\mathrm{d}}{\mathrm{d}x} + \mathrm{m}c^2 \hat{\sigma}_z + \phi$$

($x \in \mathbb{R} - \{0\}$), with the following domain:

$$D(\hat{H}) \ : \ \left\{ \varphi(0+) + \mathrm{i}\cot\left(\frac{\mu+\tau}{2}\right)\chi(0+) = 0, \quad \varphi(0-) + \mathrm{i}\tan\left(\frac{\mu-\tau}{2}\right)\chi(0-) = 0 \right\}$$

($0 \leq \mu, \tau < 2\pi$) is self-adjoint! [i.e., $\hat{H} = \hat{H}^\dagger$ and $D(\hat{H}) = D(\hat{H}^\dagger)$][1]

(b) For all these boundary conditions, we have that

$$j(0-) = j(0+) \equiv j(0) = 0\,,$$

i.e., all these boundary conditions define different impenetrable barriers at $x = 0$!

(c) Note that

$$\varphi(0-) = \varphi(0+) \equiv \varphi(0) = 0$$

is inside $D(\hat{H})$ (make $\mu = \tau = \pi/2, 3\pi/2$), but

$$\psi(0-) = \psi(0+) \equiv \psi(0) = 0$$

is not!

[1] For example, use von Neumann's theory of self-adjoint extensions

Some concluding remarks

- In the 1D Schrödinger theory, the impenetrable barrier limit, i.e., the infinite-potential limit, leads to the Dirichlet boundary condition for the respective (one-component) wavefunction

- 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)

- The limit $V_0 \to E + \mathrm{m}c^2$, for a given energy, is the impenetrable barrier limit in the 1D Dirac theory. This is because it leads to the cancellation of the probability current density at the barrier.

- In this limit, the impenetrability boundary condition for the wavefunction arises naturally, namely, its upper or large component -in the Dirac representation- satisfies the Dirichlet boundary condition at the barrier

- Similarly, in this limit, we calculated the mean value of the force exerted by the impenetrable barrier on the particle and the result tends to the required result when its nonrelativistic limit is taken

Thanks!

Grazie!

¡Gracias!