Quantum Mechanics II: PHYS 314 (Spring 2021)
Problem Set 5–Solutions.

Overview

In this Problem Set you will start to understand why we can't apply the logic that we used for the Schrödinger equation to relativistic particles in quantum mechanics, through the lens of Klein's paradox.

Introduction One way of motivating the free-particle Schrödinger equation is to take the non-relativistic dispersion relation $E = \vec{p}^2/(2m)$ and to make the replacements,

$$E \to i\hbar\frac{\partial}{\partial t}, \vec{p} \to -i\hbar\vec{\nabla}$$

so that when the wavefunction ψ satisfies

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi,$$

it necessarily has the right energy-momentum relationship.

If we follow the same procedure for the relativistic dispersion relation, $E^2 = |\vec{p}|^2c^2 + m^2c^4$, we get the free Klein-Gordon equation

$$-\hbar^2\frac{\partial^2\psi}{\partial t^2} = -c^2(\hbar^2\vec{\nabla}^2 - m^2c^2)\psi$$

and we are tempted to identify ψ with the wavefunction of a single particle (as we did in the Schrödinger case). Is this so bad?

Unfortunately this doesn't work as a consistent theory–in this question we will start to understand why.

The first mathematical issue is that the Klein-Gordon equation is second order in time derivatives, while the Schrödinger equation is first order. This means we'll need to specify both the state of the quantum system and its rate of change at an initial time to get the time-evolution. But suppose we brush this under the carpet. The second issue is that the Klein-Gordon equation admits solutions of negative energy, $E_p = \pm\sqrt{|\vec{p}|^2c^2 + m^2c^4}$. How do we interpret them? It turns out that things get even worse: these negative energy states have negative probability (densities)!

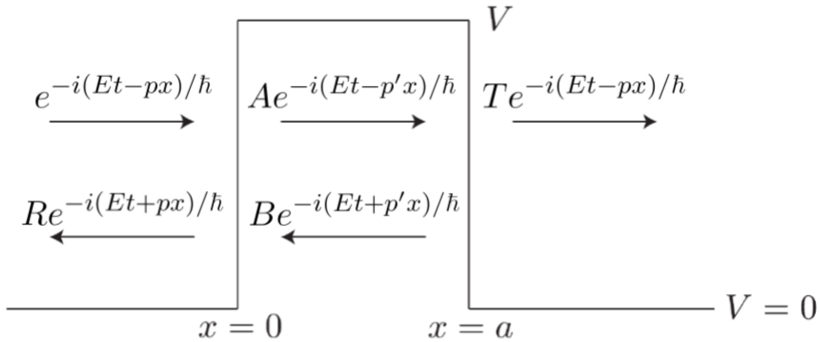

Figure 1: Rectangular barrier used in the question.

Suppose we brush this issue of negative probabilities under the carpet, too. Let's see what happens if we introduce "interactions" in the way we would in the Schrödinger equation, by introducing a potential,

$$i\hbar\frac{\partial}{\partial t} \to i\hbar\frac{\partial}{\partial t} - V.$$

Question **50pts**

Consider the rectangular barrier shown below, in Figure 1. For this question, assume that we're working in one spatial dimension.

For positive energy waves of energy E incident from the left we have

$$p = \frac{1}{c}\sqrt{E^2 - m^2c^4}, \qquad p' = \frac{1}{c}\sqrt{(E - V - mc^2)(E - V + mc^2)}.$$

(a) Using the continuity of $\psi(x)$ and $\partial\psi(x)/\partial x$ at $x = 0$, show that

$$A = \frac{2}{1 + p'/p} - \frac{1 - p'/p}{1 + p'/p}B.$$

(b) Using your result from part (a) and the continuity of $\psi(x)$ and $\partial\psi(x)/\partial x$ at $x = a$, show that

$$T = \frac{\rho\,(\lambda_+ + \lambda_-)}{\lambda_+ + \frac{p}{p'}\lambda_-},$$

where

$$\lambda_- = e^{-i(p'+p)a/\hbar} - \frac{1-p'/p}{1+p'/p} e^{i(p'-p)a/\hbar},$$
$$\lambda_+ = e^{-i(p'+p)a/\hbar} + \frac{1-p'/p}{1+p'/p} e^{i(p'-p)a/\hbar},$$
$$\rho = \frac{2}{1+p'/p} e^{i(p'-p)a/\hbar}.$$

(c) Use these results to show that the transmitted fraction is

$$|T|^2 = \left| \cos\left(\frac{ap'}{\hbar}\right) - \left(\frac{p'}{p} + \frac{p}{p'}\right) \frac{i}{2} \sin\left(\frac{ap'}{\hbar}\right) \right|^{-2}.$$

(d) Comment on the behaviour (and, in particular, whether it matches our nonrelativistic expectations) of the transmission coefficient, $|T|$, and the momentum, p', in the three regimes

- **(i)** Energies greater than the barrier, $E - mc^2 > V$.
- **(ii)** Energies below a relatively low barrier, $E - mc^2 < V < E + mc^2$.
- **(iii)** Energies below a high barrier, $E + mc^2 < V$.

Solution

(a) 5 points

The wavefunction ψ and the first derivative $\partial\psi/\partial x$ must both be continuous at $x = 0$ and $x = a$. Note that we are working in one spatial dimension! Continuity at $x = 0$ implies

$$1 + R = A + B, \tag{1}$$
$$ip(1 - R) = ip'(A - B), \tag{2}$$

where the first equation comes from continuity of the wavefunction and the second from the continuity of its derivative.

Now we can use Equations (1) and (2) to eliminate R, by multiplying Equation (1) by p and then adding the result to Equation (2). This leads to

$$2p = (p + p')A + (p - p')B.$$

Rearranging this gives

$$A = \frac{2}{1+p'/p} - \frac{1-p'/p}{1+p'/p} B. \tag{3}$$

(b) 15 points

At $x = a$ we have

$$Ae^{ip'a/\hbar} + Be^{-ip'a/\hbar} = Te^{ipa/\hbar}, \tag{4}$$

$$ip'(Ae^{ip'a/\hbar} - Be^{ip'a/\hbar}) = ipTe^{ipa/\hbar}. \tag{5}$$

We can now insert Equation (3) into Equation (4) to obtain

$$\begin{aligned} T &= Ae^{i(p'-p)a/\hbar} + Be^{-i(p'+p)a/\hbar} \\ &= \frac{2}{1+p'/p}e^{i(p'-p)a/\hbar} + B\left[e^{-i(p'+p)a/\hbar} - \frac{1-p'/p}{1+p'/p}e^{i(p'-p)a/\hbar}\right], \end{aligned} \tag{6}$$

where we've multiplied Equation (4) by $e^{-ipa/\hbar}$ to obtain the first equality.

Applying similar logic to Equation (5), we find

$$\frac{p}{p'}T = \frac{2}{1+p'/p}e^{i(p'-p)a/\hbar} - B\left[e^{-i(p'+p)a/\hbar} + \frac{1-p'/p}{1+p'/p}e^{i(p'-p)a/\hbar}\right]. \tag{7}$$

Let's tidy this up a bit, by defining

$$\begin{aligned} \lambda_- &= e^{-i(p'+p)a/\hbar} - \frac{1-p'/p}{1+p'/p}e^{i(p'-p)a/\hbar}, \\ \lambda_+ &= e^{-i(p'+p)a/\hbar} + \frac{1-p'/p}{1+p'/p}e^{i(p'-p)a/\hbar}, \\ \rho &= \frac{2}{1+p'/p}e^{i(p'-p)a/\hbar}. \end{aligned}$$

With these definitions, we can write Equations (6) and (7) as

$$T - \rho = B\lambda_-, \tag{8}$$

$$\frac{p}{p'}T - \rho = -B\lambda_+. \tag{9}$$

Dividing Equations (8) and (9) we obtain

$$\frac{T-\rho}{\frac{p}{p'}T - \rho} = -\frac{\lambda_-}{\lambda_+}.$$

Rearranging this gives

$$T - \rho = -\frac{p}{p'}T\frac{\lambda_-}{\lambda_+} + \rho\frac{\lambda_-}{\lambda_+},$$

or

$$T\left(1+\frac{p}{p'}\frac{\lambda_-}{\lambda_+}\right)=\rho\left(1+\frac{\lambda_-}{\lambda_+}\right).$$

Multiplying by λ_+ we finally find

$$T=\frac{\rho\left(\lambda_++\lambda_-\right)}{\lambda_++\frac{p}{p'}\lambda_-}. \tag{10}$$

(c) 20 points

First note that

$$\lambda_++\lambda_-=2e^{-i(p+p')a/\hbar}, \tag{11}$$

and second that

$$\lambda_++\frac{p}{p'}\lambda_-=\left(1+\frac{p}{p'}\right)e^{-i(p'+p)a/\hbar}+\frac{1-\frac{p'}{p}}{1+\frac{p'}{p}}\left(1-\frac{p}{p'}e^{i(p'+p)a/\hbar}\right). \tag{12}$$

Substituting Equations (11) and (12) into Equation (10), we obtain

$$\begin{aligned}
T&=\frac{2e^{ia(p'-p)/\hbar}}{1+p'/p}\cdot 2e^{-i(p+p')a/\hbar}\left[\left(1+\frac{p}{p'}\right)e^{-i(p'+p)a/\hbar}+\frac{1-\frac{p'}{p}}{1+\frac{p'}{p}}\left(1-\frac{p}{p'}\right)e^{i(p'+p)a/\hbar}\right]^{-1}\\
&=4e^{-2iap/\hbar}\left[\left(1+\frac{p'}{p}\right)\left(1+\frac{p}{p'}\right)e^{-i(p'+p)a/\hbar}+\left(1-\frac{p'}{p}\right)\left(1-\frac{p}{p'}\right)e^{i(p'+p)a/\hbar}\right]^{-1}\\
&=4e^{-ipa/\hbar}\left[\left(2+\frac{p'}{p}+\frac{p}{p'}\right)e^{-ip'a/\hbar}+\left(2-\frac{p'}{p}-\frac{p}{p'}\right)e^{ip'a/\hbar}\right]^{-1}\\
&=4e^{-iap/\hbar}\left[2\left(e^{-ip'a/\hbar}+e^{ip'a/\hbar}\right)+\left(\frac{p'}{p}+\frac{p}{p'}\right)\left(e^{-ip'a/\hbar}-e^{ip'a/\hbar}\right)\right]^{-1}\\
&=4e^{-iap/\hbar}\left[4\cos\left(\frac{ap'}{\hbar}\right)+\left(\frac{p'}{p}+\frac{p}{p'}\right)(-2i)\sin\left(\frac{ap'}{\hbar}\right)\right]^{-1}.
\end{aligned}$$

Thus we finally, finally get to

$$|T|^2=\left|\cos\left(\frac{ap'}{\hbar}\right)-\left(\frac{p'}{p}+\frac{p}{p'}\right)\frac{i}{2}\sin\left(\frac{ap'}{\hbar}\right)\right|^{-2}.$$

□

(d) 10 points

(i) For (kinetic) energies above the barrier, $E-mc^2>V$, p' is real and $|T|<1$, which corresponds to some reflection of flux. This is in accord with non-relativistic intuition.

(ii) For energies below a relatively low barrier, $E - mc^2 < V < E + mc^2$, p' is imaginary and we have tunnelling wavefunctions between $x = 0$ and $x = a$. This is also in accord with non-relativistic intuition.

(iii) For a very high barrier, we'd expect to continue to have tunnelling, but with an exponentially decreasing amplitude. In fact we get something completely different: For $V > E + mc^2$ (which implies $V > E - mc^2$ necessarily), p' is real again, and we have propagating solutions between $x = 0$ and $x = a$. The probability density in this region is also negative. This is known as Klein's paradox and it cannot be resolved without realising that the KG equation is a field equation associated with an indefinite number of particles, and not a single-particle wave equation.