(11) Scattering, Part 1

1 Thus Far

- A wavefunction describes our system
- The Schrödinger equation tells us how our system evolves
- Writing the wavefunction as a superposition of EESs (Energy EigenStates) makes life easier by removing time dependence
- Piecewise flat 1D potentials are nice because we already know the EESs in the flat regions, so we just need to match them at the boundaries

2 This Time

- The finite step potential
- Particle scattering
- Probability current

3 The Finite Step

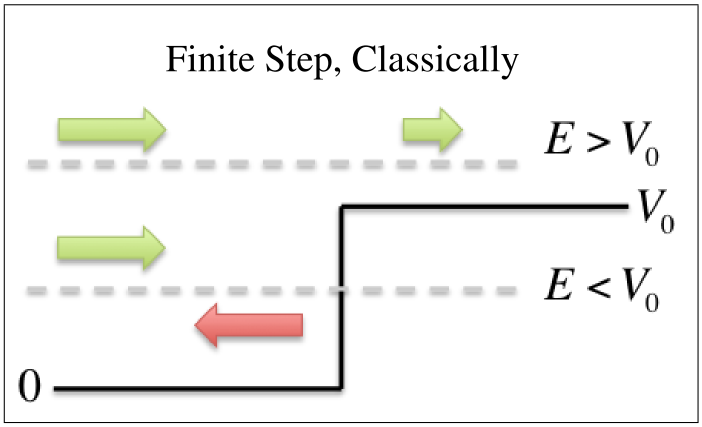
Last time we looked into a couple of piecewise flat potentials; the delta function well and the finite square well. And at the end we saw how the finite square well solution could be used to reproduce the delta and infinite square well results in the right limits.

This time we will consider a simpler potential; the finite step.

$$\text{Finite Step: } V(x) = \begin{cases} V_0 & x > 0 \\ 0 & x \leq 0 \end{cases}$$

(This is kind of like half of a finite well.) Unlike in previous lectures, this time we will not be working with bound states, but rather with unbound states. While it is always possible to make real energy eigenstates from sines, cosines, and decaying exponentials, unbound states are easier to describe in terms of traveling waves represented by complex exponentials.

We start by asking what we would expect classically from the 2 different scattering regimes. In one case, we have the total energy less than the potential step height, $E < V_0$, which would classically mean that the particle bounces off of step. In the other case, we have enough energy to surmount the step, $E > V_0$, which would classically mean that the particle slows down, but continues on in the same direction as before.

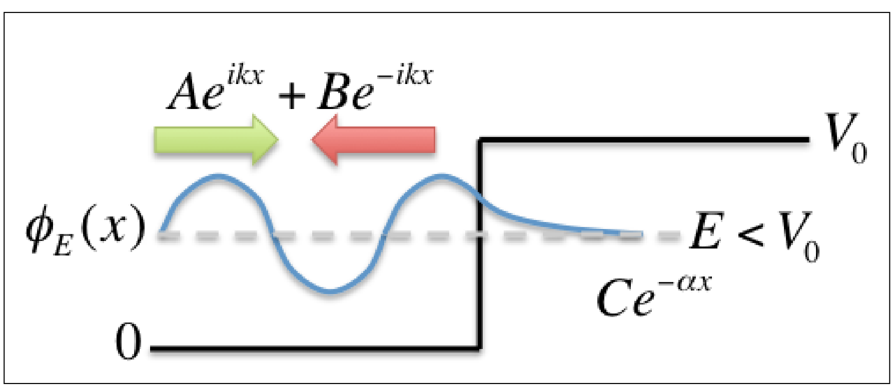


Let's look at what happens in QM in each of these cases, starting with $E < V_0$.

Show Matlab animation!

In terms of energy eigenstates, which idealize a particle as an extended (actually infinite) plane-wave, the solutions are relatively easy to write.

$$\phi_E(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x \leq 0\ ,\ k^2 = \frac{2m}{\hbar^2}E \\ Ce^{-\alpha x} & x \geq 0\ ,\ \alpha^2 = \frac{2m}{\hbar^2}(V_0 - E) \end{cases}$$



Continuity of

$$\begin{aligned} \phi(x) \quad &\Rightarrow \quad A + B = C \\ \partial_x \phi(x) \quad &\Rightarrow \quad ik(A - B) = -\alpha C \end{aligned}$$

$$\Rightarrow B = \frac{k - i\alpha}{k + i\alpha} A \quad \text{and} \quad C = \frac{2k}{k + i\alpha} A$$

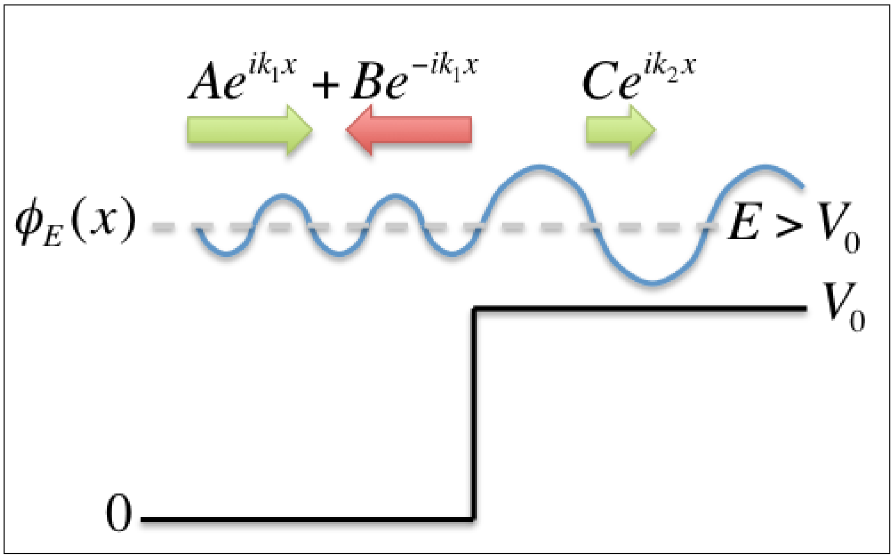
$$\text{note that} \quad |B| = |A| \quad \text{since} \quad \left| \frac{k - i\alpha}{k + i\alpha} \right|^2 = \frac{k - i\alpha}{k + i\alpha} \frac{k + i\alpha}{k - i\alpha}$$

Which tells us pretty much what we would expect classically; a particle which doesn't have enough energy to get over the step bounces off.

What about the more energetic particle with $E > V_0$? Here the solutions we need are oscillatory on both sides of the step, but the wave-numbers differ.

Show Matlab animation!

$$\phi_E(x) = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & x \le 0 \,, \; k_1^2 = \frac{2m}{\hbar^2} E \\ Ce^{ik_2 x} + De^{-ik_2 x} & x \ge 0 \,, \; k_2^2 = \frac{2m}{\hbar^2} (E - V_0) \end{cases}$$



As before, continuity will give us 2 constraints, and normalization will give us another, but this time we have 4 unknowns. The extra degree of freedom describes the type of experiment we are modeling; is the particle coming from the right or from the left? If we wanted the incoming wave to be from the right, we would choose $A = 0$ and use D for normalization. For a particle coming from the left, as before, we choose $D = 0$ and leave A to provide the normalization.

Continuity of

$$\begin{aligned} \phi(x) \quad &\Rightarrow \quad A + B = C \\ \partial_x \, \phi(x) \quad &\Rightarrow \quad ik_1(A - B) = ik_2 C \end{aligned}$$

$$\Rightarrow B = \frac{k_1 - k_2}{k_1 + k_2} A \quad \text{and} \quad C = \frac{2k_1}{k_1 + k_2} A$$

We can see from this that $|C| > |A|$ and $|B| < |A|$, since $k_1 > k_2$, but it is hard to say really what that means about where our particle ended up. Did it bounce off? Did it continue on? Did it do both?

The answers are not as obvious as in classical mechanics, but QM does offer an answer to the question of how our particle is moving, at least probabilistically. The answer comes in the form of something known as "probability current", which is the topic of the next section.

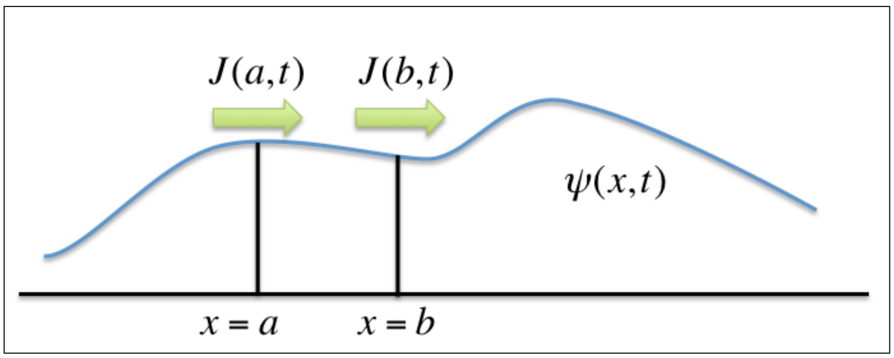
4 Probability Current

To answer the question of how a particle is moving in QM, one could reasonably look to $\langle x \rangle$, and this will work for a particle which is localized. $\langle x \rangle$ will not, however, be of much help if you have a wavefunction like e^{ikx}, and yet I keep telling you that this wavefunction represents "a particle moving to the right." What exactly do I mean by that?

The probability density $\mathbb{P}(x)$ tells me where I might find my particle at any given time, so changes in this must tell me how it is moving. We can define a probability flux, or probability current, as

Probability Current

$$
\begin{aligned}
\partial_t \mathbb{P}(x,t) &= -\partial_x \mathcal{J}(x,t) \\
\Rightarrow \partial_t \int_a^b \mathbb{P}(x,t) &= \underbrace{\mathcal{J}(a,t)}_{\text{flow in}} - \underbrace{\mathcal{J}(b,t)}_{\text{flow out}} \\
\text{SE } \Rightarrow \mathcal{J}(x,t) &= \frac{i\hbar}{2m}\left(\psi\, \partial_x \psi^* - \psi^*\, \partial_x \psi\right)
\end{aligned}
$$



The probability current has a noteworthy connection to momentum.

$$
\begin{aligned}
\mathcal{J}(x) &= \frac{1}{2m}\left[\psi(i\hbar\partial_x)\psi^* - \psi^*(i\hbar\partial_x)\psi\right] \\
&= \frac{1}{2m}\left[\psi(-i\hbar\partial_x\psi)^* + \psi^*(-i\hbar\partial_x\psi)\right] \\
&= \frac{1}{2m}\left[\psi(\hat{p}\psi)^* + \psi^*\hat{p}\psi\right] \\
&= \frac{1}{m} Re[\psi^*\hat{p}\psi] \\
\Rightarrow \int_{-\infty}^{\infty} \mathcal{J}(x) &= \frac{\langle p \rangle}{m} = v
\end{aligned}
$$

Such that the integral of the probability current over the whole region containing our particle gives the particle's classical velocity.

In the case of right and left moving plane-waves,

$$\begin{aligned}
\text{for }\ \psi(x) &= Ae^{ikx} + Be^{-ikx} \\
\mathcal{J}(x) &= \mathcal{J}_{\text{right}}(x) + \mathcal{J}_{\text{left}}(x) \\
\text{where }\ \mathcal{J}_{\text{right}}(x) &= |A|^2 \left[e^{ikx}\,\partial_x e^{-ikx} - e^{-ikx}\,\partial_x e^{ikx}\right] \\
&= |A|^2 \frac{i\hbar}{2m}(-2ik) = |A|^2 \frac{\hbar k}{m} = |A|^2 v \\
\text{and }\ \mathcal{J}_{\text{left}}(x) &= |B|^2 \left[e^{-ikx}\,\partial_x e^{ikx} - e^{ikx}\,\partial_x e^{-ikx}\right] \\
&= |B|^2 \frac{i\hbar}{2m}(2ik) = -|B|^2 v \\
\Rightarrow \mathcal{J}(x) &= \left(|A|^2 - |B|^2\right) v
\end{aligned}$$

such that the probability current is just the flux of the right moving wave minus the flux of the left moving wave. (Note, this is not true in general, but works only because we have $k_{\text{right}} = -k_{\text{left}}$. Fortunately, this condition is met for any energy eigenstate in a piecewise flat potential.)

The probability current, on the other hand, for any real wavefunction is zero.

For $\psi = \psi^*$

$$\mathcal{J}_{\text{real}}(x) = \frac{i\hbar}{2m}\left(\psi\,\partial_x\psi^* - \psi^*\,\partial_x\psi\right) = 0$$

So our exponentially decaying functions have no probability current associated with them.

5 Transmission and Reflection Coefficients

With the concept of probability current in hand, we are now in a position to talk about where out particle is likely to be found after interacting with a step potential. We can define the probability that the particle bounces off of the step, or is "reflected" as

Reflection Probability

$$R = \frac{-\mathcal{J}_{\text{left}}(x_-)}{\mathcal{J}_{\text{right}}(x_-)} \quad \text{with} \quad x_- < 0$$

$$= \left|\frac{B}{A}\right|^2 = \left(\frac{k_1 - k_2}{k_1 + k_2}\right)^2$$

Similarly, we can compute the probability that the particle continues past the step, or is "transmitted" as

Transmission Probability

$$T = \frac{\mathcal{J}_{\text{right}}(x_+)}{\mathcal{J}_{\text{right}}(x_-)} \quad \text{with} \quad x_+ > 0$$

$$= \left|\frac{C}{A}\right|^2 \frac{\hbar k_2}{\hbar k_1} = \frac{4k_1 k_2}{(k_1 + k_2)^2}$$

It is a little more illuminating to write this in terms of the energy of the incident particle

In terms of Energy

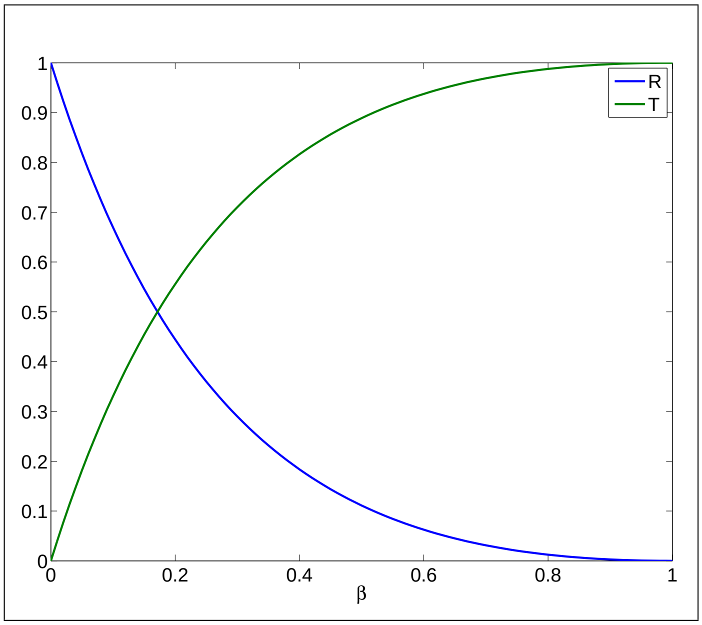
$$\text{recall} \quad k_1^2 = \frac{2m}{\hbar^2}E \quad \text{and} \quad k_2^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$$\Rightarrow \frac{k_2}{k_1} = \sqrt{1 - \frac{V_0}{E}} \equiv \beta$$

$$\text{note} \quad \beta = 0 \quad \text{for} \quad E = V_0 \quad \text{and} \quad \beta \simeq 1 \quad \text{for} \quad E \gg V_0$$

$$\Rightarrow R = \left(\frac{1-\beta}{1+\beta}\right)^2$$

$$\text{and} \quad T = \frac{4\beta}{(1+\beta)^2}$$



From which it can easily be shown that $R + T = 1$, which is just to say that no probability is lost.

---

6 Next Time

- Scattering from a more interesting potential
- All there is to know about a 1D potential in a simple 2x2 matrix