Physics 342 Lecture 20

Welcome back to more quantum mechanics! On Monday, we had constructed the analysis of the quantum free particle. We noted a few strange things about this system as compared to the infinite square well or harmonic oscillator. First, because the position of a free particle is unbounded for <u>any</u> energy, $x \in (-\infty, \infty)$, the momentum eigenstate

$$\psi_p(x,t) = e^{-\frac{i}{\hbar}(E_p t - px)}$$

is <u>not</u> normalizable, and therefore this momentum eigenstate is not in the Hilbert space. Further, the velocity of this state is

$$v_{phase} = \frac{E_p}{p} = \frac{p^2}{2mp} = \frac{p}{2m},$$

in analogy with the familiar sinusoidal waves. This is called the <u>phase velocity</u> and is 1/2 of what you would expect for a classical particle: $v = p/m$.

We found that both of these idiosyncrasies were addressed and corrected when we consider linear combinations of momentum eigenstates that are normalizable; so-called <u>wavepackets</u>. For a wavefunction expressed as:

$$\psi(x,t) = \int_{-\infty}^{\infty} dp\, g(p)\, e^{-\frac{i}{\hbar}(E_p t - px)},$$

it is normalized iff: $\displaystyle\int_{-\infty}^{\infty} dx\, |\psi(x,t)|^2 = 1 = 2\pi \int_{-\infty}^{\infty} dp\, |g(p)|^2.$

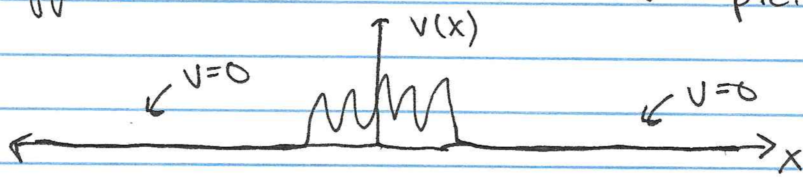
Further, the center-of-probability; the expectation value of $\hat{x}$, travels at velocity:

$$v_{group} = \frac{dE_p}{dp} = \frac{p}{m},$$

called the <u>group velocity</u>.

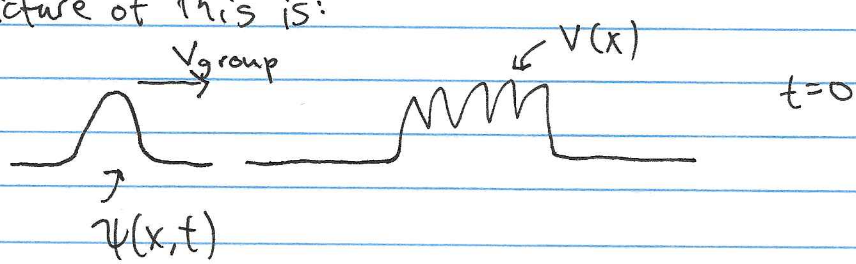
The group velocity is the speed that a wave packet, i.e., group of waves, travels at.

In this lecture, we're going to introduce the theory of scattering, starting from our understanding of the free particle. The idea of scattering is the following. Let's assume that we can model some system as a potential $V(x)$ that is localized around $x=0$. That is, for $|x| \to \infty$, $V(x) \to 0$ sufficiently fast. We won't discuss the mathematical properties or requirements of "sufficiently fast", but in language we introduced on Monday, the potential should have compact support around $x=0$. We'll draw a picture of this as:



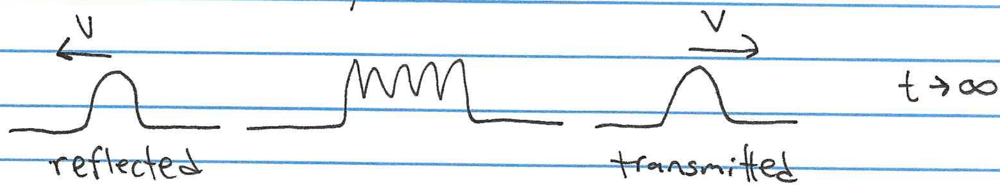
There's some craziness in the potential that's going on around $x=0$, but we can go far enough away to not be affected.

Now, let's imagine we have prepared a wave packet far to the left (negative x) of where the potential is. This wave packet is given a right-moving velocity, so that it will eventually hit the potential. A picture of this is:



Scattering theory asks the question: what happens?

specifically, scattering theory answers the question what happens long after the wave packet hits the potential, and continues traveling onward. In this scenario, if we wait a long enough time $t \to \infty$, part of the wave packet will be transmitted (continue moving right toward $x = +\infty$) and part will be reflected (bounce off the potential and move left toward $x = -\infty$):



Scattering theory answers the question of how much of the initial wave packet, i.e., how much probability amplitude, is reflected and how much is transmitted.

Note that scattering theory only asks questions when the wave packets are far away from the region where the potential is non-zero. Thus, a nice way to represent the wave packets is through linear combinations of momentum eigenstates, as we introduced earlier. Thus, we would write the initial, $t=0$, wave packet as:

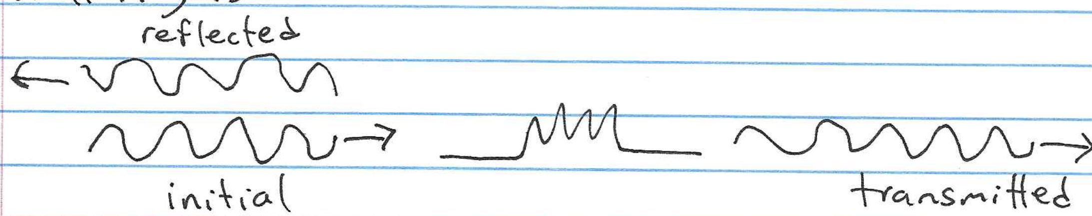
$$\psi(x, t=0) = \int dp\, g(p)\, e^{\frac{ipx}{\hbar}},$$ for some other complex function $g(p)$.

Now, we could ask how this initial wave packet reflects and transmits off of a potential V for each and every $g(p)$, but there are a continuous infinity of them. So, we use the linear combination to our advantage. We imaging sending in a momentum eigenstate from the left to hit the potential. While technically unphysical, because momentum eigenstates are not in the Hilbert space, if we know how every momentum eigenstate scatters off of the potential, we can reconstruct how a wave packet would scatter, by linearity.

So, this is what we will do. We will scatter the momentum eigenstate

$$\psi_p(x,t) = e^{-\frac{i}{\hbar}(E_p t - px)}$$

on the potential $V(x)$ and determine how much reflects and transmits. Note that I have written the argument of the exponential as $E_p t$ minus px, corresponding to moving right for $p>0$. Now, the picture we have of this scattering is:



Because the reflected and transmitted waves are also only in the region where $V=0$, we can write them as:

$$\text{reflected: } \psi_R(x,t) = A_R e^{-\frac{i}{\hbar}(E_p t + px)}, \quad x \to -\infty$$

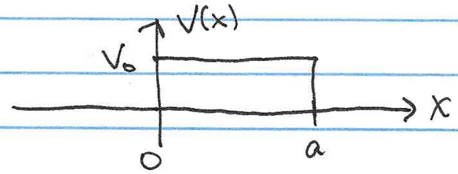
$$\text{transmitted: } \psi_T(x,t) = A_T e^{-\frac{i}{\hbar}(E_p t - px)}, \quad x \to +\infty$$

for amplitudes A_R, A_T. Note the different sign for momentum in reflection: it's traveling to the left.

In the regions where $V=0$, momentum eigenstates are also energy eigenstates, and where $V \neq 0$, energy eigenstates are still relevant, but momentum is less well defined in general. So, it will be more natural in what follows to relate everything to a fixed energy, and then write as momentum, if you like. For most of the rest of this lecture, we will use this formalism to calculate transmission and reflection waves for the example of a constant potential:

$$V(x) = \begin{cases} V_0, & 0 < x < a \\ 0, & \text{else} \end{cases}$$

That is, the potential looks like:



We'll discuss a classical analogy for this potential later.

Now, we will break up position into three regions:

I) $x < 0$, where the wavefunction is a linear combination of incident and reflected:

$$\psi_{I}(x) = e^{\frac{ikx}{\hbar}} + A_R e^{-\frac{ikx}{\hbar}}$$

III) $x > a$, where the wave function is just the transmitted wave:

$$\psi_{III}(x) = A_T e^{\frac{ikx}{\hbar}}$$

II) $0 < x < a$, where the wave function is a linear combination of the two possible momenta, $k_{II} = \pm\sqrt{2m(E - V_0)}$, where $E = \frac{k^2}{2m}$, the energy of the incident wavefunction. We have:

$$\psi_{II}(x) = Be^{\frac{i}{\hbar}\sqrt{2m(E-V_0)}\,x} + Ce^{-\frac{i}{\hbar}\sqrt{2m(E-V_0)}}$$

Note that this intermediate wavefunction is not ultimately what we want, but it is necessary for matching the wavefunctions in regions I and III that we do want.

For the wavefunction to satisfy the Schrödinger equation everywhere, it must be continuous and smooth. So, to determine A_R and A_T, we just demand continuity and smoothness at both $x=0$ and $x=a$.

Continuity requires: $\psi_I(x=0) = \psi_{II}(x=0)$

$$\hookrightarrow 1 + A_R = B + C$$

$$\psi_{II}(x=a) = \psi_{III}(x=a) \Rightarrow B e^{\frac{i\sqrt{2m(E-V_0)}\,a}{\hbar}} + C e^{-\frac{i\sqrt{2m(E-V_0)}\,a}{\hbar}} = A_T e^{\frac{ika}{\hbar}}$$

Smoothness requires: $\psi_I'(x=0) = \psi_{II}'(x=0)$

$$ik - ikA_R = i\sqrt{2m(E-V_0)}\,B - i\sqrt{2m(E-V_0)}\,C$$

$$\psi_{II}'(x=a) = \psi_{III}'(x=a) \Rightarrow i\sqrt{2m(E-V_0)}\,B e^{\frac{i\sqrt{2m(E-V_0)}\,a}{\hbar}} - i\sqrt{2m(E-V_0)}\,C e^{-\frac{i\sqrt{2m(E-V_0)}\,a}{\hbar}}$$

$$= ikA_T e^{\frac{ika}{\hbar}}$$

We thus have four equations for four (A_R, A_T, B, C) unknowns. Thus, we can completely solve for what we want: A_R and A_T.

It's now just algebra to solve for A_R and A_T, so I won't provide the details here. We find:

$$A_R = \frac{mV_0}{k^2 - mV_0 + ik\cot\left(a\sqrt{k^2-2mV_0}\right)\sqrt{k^2-2mV_0}}$$

$$A_T = \frac{k\sqrt{k^2-2mV_0}}{e^{\frac{iak}{\hbar}} k\sqrt{k^2-2mV_0}\cos\left(\frac{a}{\hbar}\sqrt{k^2-2mV_0}\right) - ie^{\frac{iak}{\hbar}}(k^2-mV)\sin\left(\frac{a}{\hbar}\sqrt{k^2-2mV}\right)}$$

While these expressions are big and unwieldy, they importantly are non-zero, generically.

First, by conservation of probability, the sum of the reflected and transmitted amplitude squared must be unity: $|A_T|^2 + |A_R|^2 = 1$. You can show this is true in this explicit example. We also call these squared amplitudes the reflection and transmission coefficients:

$R = |A_R|^2$, $T = |A_T|^2$, and they represent the fraction of the initial wave that was reflected or transmitted.

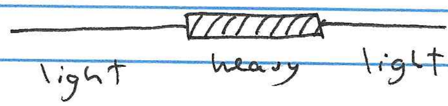
Second, note that A_R is 0 if $V_0 = 0$: that is, if there is no intermediate potential, nothing scatters off of it. Further, A_R is only 0 if $V_0 = 0$. For any non-zero value of V_0, A_R is non-zero: generically, a wave is always reflected. This is true even if $V_0 < 0$: a wave reflects off of a boundary that has less energy than where it came from! This is perhaps a bit strange from our classical, particle intuition.

Third, the transmission amplitude is only 0 if $k = 0$: if the particle has 0 momentum. Otherwise it is non-zero. In particular, A_T is non-zero if $V_0 > E = \frac{k^2}{2m}$. There is non-zero probability for transmission even if the energy is less than the height of the potential barrier. This doesn't seem like it's possible classically, and is referred to as quantum tunneling. The particle tunnels through a potential, even if it has insufficient energy. Note, however, that as it tunnels, the amplitude exponentially decays. If $E < V_0$, then, the intermediate wavefunction in region 2 is:

$$\psi_{II}(x) \sim e^{\frac{i}{\hbar}\sqrt{2m(E-V_0)}\,x} \sim e^{-\frac{\sqrt{2m(V_0-E)}}{\hbar}x}.$$

The further you have to tunnel the more you are penalized, and correspondingly the smaller A_T will be.

Perhaps this seems unfamiliar, but each of these phenomena occur for scattering of classical waves. Consider first a light rope connected on two ends to a heavy rope:



Send in a wave on the light rope (by shaking it, say). What happens? Does a wave make it to the right? Is a wave reflected? What happens if the mass of the heavy rope gets very large? I claim that this system can be analyzed almost exactly like our quantum tunneling.

Further, what if we connect two heavy ropes by a light rope:

Now what happens if we shake the rope on the left? Is there a reflection? What type of interface is heavy-to-light? Like a fixed or free end? What is its analogy in quantum mechanics?

We'll do a bit more next lecture to understand the properties of the case when $V_0 < 0$, called the finite square well.