Modern Physics notes – Spring 2007
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Lecture 25

- the Schrödinger equation
- finite-depth well

- Feynman, chapters 7, 16, 19
- Fowler, "Electron in a box","Finite square well"

The Schrödinger equation

Let's review the situations where we already know how the states and amplitudes depend on space and time. First of all, there's a stationary state. If the system is in a stationary state, the amplitude is of magnitude 1: it is at most a phase. In fact, we know what this phase is: it is $e^{-iEt/\hbar}$, where E is the energy of the state. Thus if $|\phi\rangle$ is a stationary state, we can write it at an arbitrary time as

$$|\phi\rangle = e^{-iEt/\hbar}|\phi_0\rangle$$

where $|\phi_0\rangle$ is the state at $t = 0$. In this notation, the amplitude $\phi(t) = e^{-iEt/\hbar}$.

We already noted that the amplitudes for stationary states obey the differential equation

$$i\hbar\frac{\partial\phi(t)}{\partial t} = E\phi(t)$$

By plugging the above $\phi(t)$ in you can check this.

Now let's remember what we said about the dependence of $\phi(x)$ on position. If a particle of mass m is moving in some constant potential V_0, then we said that the amplitude $\phi(x,t)$ for a stationary state depends on space as e^{ikx} for some k. The energy of this stationary state is

$$E = \frac{\hbar^2 k^2}{2m} + V_0$$

The reason we said this is that $|e^{ikx}|^2 = 1$, so that if the particle were in an infinite box, its probability to be at any given place would be the same. This means that the uncertainty principle holds properly. If we look at the stationary states in a box of finite size, then knowing E doesn't determine k exactly: it can be $\pm k$, as long as the relation for the energy still holds. We thus have an uncertainty of momentum of $2k$.

In our slightly new notation, we would say that the state $|\phi\rangle$ has probability amplitude

$$\langle x|\phi\rangle = \phi(x) = e^{ikx}$$

One thing we didn't note before was this is also the solution of a differential equation: we have

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi(x)}{\partial x^2} + V_0\phi(x) = E\phi(x)$$

It's easy to check that this is true if the above relation between E, V_0 and k holds.

Note that the right-hand-side of both of these differential equations is the same. Thus for a stationary state, let's write the probability amplitude including both spatial (e^{ikx}) and time dependence ($e^{-iEt/\hbar}$) as $\phi(x,t)$. We have

$$i\hbar\frac{\partial\phi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x,t)}{\partial x^2} + V_0\phi(x,t)$$

On the homework you'll check that $\phi(x,t) = Ae^{ikx}e^{-iEt/\hbar}$ is a solution of this equation.

The above differential equation was derived for constant $V(x) = V_0$, and for stationary states. But note first that E never appears in the equation, so we can hope that it applies also to probability amplitudes which are not just those of stationary states (i.e. those with amplitudes having a more complicated time dependence). Also, one might hope that this still applies for non-constant potential, i.e. V depending on x instead of a constant V_0. Making these two assumptions gives us the *Schrödinger* equation

$$i\hbar\frac{\partial\phi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x,t)}{\partial x^2} + V(x)\phi(x,t)$$

This works! You can find the probability amplitude for a single-particle system in any potential by solving this equation. Note that it is a linear equation for $\phi(x,t)$, so that any solution multiplied by a time- and space-independent constant is still a solution, and that the sum of any two solutions is still a solution.

The stationary states have time-dependence $e^{iEt/\hbar}$ as before. For stationary states, the Schrödinger equation therefore simplifies to

$$E\phi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\phi(x,t)}{\partial x^2} + V(x)\phi(x,t)$$

You should therefore think of the right-hand-side as another way of writing the energy, just like $p^2/2m + V$. In fact, in later quantum-mechanical courses, you will call

$$\widehat{p} \equiv -i\hbar\frac{\partial}{\partial x}$$

the momentum *operator*.

Finite-depth well

In a separate lecture you'll find a review of states and amplitudes, in both the discrete situation (the two-state system), and in the continuous one (a particle in box).

Now let's make the particle in a box a little more complicated (and realistic). No walls are infinitely high, so let's consider a situation where there are two different constant and finite potentials, say $V(x) = 0$ for $x < 0$ and $V(x) = V_0$ for $x > 0$. Again, consider a state independent of time so that the energy is definite. Then the probability amplitude may still be a sum of different pieces, but they all have the same dependence on time. Thus we can write

$$\phi(x,t) = \psi(x)e^{-iEt/\hbar}$$

where $\psi(x)$ is independent of time. It's easy to check then that the solutions of Schrodinger's equation for $x \neq 0$ are

$$\psi(x) = \begin{cases} Ae^{ip_1x/\hbar} + Be^{-ip_1x/\hbar} & x < 0 \\ Ce^{ip_2x/\hbar} + De^{-ip_2x/\hbar} & x > 0 \end{cases}$$

The fact that we're looking at a stationary state means that there's only one E in the problem: $\psi(x)$ solves the same equation for both $x < 0$ and $x > 0$. (We'll worry about what happens at $x = 0$ below). This means that

$$E = \frac{(p_1)^2}{2m}$$

and also

$$E = \frac{(p_2)^2}{2m} + V_0$$

Comparing the two relates p_1 and p_2:

$$\frac{(p_1)^2}{2m} = \frac{(p_2)^2}{2m} + V_0$$

We can solve this for p_2:

$$p_2 = \sqrt{(p_1)^2 - 2mV_0}$$

This last equation looks fairly innocuous, but note something funny happens if V_0 is too large: the argument of the square root becomes negative, so p_2 becomes imaginary! This isn't a bug, it's a feature. Look at the energy. When $2mV_0 > p_1^2$, you see that $E < V_0$. Thus we would say that the particle doesn't have enough energy to enter a region with potential energy V_0. In classical physics, that's the end of the story. But in quantum mechanics, it's not. Let $p' = -ip_2$. Then notice that the i in the exponent of the amplitude cancels, and we have

$$\psi(x) = Ce^{-p'x/\hbar} + De^{+p'x/\hbar} \qquad \text{for } x > 0$$

The first term falls off as x increases, the second increases. Now even though quantum mechanics is weird, it's not so weird that it will predict an increasing amplitude as the particle goes into a classically forbidden region. So we need to set $D = 0$, but since the first term falls off nicely, we do not need to set $C = 0$. Thus in quantum mechanics *there can be a non-zero probability of finding a particle in a classically forbidden region.* The amplitude does not have to vanish.

This means in particular that a particle can "tunnel" through a barrier, even though it has less energy. For example, some radioactive atoms are incredibly long-lived; for example, uranium decays by emitting an α-particle with a half-life of 4.5 billion years. Nuclei are incredibly small ($\sim 10^{-14}m$), so the frequency of oscillations of the nucleus is incredibly large: $\nu = c/\lambda \sim 10^{22}/s$. So how do we get half life of 10^9 years $\sim 10^{16}$ seconds from a period of around 10^{-22} seconds? The reason is that there is a potential barrier which holds the α particle in. It can tunnel out, but since the α particle is classically forbidden in the barrier, the amplitude is exponentially suppressed, as we saw above.

Notice the Schrodinger equation for a stationary state is a second-order differential equation in space. This means that when studying a particle in a finite-depth box, one must make sure both the probability amplitude and its first derivative are continuous at the edges of the box. For the example here, we have

$$\psi(0) = A + B = C$$

for the function, and

$$\psi'(0) = \frac{ip_1}{\hbar}(A - B) = -C\frac{p'}{\hbar}$$

When you're doing the finite-depth box on the homework, you do the same at the other end of the box as well. Then you have enough relations to find an equation just for p_1. This relation is the generalization to the finite-depth box of our earlier $\sin(pL/\hbar) = 0$, whose solution gave $p = n\pi\hbar/L$ (i.e. $\lambda = 2L/n$) for the infinite-depth box. Once you solve the relation for p_1 (which can be done in general only numerically), you can then find the energy levels of the finite-depth box! Thus making the walls of finite height changes the wavelength and energies of the particles trapped within.