Modern Physics notes – Spring 2006

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Lecture 24a

- A review of states and amplitudes
- A review of a particle in a box

States and Amplitudes

Let's do a mini-review of how quantum mechanics works, and introduce a little bit of new notation. A given physical system at a given time is described by a *state*. A special bunch of states is called the *basis*. All states can be described by linear combinations of the basis states. The set of basis states is not unique, but it is often convenient to use the *stationary states* as a basis. If a system is in a stationary state, it remains in this stationary state with probability 1 for all time, and has definite energy. However, if the system is in a linear combination of stationary states with different energies, then it does not stay in this exact state: but rather oscillates back and forth between states.

We've discussed a number of systems, but they all fall into one of two classes: the basis states are *discrete* or *continuous*. Example of the discrete ones are the two-state systems like the spin-1/2 particle or the ammonia molecule. A continuous system is the particle in a box: it can be anywhere in the box. The basis states for the particle in a box can be written $|x\rangle$. This means that if you measure the position of the particle, it is precisely at a location labeled by the position x.

There's a very important distinction to make in quantum mechanics. This is between *states* and *amplitudes*. A state tells you the whole thing: this is what the precise physical description of the system is. An amplitude is a number: it tells you the probability (when you take its magnitude squared) if the system is in a particular state. You can determine the amplitudes from the states. The notation we use nicely reflects this. Let's first review this for a discrete system. For example, say we know that a spin-1/2 particle has $S_x = -\hbar/2$. The state is then $|\downarrow x\rangle$. If desired, we can equivalently write this state as

$$|\downarrow x\rangle = \frac{1}{\sqrt{2}}|\uparrow z\rangle - \frac{1}{\sqrt{2}}|\downarrow z\rangle$$

This is useful if we ask the following question: what is the probability that this same particle (in state $|\uparrow x\rangle$) has spin $S_z = \hbar/2$. Then this particular *amplitude* is

$$\langle\uparrow z|\downarrow x\rangle = \langle\uparrow z|\left(\frac{1}{\sqrt{2}}|\uparrow z\rangle - \frac{1}{\sqrt{2}}|\downarrow z\rangle\right) = \frac{1}{\sqrt{2}}$$

The probability is thus $|1/\sqrt{2}|^2 = 1/2$. Likewise, we can also determine the amplitude for the spin $S_z = -\hbar/2$ for this same state $|\downarrow x\rangle$. It is

$$\langle\downarrow z|\downarrow x\rangle = \langle\downarrow z|\left(\frac{1}{\sqrt{2}}|\uparrow z\rangle - \frac{1}{\sqrt{2}}|\downarrow z\rangle\right) = -\frac{1}{\sqrt{2}}$$

The *state* is $|x\rangle$. The *amplitudes* are $\langle\downarrow z|\downarrow x\rangle = -1/\sqrt{2}$ and $\langle\uparrow z|\downarrow x\rangle = 1/\sqrt{2}$.

If we know all the amplitudes, we know the state. If we know the state, we can work out all the amplitudes. We can write this out precisely by labeling the basis states $|j\rangle$, with $j = 1, 2, \ldots$. (For the spin-s particle, $j = 1, 2, \ldots 2s + 1$.) Then we can write any state $|\psi\rangle$ as

$$|\psi\rangle = \sum_j \psi_j |j\rangle$$

where the ψ_j are the amplitudes

$$\psi_j = \langle j|\psi\rangle$$

If this isn't clear to you just look at the explicit example we did above.

Now let's turn to the continuous case. There we can't label the states by integers like we just did for the discrete case. But the idea is the same. The basis of states are $|x\rangle$, where x is a continuous variable. We've discussed amplitudes already: we called them $\psi(x)$. To make this notation look like the discrete case, label the state to be $|\psi\rangle$ when the probability amplitude $\psi(x)$. Then we also have

$$\psi(x) = \langle x|\psi\rangle$$

Note that this is just like the discrete case. The only difference is that instead of having discrete numbers $\psi_j, j = 1\ldots$, we have a function $\psi(x)$, with a continuous variable x.

To reiterate, when a particle is in state $|\psi\rangle$, it has probability amplitude $\psi(x) = \langle x|\psi\rangle$. The probability it is in the region between x_1 and x_2 is still

$$P(x_2 < x < x_1) = \int_{x_1}^{x_2} |\psi(x)|^2$$

Dependence on space

We're now going to leave the two-state system and go back to understanding what happens to a particle moving around. We'll understand the energy levels of a particle in a box where the sides aren't infinitely high, so that the particle isn't strictly confied to the box.

A while back I discussed how the amplitude of a "free" particle $\psi(x)$ depends on space as

$$\psi(x) \propto e^{i\vec{p}\cdot\vec{x}/\hbar}$$

If probability is independent of both space and time, then we have definite momentum and energy, with the amplitude proportional to

$$\psi(x) \propto e^{i(\vec{p}\cdot\vec{x}-Et)/\hbar}$$

This is called a *plane wave*; as we saw this satisfies the wave equation. So that's pretty easy. Quantum mechanics doesn't fix E or p, but if this is to describe a single free particle of mass m with velocity much smaller than the speed of light, we have

$$E = \frac{|\vec{p}|^2}{2m}$$

The universe would be a boring place if probabilities didn't depend on space or time, so we need to make this problem a little more complicated. Let's still consider stationary states, so that they have a definite energy, but now let's include a particle moving in a potential depending on space. The simplest example of this is a particle confined to a one-dimensional box. We've already studied this, but it's useful to redo it in a more general language.

A particle in a box is equivalent to a particle moving in a potential $V(x)$, where $V(x) = \infty$ for $x < 0$, $V(x) = 0$ for $0 < x < L$, and $V(x) = \infty$ for $x > L$. When the potential energy is infinite, no particle can go there, so the particle is confined to the box $0 < x < L$. The crucial point is that for a stationary state of energy E within the box, the relation $E = p^2/2m$ still holds. This almost fixes p, but not quite: both p and $-p$ give the same energy. Thus this stationary state can have spatial dependence $e^{ipx/\hbar}$ and/or $e^{-ipx/\hbar}$. Since this is quantum mechanics, we can have both! The general stationary state for a definite energy $E_p = p^2/(2m)$ has amplitude

$$\psi(x) = \begin{cases} 0 & x < 0 \\ Ae^{ipx/\hbar} + Be^{-ipx/\hbar} & 0 < x < L \\ 0 & x > L \end{cases}$$

where A and B are (so far) arbitrary coefficients.

So how do we fix A, B and p? The way is to require that the amplitude $\psi(x)$ be continuous in space. The above formula is obviously continuous except at $x = 0$ and $x = L$. To make it continuous at $x = 0$, we must have

$$A + B = 0$$

To make it continuous at $x = L$, we must have

$$Ae^{-ipL/\hbar} + Ae^{ipL/\hbar} = 0$$

The first condition means that $A = -B$; the second then implies that either $A = B = 0$ (i.e. no particle!) or

$$\sin(pL/\hbar) = 0$$

This is solved by requiring

$$pL = n\hbar\pi$$

for some integer n. We have recovered the quantization of momenta in a box: using $p = h/\lambda$ gives the familiar quantization formula $\lambda = 2L/n$. Thus for every integer n, there is an allowed amplitude

$$\psi_n(x) = A_n \sin\left(\frac{n\pi x}{L}\right) \qquad \text{for } 0 < x < L$$

Look familiar? This is our standing wave. Even without determining A_n, we now know the energy levels of a particle in a box: the nth level has definite energy

$$E_n = \frac{n^2\hbar^2}{2mL^2}$$

One thing to remember about the amplitude is that by definition the probability that the particle is in any given region $a < x < b$ is

$$P(a < x < b) = \int_a^b |\psi(x)|^2 dx$$

To fix the normalization A_n, we require that the probability that the particle is somewhere is 1, so

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$$

In this example, we therefore have

$$\begin{aligned} 1 &= |A_n|^2 \int_0^L \sin^2(n\pi x/L) dx \\ &= |A_n|^2 \int_0^L \frac{1}{2}\left(1 - \cos(2n\pi x/L)\right) dx \\ &= |A_n|^2 L/2 \end{aligned}$$

where I used the trigonometric identity $2\sin^2(a) = 1 - \cos(a)$, which you can easily prove from the definitions of sine and cosine in terms of $e^{\pm ia}$. This means that A_n in this example is independent of n, and is $A_n = \sqrt{2/L}$.