

We said last lecture that $\Psi^2(x, t)dx =$ probability of finding particle within dx of x at time t . For this to work then our wavefunction must be NORMALISED such that $\int \Psi^2(x, t)dx = 1$ (the particle must be SOMEWHERE!). so lets do some examples of this:

1.4.1 $\Psi(x, t = 0) = N \exp(-ax^2/2)$

Normalisation condition is

$$\int_{-\infty}^{+\infty} N^* e^{-ax^2/2} N e^{-ax^2/2} dx = 1$$

$$N^2 \int_{-\infty}^{+\infty} e^{-ax^2} dx = 1$$

Wolfram alpha site lets you calculate definite integrals

<http://www.wolframalpha.com/>

functions have capital letters, so here type integrate Exp[-a x^ 2] between -infty and infty in the box and hit return to get $= \sqrt{\frac{\pi}{a}}$ hence

$$N^2 \sqrt{\frac{\pi}{a}} = 1$$

$$N = \left(\frac{a}{\pi}\right)^{1/4}$$

so then the probability I will find the particle between $0 < x < a$ is $\int_0^a \Psi^* \Psi dx = \sqrt{a/\pi} \sqrt{\pi/a} \text{erf}(a^{3/2})/2 = \text{erf}(a^{3/2})/2$

1.4.2 Normalisation is independent of time

In the example above we see that the normalisation is independent of time - this is actually a general property of all systems, not limited to the specific example of a free particle. its possible, if tedious, to show very generally from the Schroedinger equation that $d/dt \int \Psi^* \Psi dx = 0$. I'm not going to go through it if you are really interested see the derivation in section 1.4 of griffiths. But the fact that $d/dt \int \Psi^* \Psi dx = 0$ means that I only need to normalise at $t = 0$ and then my wavefunction has the same normalization for all subsequent times.

2 Expectation values and operators

If we only have a probability then we don't have a clear answer to the question 'what value do we get when we measure something'. but we have a probability distribution. so if we had multiple identical systems and measured some quantity, say position, we would get a distribution of values. we could average this, and say this is the expected value we would measure. expectation value = average value from multiple measurements of identical systems NOT the value we will get if we make one measurement. To get an average, we multiply each possible value by the probability of getting that value - eg height of people on the front row!

2.1 Position

The expectation, or average, value of position will be denoted by angle brackets and is simply

$$\begin{aligned}\langle x(t) \rangle &= \int xP(x, t)dx = \int x\Psi^*(x, t)\Psi(x, t)dx \\ &= \int \Psi^*(x, t)x\Psi(x, t)dx\end{aligned}$$

where the reason for the ordering will become apparent soon.

So for the free electron we have

$$\langle x(t) \rangle = 1/L \int_0^L e^{-i(kx-\omega t)} x e^{i(kx-\omega t)} dx = 1/L \int_0^L x dx = 1/L [x^2/2]_0^L dx = L/2$$

and for $\Psi(x, t = 0) = (\frac{a}{\pi})^{1/4} \exp(-ax^2/2)$ we have

$$\langle x \rangle = (\frac{a}{\pi})^{1/2} \int_{-\infty}^{+\infty} \exp(-ax^2/2) x \exp(-ax^2/2) dx = (\frac{a}{\pi})^{1/2} \int_{-\infty}^{+\infty} x \exp(-ax^2) dx$$

this is another standard integral we could look up on wolfram alpha - or actually we can simply look at the symmetry and see that its zero!! which makes a lot of sense when we draw it

2.2 Momentum

Going back to our free space wavefunction, we know that $\partial\Psi/\partial x = \partial A e^{i(kx - \omega t)}/\partial x = ik\Psi = ip/\hbar\Psi$. we know $p = h/\lambda = \hbar k$. Hence

$$\frac{\hbar}{i} \frac{\partial\Psi}{\partial x} = p\Psi$$

$$-i\hbar \frac{\partial\Psi}{\partial x} = p\Psi$$

So there is an association between the dynamical quantity p and the differential operator $-i\hbar\partial/\partial x$. The effect of multiplying Ψ by p is the same as the effect of operating on it with the differential operator $p\Psi = -i\hbar\partial\Psi/\partial x$. So we can define a momentum operator $\hat{p} = -i\hbar\partial/\partial x$.

Since this is an operator, it matters which ORDER we use $\int \Psi^*(\partial\Psi/\partial x)dx \neq \int \partial/\partial x(\Psi^*\Psi)dx$, and putting it at the end makes no sense at all $\int[\Psi^*\Psi]\partial/\partial x dx$ as it doesn't have anything to operate on! This is unlike position, where although we call \hat{x} an operator, it doesn't actually make a difference $\int \Psi^*\hat{x}\Psi dx = \int \hat{x}\Psi^*\Psi dx = \int \Psi^*\Psi\hat{x} dx$.

So the only choice is whether to put it at the start or in the middle. suppose we'd put it at the start then we can integrate to get:

$$\langle p \rangle = \int_{-\infty}^{+\infty} -i\hbar \frac{\partial}{\partial x} [\Psi^*\Psi] dx = -i\hbar [\Psi^*\Psi]_{-\infty}^{\infty}$$

But this is zero by construction as the wavefunction must go to zero at $\pm\infty$ as the particle would never be found there. so the only way to get a non-trivial, meaningful answer is to put it in the middle.

so for $\Psi(x, t = 0) = (\frac{a}{\pi})^{1/4} \exp(-ax^2/2)$ we get

$$\langle p \rangle = \left(\frac{a}{\pi}\right)^{1/2} \int \exp(-ax^2/2) -i\hbar\partial/\partial x \exp(-ax^2/2) dx$$

$$= -\left(\frac{ia\hbar}{\pi}\right)^{1/2} \int \exp(-ax^2/2) -ax \exp(-ax^2/2) dx = \left(\frac{ia^2\hbar}{\pi}\right)^{1/2} \int x \exp(-ax^2) dx$$

Again, go to wolfram alpha or do it by inspection - its zero! so here the mean momentum is actually zero, even though it didn't have to be by construction. and this is telling us physically that its a standing wave!

2.3 Operator Momentum and Ehrenfest's theorem

With this operator notation we can prove quite formally and rigorously (see section 1.5 Griffiths) that

$$\langle p \rangle = \int \Psi^*(x, t) \cdot -i\hbar \frac{\partial \Psi(x, t)}{\partial x} dx = \frac{1}{m} \frac{d \langle x \rangle}{dt}$$

i.e. the expectation value of velocity is equal to the rate of change of the expectation value of position $\langle v \rangle = d \langle x \rangle / dt$, and the expectation value of momentum is $\langle p \rangle = m \langle v \rangle$.

This is what we *should* get. At some point we have to make a transition from the quantum world to the classical one. Roughly, that's when we go to macroscopic rather than microscopic scales. And then quantum mechanics HAS to give the same answer as classical mechanics! In classical mechanics we have $p = mdx/dt$, so quantum has to have $\langle p \rangle = md \langle x \rangle / dt!!$ and it does.

Similarly, we could prove in a very general way that $d \langle p \rangle / dt = \langle F \rangle = - \langle \partial V / \partial x \rangle$ which is Newton's law for a conservative force.

Expectation values obey classical laws, even though the wavefunction itself is probabilistic and thoroughly quantum in nature which is called Ehrenfest's theorem. This is required for any theory - we know classical laws work in the macroscopic regime (and velocity and gravity are small so we don't have to do relativity).

2.4 General operators

Any dynamical variable $A(x, p, t)$ can be written classically as some function of position, momentum and time. We can associate this with an operator $\hat{A}(x, p, t)$ by substituting $-i\hbar \partial / \partial x$ for p . Then the expectation value of this variable is

$$\langle A(x, t) \rangle = \int \Psi^*(x, t) \hat{A}(x, -i\hbar \partial / \partial x, t) \Psi(x, t) dx$$

2.5 Equations from operators

The Schrödinger equation is $E = T + V$. We saw how to do T above and we saw in our justification of Schrödinger that we could associate energy with

the operator is $i\hbar\frac{\partial}{\partial t}$. Hence we write this energy equation as

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

In classical mechanics the sum of kinetic and potential energy is called the Hamiltonian. Hence we have

$$H = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V$$

to illustrate how to apply this to a new equation, we know that the fully relativistic equation for a free particle energy is $E^2 = p^2c^2 + m^2c^4$. If we write this in operator form (operating on a wavefunction!) we have

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}i\hbar\frac{\partial\Psi}{\partial t} &= c^2 \times -i\hbar\frac{\partial}{\partial x} \times -i\hbar\frac{\partial\Psi}{\partial x} + m^2c^4\Psi \\ -\hbar^2\frac{\partial^2\Psi}{\partial t^2} &= -\hbar^2c^2\frac{\partial^2\Psi}{\partial x^2} + m^2c^4\Psi \end{aligned}$$

this is the relativistic equation Schroedinger (Klein Gordon equation) for a free particle! and we can see this makes sense by looking at what it does for massless relativistic particles (ie photons!!)

$$\begin{aligned} -\hbar^2\frac{\partial^2\Psi}{\partial t^2} &= -\hbar^2c^2\frac{\partial^2\Psi}{\partial x^2} \\ \frac{\partial^2\Psi}{\partial x^2} &= \frac{1}{c^2}\frac{\partial^2\Psi}{\partial t^2} \end{aligned}$$

which is of course a wave equation with velocity c !

2.6 Reality check...

The next few sections take a bodyswerve into more formal language. But they make some very important points, so its worth while to do them! One thing that might worry us is whether our expectation values are real!! Our fundamental operator for p is $-i\hbar\partial/\partial x$ and thats got complex numbers in it, and we know that wavefunctions themselves can be complex. but anything we can measure has to be real - $\langle p \rangle, \langle H \rangle$ etc....

We can take the time derivative of the normalisation constraint

$$\frac{d}{dt} \left[\int \Psi^*(x, t) \Psi(x, t) dx \right] = \frac{d}{dt} [1] = 0$$

take the differential inside the integral (so its now a partial derivative not a total derivative)

$$\int \frac{\partial}{\partial t} [\Psi^*(x, t) \Psi(x, t)] dx = 0$$
$$\int \frac{\partial \Psi^*(x, t)}{\partial t} \Psi(x, t) + \Psi^*(x, t) \frac{\partial \Psi(x, t)}{\partial t} = 0$$

But our Schroedinger equation says

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