Introduction To Quantum Mechanics

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Chapter 1

Wavefunctions and the Schroedinger Equation

1.1 Wavefunctions

By adding waves with lots of different momenta prevents us from knowing the position and momentum at the same time. By decreasing the uncertainty in position we increase it in momentum. This gives us a weak idea of Heisenberg Uncertainty!

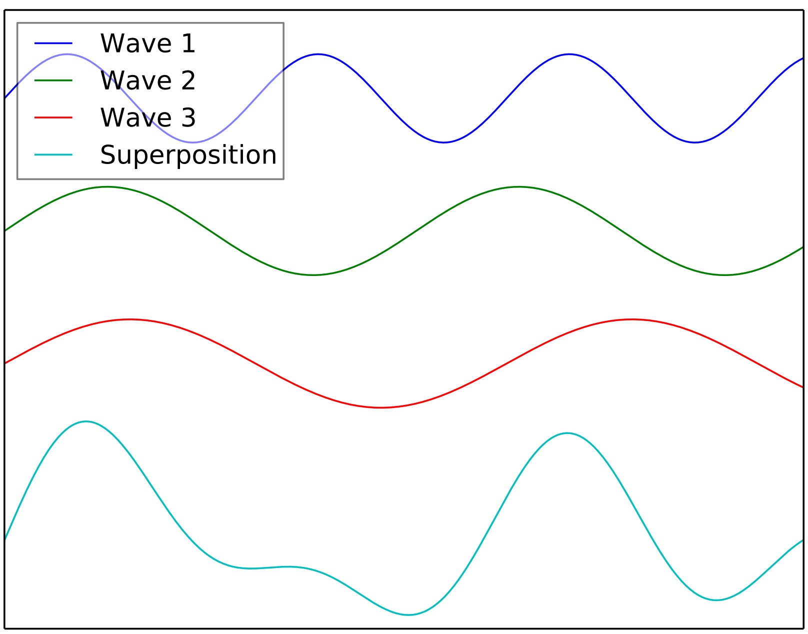

Figure 1.1: Adding waves together "localises" them more in space.

$$\Delta x \Delta p \geq \frac{\hbar}{2}$$

1.1.1 Classical Waves

We expect classical waves to move in a certain way, in accordance with the wave equation:

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 y}{\partial t^2}$$

and have the following properties:

- $v = \omega/k$
- $\omega = 2\pi f$
- $f = 2\pi/\lambda$

For example:

$$y(x,t) = A\cos(kx - \omega t) + B\sin(kx - \omega t)$$

Which satisfies the above wave equation.

However, here, momentum (mv) is not dependent on wavelength. This must be different in the quantum world, because of De Broglie's relation:

$$\lambda = \frac{h}{p}$$

1.1.2 Quantum Waves

Let's just begin by studying a random wave:

$$\Psi(x,t) = A\cos(kx - \omega t) + B\sin(kx - \omega t)$$

From the quantum world, we can use that:

- $p = h/\lambda = \hbar k$
- $E = hf = \hbar\omega$

And from the classical world:

- $E = p^2/2m = \hbar^2 k^2/2m$

Let's begin by getting a k^2 out by differentiating the wavefunction with respect to x twice:

$$\frac{\partial^2 \Psi}{\partial x^2} = -k^2\Psi$$

Plugging into the above formulae:

$$\Psi E = \Psi\hbar^2 k^2 = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Now we need to get ω. Let's try differentiating with respect to time.

$$\frac{\partial \Psi}{\partial t} = \omega\left[A\sin(kx - \omega t) - B\cos(kx - \omega t)\right]$$

However, this isn't really that useful. We want it to equal a multiple of our original wavefunction, or the maths is really hard to do.

$$\omega\left[A\sin(kx-\omega t)-B\cos(kx-\omega t)\right]=C\Psi=C\left[A\cos(kx-\omega t)+B\sin(kx-\omega t)\right]$$

We can now equate coefficients and find that (sub $\sin(kx-\omega t)=s$):

$$\omega[As-Bc]=C[Ac+Bs]\ \rightarrow\ C=\frac{\omega A}{B}$$

And as such

$$B^2=-A^2\quad\rightarrow\quad B=\pm iA$$

From this we find that:

$$\Psi(x,t)=A\left[\cos(kx-\omega t)+i\sin(kx-\omega t)\right]=Ae^{i(kx-\omega t)}$$

And now we can put it all together to find the *Schroedinger Equation for a free particle*:

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

This can be easily generalised to find *The Schroedinger Equation!*:

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

We can notice that the Schroedinger Equation is *linear* and *homogeneous*! This means that the linear sum of any two solutions is also a solution.

For the classical wave equation we needed two boundary conditions to solve, however here we only need one.

1.2 Interpretation of Ψ

This equation leads us to believe that there is an underlying statistical nature to The Universe.

Classically, we know that $I\propto A^2$. Quantum mechanically we think of this square of the wavefunction as the probability of finding the particle at that point.

$$P(particle)=|\Psi(x,t)|^2=\Psi^*\Psi$$

We choose this because it will *always* be real - like probabilities must be.

1.3 Normalisation

Suppose we want to normalise some function $f(x,t)$. We need to find the total area under the function and then divide through by a constant to make sure this is unity:

$$|N|^2\int_{-\infty}^{\infty}f^*(x,t)f(x,t)\cdot\mathrm{d}x=1$$

And so we can find the normalisation constant, N:

$$N=\frac{1}{\sqrt{\int_{-\infty}^{\infty}f^*(x,t)f(x,t)\cdot\mathrm{d}x}}$$

We simply need to do this for the wavefunction to normalise it.

1.3.1 Normalizatiof condition

For the unboud particle, it is trivial to work out the normalization condition.

$$\int_{-\infty}^{\infty} \Psi^* \Psi \cdot \mathrm{d}x = 1$$

$$A^2 \int_{-\infty}^{\infty} \exp(-i[kx - \omega t]) \exp(i[kx - \omega t]) \cdot \mathrm{d}x = 1$$

$$A^2 \cdot \infty = 1$$

Oh dear! This is when we assume that the particle is not confined at all, when it is really confined to the length of our lab, L, giving:

$$A = \frac{1}{\sqrt{L}}$$

1.3.2 Gaussian wavefunction

What happens when we try to find the normalisation condition for a gaussian? The equation

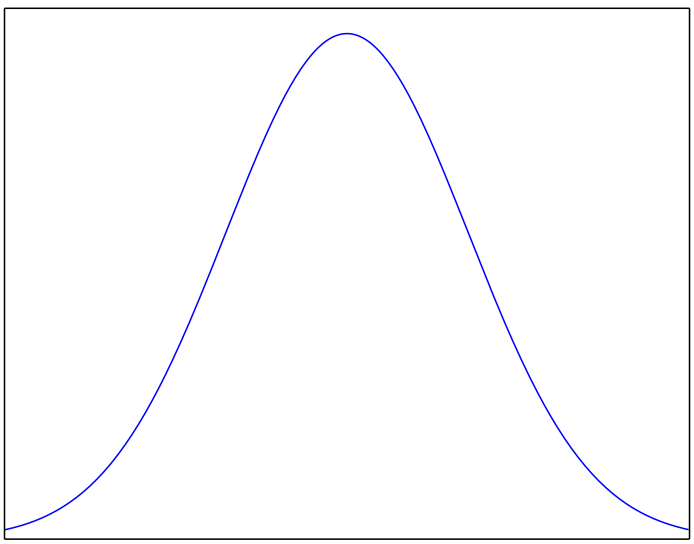

Figure 1.2: A Gaussian function

for a gaussian:

$$\Psi = N \exp\left(-\frac{ax^2}{2}\right)$$

To find the normalisation:

$$\int \Psi^* \Psi \cdot \mathrm{d}x = 1 = \int_{-\infty}^{\infty} N^2 \exp\left(-ax^2\right) \cdot \mathrm{d}x$$

Using WolframAlpha:

$$N^2 \frac{\sqrt{\pi}}{\sqrt{a}} = 1 \;\rightarrow\; N = \left(\frac{a}{\pi}\right)^{\frac{1}{4}}$$

Now, let's work out what the probability of finding the particle in the range of $0 \to a$!

$$\int_0^a P(x) \cdot \mathrm{d}x = \left(\frac{a}{\pi}\right)^{\frac{1}{2}} \int_0^a \exp(-ax^2) \cdot \mathrm{d}x = \frac{\mathrm{Erf}\left(a^{\frac{3}{2}}\right)}{2}$$

1.3.3 Normalization is time-independent

It is possible to show that:

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} \Psi^* \Psi \cdot \mathrm{d}x = 0$$

This means you only need to normalize once!

1.4 Position

What's the average position of the particle with our Gaussian wavefunction? Let's denote it $< x >$:

$$< x >= \int P(x) x \cdot \mathrm{d}x = \int \Psi^* x \Psi \cdot \mathrm{d}x$$

Substituting in the Gaussian:

$$< x >= \left(\frac{a}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x \exp(-ax^2) \cdot \mathrm{d}x$$

Which we can solve to find:

$$< x >= 0!$$

Which is exactly what you would expect, as the Gaussian is symmetric about 0.

1.4.1 Momentum

Similarly to how we worked out the average position, we must be able to work out the average momentum. Let's start with:

$$E\Psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

From the definition of kinetic energy:

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

We can put these together to show:

$$\Psi p^2 = \Psi p \cdot p = -\hbar^2 \frac{\partial^2 \Psi}{\partial x^2}$$

And extract:

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

From this, we can try to find what the average momentum in the Gaussian is!

$$< p >= \int p(x) P(x) \cdot \mathrm{d}x$$

Now we substitute in for $p\Psi$:

$$-i\hbar \int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} \cdot \mathrm{d}x$$

We already have the wavefunction, meaning we can substiute in to give:

$$< p >= \left(\frac{a}{\pi}\right)^2 (-i\hbar) \int_{-\infty}^{\infty} -ax \exp(-ax^2) \cdot \mathrm{d}x = 0$$

We can see that this is going to be 0 because of the fact that it is an odd function multiplied by an even function.

The reason that we would expect this result is because this is clearly a bound wavefunction. This means that there will be standing waves set up inside the two potential barriers leading to standing waves which, clearly, aren't going anywhere and as such have a mean momentum of zero.

1.4.2 Ehrenfrest's Theorem

This theorem describes that these small quantum effects must add up to create the same overall behaviour as classical mechanics for a large system.

We can show that:

$$< p >= m \frac{\mathrm{d} < x >}{\mathrm{d}t}$$

and that:

$$\frac{\mathrm{d} < p >}{\mathrm{d}t} =< F >= -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

1.4.3 General operators

This subsection deals with us generalising the discussion on momentum above. If we have a dynamical variable $A(x, p, t, \ldots)$ we can calculate an expectation of that quantity just by generalising to:

$$< A(x, p, t, \ldots) = \int_{-\infty}^{\infty} \Psi^* A(x, p, t, \ldots) \Psi \cdot \mathrm{d}x$$

This is best demonstrated with an example:

Example: Kinetic Energy

$$E\Psi = \frac{p \cdot p}{2m} \Psi = -\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

Now we will start from the original expression:

$$< E >= \int E(x) P(x) \mathrm{d}x = \int_{-\infty}^{\infty} \Psi^* E \Psi \cdot \mathrm{d}x$$

Substituting in:

$$< E >= -\frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Psi^* \frac{\partial^2 \Psi}{\partial x^2} \cdot \mathrm{d}x$$

From here we can substitute any wavefunction in, for example with the Gaussian above we get an answer of