15 Momentum space wavefunctions

15.1 free particles

in free space we saw that the time-independent Schroedinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

which has the solution $\psi(x,0) = Ae^{ikx}$ for a wave travelling from left to right, or Ae^{-ikx} for a wave travelling from right to left, both with energy $E_k = \hbar^2k^2/2m$. so we could in fact simplify this a bit with $k = \pm\sqrt{2mE}/\hbar$. And then we have $\psi(x,0) = Ae^{ikx}$ as a particular solution for any direction.

we get more physical insight into this by writing the momentum operator as an eigenvalue equation - $\hat{p}f(x) = pf(x)$

$$-i\hbar\frac{df(x)}{dx} = pf(x)$$

$$\int \frac{df(x)}{f} = \frac{p}{-i\hbar}\int dx$$

$\log f = ipx/\hbar + c$ where c is a constant so $f = e^{ipx/\hbar+c} = Be^{ipx/\hbar}$ where $B = e^c$ is a normalisation constant. so plane waves which are eigenfunctions of the energy operator for free space ($V = 0$) are also eigenfunctions of the momentum operator - so these conserve momentum! which is what you would hope as this is free space so we should conserve momentum as there are no external forces ($F = dV/dx$, so no forces means no potential i.e. $V = 0$ is Schroedinger.)!

but this was just the time independent energy equation. we also know that $\Psi(x,t) = \psi(x,0)e^{-iE_kt/\hbar} = Ae^{i(kx-E_kt/\hbar)}$

this is a wave, of the form $y(x,t) = Ae^{i(kx-\omega t)}$ where $\omega = E_k/\hbar$. but we know that for any function of x, t which depends on x, t in the special way $x \pm vt$ where v is a constant represents a wave of fixed profile travelling in the $\pm$ x direction at speed v, so this wave has velocity $\omega/k = \hbar k^2/(2mk) = \hbar k/2m$

but the classical velocity of a particle from its momentum $p = mv_{classical}$ is $v_{classical} = \pm p/m = \pm\hbar k/m$

so the quantum wave travels at half the velocity of the particle it is meant to represent.... not really a good start! and remember that we couldn't normalise this either! because to have a well well defined (deterministic) momentum, $\hbar k$, we can only get there by having a completely indeterminant position - a sinusoid can be anywhere in space.

So there is some sense in which this is NOT a physically realiseable state. to normalise it we needed to localise it by confining it to some lab space $-a < x < a$ but this is equivalent to adding in different momentum components!

but if we cannot have a completely definite momentum, there is some sense in which de Broglies formula simply does not work. there is no such thing as a particle with determinate momentum. But there could be a particle with a very small range of momenta - we could make a normalisable wavepacket with a range of momenta. And then if its a sum of a load of waves it has a group velocity as well as a phase velocity - the phase velocity is the velocity of individual ripples, but the group velocity is the motion of the wavepacket as a whole. so lets try it and see if we can make this work!

so what we want to do is know how to add together multiple plane waves in order to get a wavepacket of a distinct shape in space. we do this using Fourier transforms!

15.2 fourier transforms

we're going to be doing fourier transforms, so first a bit of revision you are most used to seeing them in the time-frequency domain

$$g(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} G(\omega) e^{i\omega t} df$$

$$G(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(t) e^{-i\omega t} dx$$

where $\omega = 2\pi f$. but we can just as easily do them in the position-wavenumber domain

$$g(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} G(k) e^{ikx} dk$$

$$G(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(x) e^{-ikx} dx$$

where $k = 2\pi/\lambda = p/\hbar$. So for any wavefunction in standard (configuration) space, we can write an equivalent momentum space wavefunction.

$$\psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} dk$$

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x) e^{-ikx} dx$$

lets just see an example with a $\delta(x)$ as we are about to need it!

$$G(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \delta(x) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}}$$

hence

$$\delta(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi}} e^{ikx} dk$$

$$= \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikx} dk = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} e^{ipx/\hbar} dp$$

but the more useful bit comes when we add in the time dependence. In general we have

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k,t) e^{ikx} dk$$

$$\phi(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \psi(x,t) e^{-ikx} dx$$

useful integral

$$\int e^{-\alpha u^2} e^{-\beta u} du = (\pi/\alpha)^{1/2} e^{\beta^2/4\alpha}$$

15.3 Gaussian wavepackets

and we are going to try for a gaussian travelling wave $\psi(x,0) = Ae^{-ax^2}e^{ilx}$ - gaussians are good as the FT of a gaussian is a gaussian. and we know that the travelling wavepacket has group velocty l/m.

first normalise

$$\int \psi^* \psi dx = \int A^2 e^{-2ax^2} e^{-ilx} e^{ilx} dx = A^2 \Big(\frac{\pi}{2a}\Big)^{1/2} = 1$$

$$A = \Big(\frac{2a}{\pi}\Big)^{1/4}$$

now do a fourier transform

$$\phi(k,0) = 1/\sqrt{2\pi} \int \psi(x,0) e^{-ikx} dx = 1/\sqrt{2\pi} \Big(\frac{2a}{\pi}\Big)^{1/4} \int e^{-ax^2} e^{ilx} e^{-ikx} dx$$

$$= 1/\sqrt{2\pi} \Big(\frac{2a}{\pi}\Big)^{1/4} \int e^{-ax^2} e^{-ix(k-l)} dx = 1/\sqrt{2\pi} \Big(\frac{2a}{\pi}\Big)^{1/4} \Big(\frac{\pi}{a}\Big)^{1/2} e^{i^2(k-l)^2/4a}$$

$$= \frac{1}{(2\pi a)^{1/4}} e^{-(k-l)^2/4a}$$

so now we know that the gaussian can be broken down into the infinite sum of different k values with

$$\psi(x,0) = \frac{1}{\sqrt{2\pi}} \int \phi(k,0) e^{ikx} dk = \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{1/4}} \int e^{-(k-l)^2/4a} e^{ikx} dk$$

i.e. an infinite sum of the plane wave solutions of the $t = 0$ eigenfunctions. each of these has a different time dependence $e^{-iEt/\hbar} = e^{-i\hbar k^2 t/2m}$ so

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \frac{1}{(2\pi a)^{1/4}} \int e^{-(k-l)^2/4a} e^{ikx} e^{-i\hbar k^2 t/2m} dk$$

after some tedious algebra we get

$$|\Psi(x,t)|^2 = \big(\frac{2a}{\pi}\big)^{1/4} e^{-l^2/4a} \Big(\frac{1}{(1 + 2ai\hbar t/m)}\Big)^{1/2} e^{a(l/2a+ix)^2/(1+2ai\hbar t/m)}$$

let $\theta = 2\hbar a/m$ and $w = \sqrt{a/(1+\theta^2 t^2)}$ to get

$$|\Psi(x,t)|^2 = \sqrt{\frac{2}{\pi}} w e^{-2w^2(x-\theta l t/2a)^2}$$

a gaussian has $e^{-(x-x_0)^2/2\sigma^2}$ so its a gaussian with peak position $x_0 = \theta l t/2a = 2\hbar a l t/(2ma) = \hbar l/m$ which is what you expect for the classical particle!! so the peak of the wavepacket has a group velocity which is what we want.

the wavepacket also spreads - its width is given by $1/(2\sigma^2) = 2w^2$ so

$$\sigma^2 = \frac{1}{4w^2} = \frac{1 + (2\hbar a t/m)^2}{4a}$$

as time progresses, the position gaussian broadens with time. this is EXACTLY what you expect - the wavefunction is made up of many different k values, ie different momenta. so the lower k move slower than the higher k and so it broadens with time.

The uncertainty in momentum is back with the $|\phi(k)|^2 \propto e^{-(k-l)^2/2a}$ this has $\sigma_k^2 = a$ so $\sigma_k = a^{1/2}$. Then $\sigma_p = \hbar\sigma_k$ so hence $\Delta x \Delta p = \hbar a^{1/2}/(2a^{1/2}) = \hbar/2$. so this one stays constant (as momentum is conserved!). so this product just gets bigger....

This is the heisenburg uncertainty principle, but now you can really see where it comes from. if we try to localise the particle, we can do it better and better by adding in more and more different k values. So the narrower we are in position, the broader we are in momentum. but the centroid stays in the same place - the mean momentum is zero. $\Delta x \Delta p \geq \hbar/2$

15.4 Uncertainty principle $\Delta E \Delta t \leq \hbar/2$

ask how long it takes a moving wavepacket to pass a particular point. then $\Delta t = \Delta x/v = m\Delta x/p$ but $E = p^2/2m$ so $\Delta E = 2p\Delta p/2m = \Delta p/m$ Hence

$$\Delta t \Delta E = \frac{m\Delta x}{p}\frac{2p\Delta p}{2m} = \Delta x \Delta p \geq \hbar/2$$

so this is clear that there is a corresponding energy-time uncertainty relation. but this should make you feel uncomfortable. position and momentum are both dynamical varibales, measuravble characteristics of the system. As is energy. But time is emphatically not. The Δt is NOT the intrinsic dispersion we have if we make a whole load of measurements of time, its the time it takes the system to change substatially. time is not an operator belonging to the particle, it is a parameter describing the evolution of the system. As Lev Landau once joked "To violate the time-energy uncertainty relation all I have to do is measure the energy very precisely and then look at my watch!"

Nevertheless, there is something in it! A state that only exists for a short time cannot have a definite energy. To have a definite energy, the frequency of the state must accurately be defined, and this requires the state to hang around for many cycles, the reciprocal of the required accuracy. eg linewidths - a long lived transition has narrow energy width, a short one has broad energy width.

what we are really doing is saying $\Delta t = \Delta < B > /(dB/dt)$ where B is some dynamical operator and dB/dt is the rate of change of that dynamical quantity.

NOT that the conservation of energy is violated - borrow" energy from the Universe as long as it is "returned" within a short amount of time!!! ' there are many legitimate readings of the energy time uncertainty principle, but this isn't one of them! Nowehere dows QM licence violation of energy conservation and certainly no such authorzation entered the derivation. But the uncertainty principle is extrordinarily robust. it can be misused without leading to seriously incorrect results, and as a consequence, physicits are in the habit of applying it rather carelessly! (Griffiths!)