

Wave Equations, Wavepackets and Superposition

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A Challenge to Schrödinger

De Broglie's doctoral thesis, defended at the end of 1924, created a lot of excitement in European physics circles. Shortly after it was published in the fall of 1925 Pieter Debye, a theorist in Zurich, suggested to Erwin Schrödinger that he give a seminar on de Broglie's work. Schrödinger gave a polished presentation, but at the end Debye remarked that he considered the whole theory rather childish: why should a wave confine itself to a circle in space? It wasn't as if the circle was a waving circular string, real waves in space diffracted and diffused, in fact they obeyed three-dimensional wave equations, and that was what was needed. This was a direct challenge to Schrödinger, who spent some weeks in the Swiss mountains working on the problem, and constructing his equation.

There is no rigorous derivation of Schrödinger's equation from previously established theory, but it can be made very plausible by thinking about the connection between light waves and photons, and construction an analogous structure for de Broglie's waves and electrons (and, later, other particles).

Maxwell's Wave Equation

Let us examine what Maxwell's equations tell us about the motion of the simplest type of electromagnetic wave—a monochromatic wave in empty space, with no currents or charges present.

As we discussed in the last lecture, Maxwell found the wave equation

$$\nabla^2 \vec{E} - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0.$$

which reduces to

$$\frac{\partial^2 \vec{E}}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0$$

for a plane wave moving in the x -direction, with solution

$$\vec{E}(x, t) = \vec{E}_0 e^{i(kx - \omega t)}.$$

Applying the wave equation differential operator to this plane wave solution

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \vec{E}_0 e^{i(kx - \omega t)} = \left(k^2 - \frac{\omega^2}{c^2} \right) \vec{E}_0 e^{i(kx - \omega t)} = 0,$$

so

$$\omega = ck.$$

This is just the familiar statement that the wave must travel at c .

What does the Wave Equation tell us about the *Photon*?

We know from the photoelectric effect and Compton scattering that the photon energy and momentum are related to the frequency and wavelength of the light by

$$E = h\nu = \hbar\omega$$

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

Notice, then, that the wave equation tells us that $\omega = ck$ and hence $E = cp$.

To put it another way, if we think of $e^{i(kx - \omega t)}$ as describing a particle (photon) it would be more natural to write the plane wave as

$$\vec{E}_0 e^{\frac{i}{\hbar}(px - Et)}$$

that is, in terms of the energy and momentum of the particle.

In these terms, applying the (Maxwell) wave equation operator to the plane wave yields

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \vec{E}_0 e^{\frac{i}{\hbar}(px - Et)} = \left(p^2 - \frac{E^2}{c^2} \right) \vec{E}_0 e^{\frac{i}{\hbar}(px - Et)} = 0$$

or

$$E^2 = c^2 p^2.$$

The wave equation operator applied to the plane wave describing the particle propagation yields the energy-momentum relationship for the particle.

Constructing a Wave Equation for a Particle with Mass

The discussion above suggests how we might extend the wave equation operator from the photon case (zero rest mass) to a particle having rest mass m_0 . We need a wave equation operator that, when it operates on a plane wave, yields

$$E^2 = c^2 p^2 + m_0^2 c^4$$

Writing the plane wave function

$$\varphi(x, t) = A e^{\frac{i}{\hbar}(px - Et)}$$

where A is a constant, we find we can get $E^2 = c^2 p^2 + m_0^2 c^4$ by adding a constant (mass) term to the differentiation terms in the wave operator:

$$\left(\frac{\partial^2}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{m_0^2 c^2}{\hbar^2} \right) A e^{\frac{i}{\hbar}(px - Et)} = -\frac{1}{\hbar^2} \left(p^2 - \frac{E^2}{c^2} + m_0^2 c^2 \right) A e^{\frac{i}{\hbar}(px - Et)} = 0.$$

This wave equation is called the *Klein-Gordon* equation and correctly describes the propagation of relativistic particles of mass m_0 . However, it's a bit inconvenient for nonrelativistic particles, like the electron in the hydrogen atom, just as $E^2 = m_0^2 c^4 + c^2 p^2$ is less useful than $E = p^2/2m$ for this case.

A Nonrelativistic Wave Equation

Continuing along the same lines, let us assume that a nonrelativistic electron in free space (no potentials, so no forces) is described by a plane wave:

$$\psi(x, t) = A e^{\frac{i}{\hbar}(px - Et)}$$

We need to construct a wave equation operator which, applied to this wave function, just gives us the ordinary nonrelativistic energy-momentum relationship, $E = p^2/2m$. The p^2 obviously comes as usual from differentiating twice with respect to x , but the only way we can get E is by having a *single* differentiation with respect to time, so this looks different from previous wave equations:

$$i\hbar \frac{\partial \psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x, t)}{\partial x^2}.$$

This is *Schrödinger's equation* for a free particle. It is easy to check that if $\psi(x, t)$ has the plane wave form given above, the condition for it to be a solution of this wave equation is just $E = p^2/2m$.

Notice one remarkable feature of the above equation—the i on the left means that ψ *cannot* be a real function.

How Does a Varying Potential Affect a de Broglie Wave?

The effect of a potential on a de Broglie wave was considered by Sommerfeld in an attempt to generalize the rather restrictive conditions in Bohr's model of the atom. Since the electron was orbiting in an inverse square force, just like the planets around the sun, Sommerfeld couldn't understand why Bohr's atom had only circular orbits, no Kepler-like ellipses. (Recall that all the observed spectral lines of hydrogen were accounted for by energy differences between *circular* orbits.)

De Broglie's analysis of the allowed circular orbits can be formulated by assuming at some instant in time the spatial variation of the wave function on going around the orbit includes a phase term of the form $e^{ipq/\hbar}$, where here the parameter q measures distance around the orbit. Now for an acceptable wave function, the total phase change on going around the orbit must be $2n\pi$, where n is an integer. For the usual Bohr circular orbit, p is constant on going around, q changes by $2\pi r$, where r is the radius of the orbit, giving

$$\frac{1}{\hbar} p 2\pi r = 2n\pi, \quad \text{so } pr = n\hbar,$$

the usual angular momentum quantization.

What Sommerfeld did was to consider a general Kepler ellipse orbit, and visualize the wave going around such an orbit. Assuming the usual relationship $p = h/\lambda$, the wavelength will vary as the particle moves around the orbit, being shortest where the particle moves fastest, at its closest approach to the nucleus. Nevertheless, the phase change on moving a short distance Δq should still be $p\Delta q/\hbar$, and requiring the wave function to link up smoothly on going once around the orbit gives

$$\oint pdq = nh.$$

Thus only certain elliptical orbits are allowed. The mathematics is nontrivial, but it turns out that *every allowed elliptical orbit has the same energy as one of the allowed circular orbits*. That is why Bohr's theory gave all the energy levels. Actually, this whole analysis is old fashioned (it's called the "old quantum theory") but we've gone over it to introduce the idea of *a wave with variable wavelength, changing with the momentum as the particle moves through a varying potential*.

The reader may well be wondering at this point why it is at all useful to visualize a real wave going round an orbit, when we have stated that any solution of Schrödinger's equation is necessarily a complex function. As we shall see, it is often possible to find solutions, including those corresponding to Bohr's energy levels, in which the complex nature of the wave function only appears in a time varying phase factor, $e^{-iEt/\hbar}$. We should also add that if the spatial dependence is a real function, such as $\sin kx$, it represents a standing wave, not a particle circling in one direction, which would be e^{ikx} , or $e^{ipx/\hbar}$. Bearing all this in mind, it is still often instructive to sketch real wave functions, especially for one-dimensional problems.

Schrödinger's Equation for a Particle in a Potential

Let us consider first the one-dimensional situation of a particle going in the x -direction subject to a "roller coaster" potential. What do we expect the wave function to look like? We would expect the wavelength to be shortest where the potential is lowest, in the valleys, because that's where the particle is going fastest—maximum momentum.

With a nonzero potential present, the energy-momentum relationship for the particle becomes the energy equation

$$E = \frac{p^2}{2m} + V(x)$$

We need to construct a wave equation which leads naturally to this relationship. In contrast to the free particle cases discussed above, the relevant wave function here will no longer be a plane wave, since the wavelength varies with the potential. However, at a given x , the momentum is determined by the “local wavelength”, that is,

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

It follows that the appropriate wave equation is:

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

This is the standard one-dimensional Schrödinger equation.

In three dimensions, the argument is precisely analogous. The only difference is that the square of the momentum is now a sum of three squared components, for the x , y and z

directions, so $\frac{\partial^2}{\partial x^2}$ becomes $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2$,

so now

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

This is the complete Schrödinger equation. So far, of course, it is based on plausibility arguments and hand-waving. Why should anyone believe that it really describes an electron wave? Schrödinger’s test of his equation was the hydrogen atom. He looked for Bohr’s “stationary states”: states in which the electron was localized somewhere near the proton, and having a definite energy. The time dependence would be the same as for a plane wave of definite energy, $e^{-iEt/\hbar}$, the spatial dependence would be a time-independent function decreasing rapidly at large distances from the proton. That is, he took

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

He took advantage of the spherical symmetry by re-expressing the spatial wave function in spherical polar coordinates, and found his equation became a standard differential equation solved in the nineteenth century. The solution gave the shape of possible wave functions, and also allowed values of energy and angular momentum. These values were exactly the same as Bohr's (except that the lowest allowed state in the new theory had zero angular momentum): impressive evidence that the new theory was correct.

Current Conservation

When Schrödinger published this result in 1926, he also wrote down the complex conjugate equation, and proved that taking them together it was not difficult to deduce a continuity equation:

$$\frac{\partial \rho}{\partial t} + \text{div } \vec{j} = 0$$

where $\rho = \psi^* \psi = |\psi|^2$

and $\vec{j} = \frac{\hbar}{2mi} (\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*)$.

But What Do These Equations Mean?

Schrödinger believed the above continuity equations represented the conservation of electric charge, and had no further significance. He thought that after all his own equation showed the electron to be just a smooth classical wave at the deepest level. In fact, he succeeded in solving the three-dimensional equation with a Coulomb potential and he found the Bohr energy levels of the hydrogen atom. Obviously, he was on the right track! This classical revival approach, however, couldn't deal with the unpredictability of quantum mechanics, such as where a single photon—or electron—would land in a two-slit diffraction pattern.

The truth is, Schrödinger didn't understand his own equation. Another physicist, Max Born, published a paper a few days after Schrödinger's in which he suggested that $|\psi(x, y, z, t)|^2 dx dy dz$ was the *relative probability* of finding the electron in a small volume $dx dy dz$ at (x, y, z) at time t . This interpretation was based directly on the analogy with light waves and photons, and has turned out to be correct.

Notation note: ψ is called the “*amplitude*” or sometimes the “*probability amplitude*”.

Photons and Electrons

We have seen that electrons and photons behave in a very similar fashion—both exhibit diffraction effects, as in the double slit experiment, both have particle like or quantum behavior. As we have already discussed, we now have a framework for understanding photons—we first figure out how the electromagnetic wave propagates, using Maxwell's equations, that is, we find E as a function of x, y, z, t . Having evaluated $E(x, y, z, t)$, the

probability of finding a photon in a given small volume of space $dx dy dz$, at time t , is proportional to $|E(x,y,z,t)|^2 dx dy dz$, the energy density.

Born assumed that Schrödinger's wave function for the electron corresponded to the electromagnetic wave for the photon in the sense that the square of the modulus of the Schrödinger wave amplitude at a point was the relative probability density for finding the electron at that point. So the routine is the same: for given boundary conditions and a given potential, Schrödinger's differential equation can be solved and the wave function $\psi(x, y, z, t)$ evaluated. Then, $|\psi(x, y, z, t)|^2 dx dy dz$ gives the relative probability of finding the electron at (x, y, z) at time t .

Notice, though, that this interpretation of the wave function is *not* essential in finding the allowed energy levels in a given potential, such as the Bohr orbit energies, which Schrödinger derived before the physical significance of his wave function was understood.

How Wave Amplitude Varies in a Roller Coaster Potential

We mentioned above that for an electron traveling along a roller coaster potential, the local wavelength is related to the momentum of the electron as it passes that point. Perhaps slightly less obvious is that the *amplitude* of the wave varies: it will be largest at the tops of the hills (provided the particle has enough energy to get there) because that's where the particle is moving slowest, and therefore is most likely to be found.

Keeping the Wave and the Particle Together?

Suppose following de Broglie we write down the relation between the "particle properties" of the electron and its "wave properties":

$$\frac{1}{2}mv^2 = E = hf, \quad mv = p = h/\lambda.$$

It would seem that we can immediately figure out the speed of the wave, just using $\lambda f = c'$, say. We find:

$$\lambda f = \frac{h}{mv} \cdot \frac{\frac{1}{2}mv^2}{h} = \frac{1}{2}v.$$

So the speed of the wave seems to be only half the speed of the electron! How could they stay together? What's wrong with this calculation?

Localizing an Electron

To answer this question, it is necessary to think a little more carefully about the wave function corresponding to an electron traveling through a cathode ray tube, say. The electron leaves the cathode, shoots through the vacuum, and impinges on the screen. At an intermediate point in this process, it is moving through the vacuum and the wave function must be nonzero over some volume, but zero in the places the electron has not possibly reached yet, and zero in the places it has definitely left.

However, if the electron has a precise energy, say exactly a thousand electron volts, it also has a precise momentum. This necessarily implies that the wave has a precise wavelength. But the only wave with a *precise* wavelength λ has the form

$$\psi(x, t) = Ae^{i(kx - \omega t)}$$

where $k = 2\pi / \lambda$, and $\omega = 2\pi f$. The problem is that this plane sine wave extends to infinity in both spatial directions, so cannot represent a particle whose wave function is nonzero in a limited region of space.

Therefore, to represent a localized particle, we must superpose waves having different wavelengths. Now, the waves representing electrons, *unlike the light waves representing photons*, travel at different speeds for different energies. Any intuition gained by thinking about superposing light waves of different wavelengths can be *misleading* if applied to electron waves!

Fortunately, there are many examples in nature of waves whose speed depends on wavelength. A simple example is water waves on the ocean. We consider waves having a wavelength much shorter than the depth of the ocean. What is the ω, k relationship for these waves? We know it's not $\omega = Ck$, with a constant C , because waves of different wavelengths move at different speeds. In fact, it's easy to figure out the ω, k relationship, known as the *dispersion relation*, for these waves from a simple dimensional argument. What physical parameters can the wave frequency depend on? Obviously, the wavelength λ . We will use $k = 2\pi / \lambda$ as our variable. k has dimensions L^{-1} .

These waves are driven by gravity, so g , with dimensions LT^{-2} , is relevant. Actually, that's all. For ocean waves, surface tension is certainly negligible, as is the air density, and the water's viscosity. You might think the density of the water matters, but these waves are rather like a pendulum, in that they are driven by gravity, so increasing the density would increase both force and inertial mass by the same amount.

For these deepwater waves, then, dimensional analysis immediately gives:

$$\omega^2 = Cgk$$

where C is some dimensionless constant we cannot fix by dimensional argument, but actually it turns out to be 1.

Wavepackets and the Principle of Superposition

To return momentarily to the electron traveling through a vacuum, it is clear physically that it must have a wave function that goes to zero far away in either direction (we'll still work in one dimension, for simplicity). A localized wave function of this type is called a "wavepacket". We shall discover that a wavepacket can be constructed by adding plane

waves together. Now, the plane waves we add together will individually be solutions of the Schrödinger equation.

But does it follow that the *sum* of such solutions of the Schrödinger equation is itself a solution to the equation? The answer is yes—in other words, the Schrödinger equation

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

is a *linear* equation, that is to say, if $\psi_1(x, y, z, t)$, $\psi_2(x, y, z, t)$ are both solutions of the equation, then so is

$$\psi(x, y, z, t) = c_1 \psi_1(x, y, z, t) + c_2 \psi_2(x, y, z, t)$$

where c_1 and c_2 are arbitrary constants, as is easy to check. This is called the *Principle of Superposition*.

The essential point is that in Schrödinger's equation every term contains a factor ψ , but no term contains a factor ψ^2 (or a higher power). That's what is meant by a "linear" equation. If the equation *did* contain a constant term, or a term including ψ^2 , superposition wouldn't work—the sum of two solutions to the equation would not itself be a solution to the equation.

In fact, we have been assuming this linearity all along: when we analyze interference and diffraction of waves, we just add the two wave amplitudes at each spot. For the double slit, we take it that if the wave radiating from one slit satisfies the wave equation, then adding the two waves together will give a new wave which also satisfies the equation.

The First Step in Building a Wavepacket: Adding Two Sine Waves

If we add together two sine waves with frequencies close together, we get beats. This pattern can be viewed as a string of wavepackets, and is useful for gaining an understanding of why the electron speed calculated from $\lambda f = c'$ above is apparently half what it should be.

We use the trigonometric addition formula:

$$\begin{aligned} & \sin((k - \Delta k)x - (\omega - \Delta\omega)t) + \sin((k + \Delta k)x - (\omega + \Delta\omega)t) = \\ & 2 \sin(kx - \omega t) \cos((\Delta k)x - (\Delta\omega)t). \end{aligned}$$

This formula represents the phenomenon of beats between waves close in frequency. The first term, $\sin(kx - \omega t)$, oscillates at the average of the two frequencies. It is modulated by the slowly varying second term, often called the “envelope function”, which oscillates once over a spatial extent of order $\pi / \Delta k$. This is the distance over which waves initially in phase at the origin become completely out of phase. Of course, going a further distance of order $\pi / \Delta k$, the waves will become synchronized again.

That is, beating two close frequencies together breaks up the continuous wave into a series of packets, the beats. To describe a single electron moving through space, we need a single packet. This can be achieved by superposing waves having a continuous distribution of wavelengths, or wave numbers within of order Δk , say, of k . In this case, the waves will be out of phase after a distance of order $\pi / \Delta k$, but since they have many different wavelengths, they will never get back in phase again.

Phase Velocity and Group Velocity

The best way to understand how these waves add up is to view my [applet](#). It will immediately become apparent that there are *two different velocities* in the dynamics: first, the velocity with which the *individual peaks* move to the right, and second the velocity at which the slowly varying envelope function—the beat pattern—moves. The $\lambda f = c'$ individual peak velocity is determined by the term $\sin(kx - \omega t)$, it is ω / k : this is called the *phase velocity*. The speed with which the beat pattern moves, on the other hand, is determined by the term $\cos((\Delta k)x - (\Delta \omega)t)$, this speed is $\Delta \omega / \Delta k = d\omega / dk$ for close frequencies.

Going back one more time to the electron wavepacket, armed with this new insight, we can see immediately that the wave speed we calculated from $\lambda f = c'$ was the *phase* velocity of the waves. The packet itself will of course move at the *group* velocity—and it is easy to check that this is just v .

Adding More Waves

We’ve seen how two sine waves of equal amplitude close together in frequency produce beats: if the waves are in phase at the origin, as we go along the x -axis they gradually fall out of phase, and cancel each other at a distance $x = \pi / 2\Delta$, where 2Δ is the difference in k of the two $\sin kx$ waves. (For the moment, we are ignoring the time development of these waves: we’re just looking at $t = 0$.) If we continue along the x -axis to π / Δ , the two waves will be back in phase again, this is the next beat. Now, if instead of adding *two* waves, we add *many* waves, all of different k , *but* with the k ’s taken from some small interval of size of order Δk , and all these waves are in phase at the origin, then, again, they will all stay more or less in phase for a distance of order $x = \pi / 2\Delta$. However, as we proceed past that point, the chances of them all getting back in phase again get rapidly smaller as we increase the number of different waves.

This suggests a way to construct a wavepacket: add together a lot of waves from within a narrow frequency range, and they will *only* be in phase in a region containing the origin.

Adding waves in this way leads to a more general derivation of the formula $d\omega/dk$ for the group velocity. The standard approach is to replace the sum over plane waves by an integral, with the wavenumber k as the variable of integration, and the convention is to put a factor 2π in the denominator:

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

Since we are constructing a wavepacket with a fairly well-defined momentum, we will take the function $\phi(k)$ to be strongly peaked at k_0 , and going rapidly to zero away from that value, so the only significant contribution to the integral is from the neighborhood of k_0 . Therefore, if $\omega(k)$ is reasonably smooth (which it is) it is safe to put

$$\omega(k) = \omega(k_0) + (k - k_0)\omega'(k_0)$$

in the exponential.

This gives

$$\begin{aligned} \psi(x, t) &= \int_{-\infty}^{+\infty} \frac{dk}{2\pi} e^{ikx - i\omega(k_0)t - i(k - k_0)\omega'(k_0)t} \phi(k) \\ &= e^{i(k_0x - \omega(k_0)t)} \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{i(k - k_0)(x - \omega'(k_0)t)} \phi(k). \end{aligned}$$

The first term just represents a single wave at k_0 , and the peaks move at the phase velocity $v_{phase} = \omega/k$.

The second term, the integral, is the *envelope function*: here x only appears in the combination

$$x - \omega'(k_0)t$$

so the envelope, and hence the wavepacket, moves to the right at the group velocity: $v_{group} = \omega'(k_0)$. Note that if the *next* term in the Taylor expansion of $\omega(k)$ is also included, that amounts to adding wavepackets with slightly different group velocities together, and the initial (total) wavepacket will gradually widen.

The Gaussian Wavepacket

Fortunately, there is a simple explicit mathematical realization of the addition of plane waves to form a localized function: the *Gaussian wavepacket*,

$$\psi(x, t = 0) = A e^{ik_0 x} e^{-x^2/2\Delta^2}$$

where $p_0 = \hbar k_0$. For this wavepacket to represent one electron, with the probability of finding the electron in a small section of length dx at x equal to $|\psi|^2 dx$, and the *total* probability of finding the electron somewhere equal to one, the constant A is uniquely determined (apart from a possible phase multiplier $e^{i\delta}$, which would not affect the probability).

Using the standard result

$$\int_{-\infty}^{+\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

we find $|A|^2 = (\pi\Delta^2)^{-1/2}$ so

$$\psi(x, t = 0) = \frac{1}{(\pi\Delta^2)^{1/4}} e^{ik_0 x} e^{-x^2/2\Delta^2}.$$

But how do we construct this particular wavepacket by superposing plane waves? That is to say, we need a representation of the form:

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

The function $\phi(k)$ represents the weighting of plane waves in the neighborhood of wavenumber k . This is a particular example of a *Fourier transform*—we will be discussing the general case in detail a little later in the course. Note that if $\phi(k)$ is a bounded function, any particular k value gives a vanishingly small contribution, the plane-wave contribution to $\psi(x)$ from a range dk is $\phi(k) dk / 2\pi$. In fact, $\phi(k)$ is given in terms of $\psi(x)$ by

$$\phi(k) = \int_{-\infty}^{+\infty} dx e^{-ikx} \psi(x).$$

It is perhaps worth mentioning at this point that this can be understood *qualitatively* by observing that the plane wave prefactor e^{-ikx} will interfere destructively with all plane wave components of $\psi(x)$ except that of wavenumber k , where it may at first appear that the

contribution is infinite, but recall that as stated above, any particular k component has a vanishingly small weight—and, in fact, this is the right answer, as we shall show in more convincing fashion later.

In the present case, the above handwaving argument is unnecessary, because both the integrals can be carried out exactly, using the standard result:

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} dx = e^{b^2/4a} \sqrt{\frac{\pi}{a}}$$

giving

$$\phi(k) = (4\pi\Delta^2)^{\frac{1}{4}} e^{-\Delta^2(k-k_0)^2/2}.$$

Putting this back in the integral for $\psi(x)$ shows that the integral equations are consistent.

Note the normalization integrals in x -space and k -space are:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1, \quad \int_{-\infty}^{\infty} |\phi(k)|^2 \frac{dk}{2\pi} = 1.$$

The physical significance of the second equation above is that if the wavepacket goes through a diffraction grating so that the different k -components are dispersed in different directions, like the colors in white light, and a detector is arranged to register the electron if it has wavenumber between k and $k + dk$, the probability of finding it in that wavenumber range is $|\phi(k)|^2 dk / 2\pi$.

Expectation Values and the Uncertainty Principle

It is clear from the expressions for $\psi(x)$ and its Fourier transform $\phi(k)$ above that the spreading of the wave function in x -space is inversely related to its spreading in k -space: the x -space wavefunction has spread $\sim \Delta$, the k -space wavefunction $\sim 1/\Delta$. This is perhaps the simplest example of Heisenberg's famous Uncertainty Principle: in quantum mechanics, both the position and momentum of a particle cannot be known precisely at the same moment; the more exactly one is specified the less well the other is known. This is an inevitable consequence of the wave nature of the probability distribution. As we have already seen, a particle with an exact momentum has a wave of specific wavelength, and the only such wave is a plane wave extending from minus infinity to infinity, so the position of the particle is completely undetermined. A particle with precisely defined position is described by a wavepacket having all wavelengths included with equal

weight—the momentum is completely undefined. We shall give more examples of the Uncertainty Principle, of efforts to evade it and of its uses in estimates, in the next lecture.

Definitions of Δx , Δp

The standard notation for the *expectation value* of an operator in a given quantum state is

$$\langle x \rangle = \int x |\psi(x)|^2 dx.$$

In other words, $\langle x \rangle$ would be the statistical average outcome of making many measurements of x on identically prepared systems all in the quantum state $\psi(x)$ (ignoring the time dependence here for the sake of simplicity).

When we talk about the “uncertainty” in x , we mean in quantum mechanics the *root mean square deviation in the measurements*. This is usually written Δx (unfortunate in view of our—also standard—use of Δ in the Gaussian function above, so the reader should watch carefully!).

Therefore

$$\Delta x = \sqrt{\int (x - \langle x \rangle)^2 |\psi(x)|^2 dx}.$$

For our wavepacket, $\langle x \rangle = 0$. It is easy to check that

$$\Delta x = \frac{\Delta}{\sqrt{2}}, \text{ and writing } p = \hbar k, \Delta p = \frac{\hbar}{\Delta\sqrt{2}} \text{ giving } \Delta x \cdot \Delta p = \frac{\hbar}{2}.$$