Tuesday 10^{th} May 2005

Quantum Physics Handout

Wavepackets and the Uncertainty Principle

Introduction

A wavepacket is any group of waves. It does not have to be neat and symmetrical and centred on the origin — all that matters is that it dies away to zero far from some centre. Because a QM particle is represented by a wavepacket of De Broglie waves, wavepackets play an important role in quantum physics.

The most interesting wavepackets have a clearly distinguishable “carrier” wave, the amplitude of which is modulated by a much more slowly varying envelope. The wavepacket in Figure 1 is of this type. If it were a sound, the

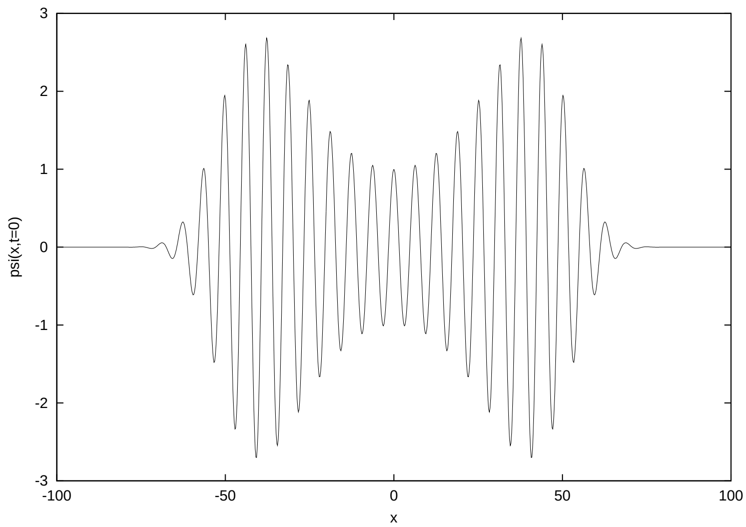

Figure 1: A wavepacket with a clear carrier wave

pitch would be the frequency of the carrier wave and the envelope would give the volume as a function of time.

Not all wavepackets are so simple. Figure 2 shows a messier one without a clear carrier wave. A sound of this type would be a noise — a hand clap or

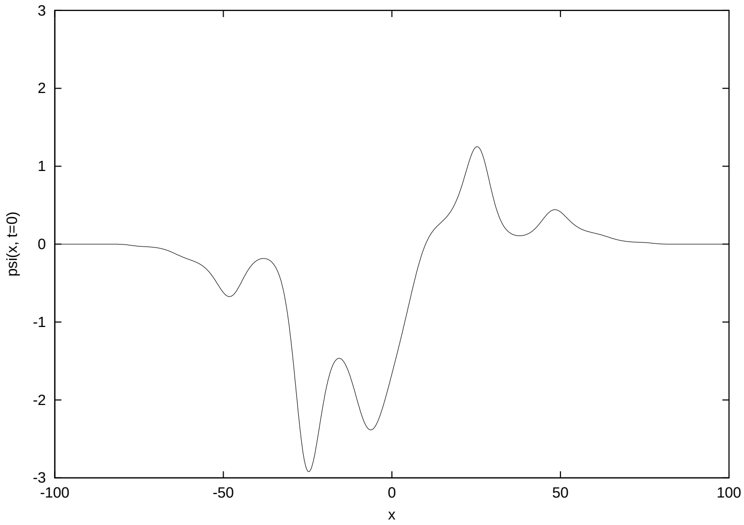

Figure 2: A wavepacket without a clear carrier wave

a door closing — rather than a musical note with a clear pitch.

Recall that the formula

$$\psi(x,t) = a\cos(kx - \omega t + \phi)$$

describes a travelling wave of amplitude a, wavelength $\lambda = 2\pi/k$, frequency $\nu = \omega/2\pi$, and phase shift ϕ. The angular frequency ω and wavevector k are linked by the dispersion relation $\omega = \omega(k)$. For light waves, for example, $\omega = ck$.

Wavepackets are not single travelling waves, but it is plausible (and true) that they can always be written as superpositions of many travelling waves:

$$\psi(x,t) \quad = \quad \sum_{n=1}^{N} a_n \cos(k_n x - \omega_n t + \phi_n)\ .$$

By choosing the wavevectors, amplitudes and phase shifts carefully, it is possible to ensure that the waves in the superposition undergo perfect destructive interference (producing a total amplitude of zero) everywhere except in one small region of space. The resulting $\psi(x,t)$ is then a wavepacket.

(Strictly, it is not possible to construct a finite wavepacket using a fixed number N of cosine waves. To ensure perfect destructive interference everywhere far away from the centre, it is necessary to let N tend to infinity and to replace the sum over wavevectors by an integral. We shall ignore this mathematical issue.)

Although the idea that wavepackets can be constructed from cosine waves is plausible enough, the prospect of having to work out all the amplitudes a_n and phase shifts ϕ_n may appear forbidding. In fact, it turns out to be quite easy, as you will learn when you study Fourier analysis at the beginning of next year. (Incidentally, you already know all the mathematics you need to understand Fourier analysis, so there is nothing to stop you looking it up in a book if you are interested.)

Now that the idea of Fourier superposition has been introduced, the difference between the wavepackets in Figures 1 and 2 can be described in mathematical terms. In Figure 1 (the musical instrument), all the wavelengths $\lambda_n = 2\pi/k_n$ appearing in the superposition are very close to the carrier wavelength. This explains why the ear is able to pick out the carrier frequency and associate a pitch with the sound. In Figure 2 (the hand clap), the wavelengths appearing in the Fourier superposition are all over the place. Since they are no longer clustered around a central carrier wavelength, the ear cannot pick out a clear pitch.

The Uncertainty Principle

The idea of Fourier superposition has several interesting repercussions. Imagine, for example, that you want to make a wavepacket that "sounds like" middle C, the frequency of which is approximately 261 Hz. If the wavepacket is to have a clearly distinguishable pitch, it has to be long enough to contain many carrier-wave oscillations of this frequency. The exact number depends on how cleverly the human brain interprets sounds, but 25 might be a reasonable guess. Such a wavepacket takes about 25/261 s to pass by. Hence, no noise significantly shorter than 0.1 seconds can possibly sound like middle C. Very short wavepackets have to contain a wide spread of component frequencies/wavelengths (otherwise how could the interference between the components change over such a short distance from constructive at the centre of the wavepacket to destructive everywhere else?) and so do not have a clear pitch. This is why most percussion instruments, which make very short sounds, have no discernible pitch.

Let us investigate some of the consequences of this idea. Suppose that a wavepacket is constructed using cosine waves with wavevectors in a narrow range $k_c \pm \Delta k$ centred on the carrier wavevector k_c. What is the minimum possible size of such a wavepacket?

To work this out, start by considering two component waves of equal amplitude which interfere constructively at position $x = 0$ at time $t = 0$:

$$\psi_1(x,t) \ = \ \cos(k_1 x - \omega_1 t) \ , \qquad \psi_2(x,t) \ = \ \cos(k_2 x - \omega_2 t) \ .$$

Figure 3 shows an example with $k_1 = 0.95\,\mathrm{m}^{-1}$ and $k_2 = 1.05\,\mathrm{m}^{-1}$. The superposition $\psi(x, t = 0) = \psi_1(x, t = 0) + \psi_2(x, t = 0)$ is also shown. The short carrier wave and the slowly varying interference envelope of the beats are clear.

How wide are the beats? At time $t = 0$, the first zero of the envelope function occurs at the point marked by the dashed vertical line on Figure 3. The functions $\cos(k_1 x)$ and $\cos(k_2 x)$ are equal and opposite at this point, and hence the phases $k_1 x$ and $k_2 x$ differ by π. This gives

$$k_1 x = k_2 x + \pi \ ,$$

or, equivalently,

$$x \ = \ \text{half-width of beat envelope} \ = \ \frac{\pi}{|k_1 - k_2|} \ .$$

Now return to the full wavepacket, which contains huge numbers of components with wavevectors between $k_c - \Delta k$ and $k_c + \Delta k$. The details are very complicated in this case, but the basic principle is the same: in order to shift from the constructive interference that occurs at the centre of the wavepacket to the perfect destructive interference that occurs everywhere outside the wavepacket, the relative phases of the components have to change by something close to π. The value of x that gives a phase difference of π between the components with wavevectors $k_c - \Delta k$ and $k_c + \Delta k$ satisfies

$$(k_c + \Delta k)x \ = \ (k_c - \Delta k)x + \pi$$

and hence

$$x \ = \ \frac{\pi}{2\Delta k} \ .$$

The half-width of the wavepacket cannot be very much smaller than this, no matter how cleverly the phases and amplitudes are chosen.

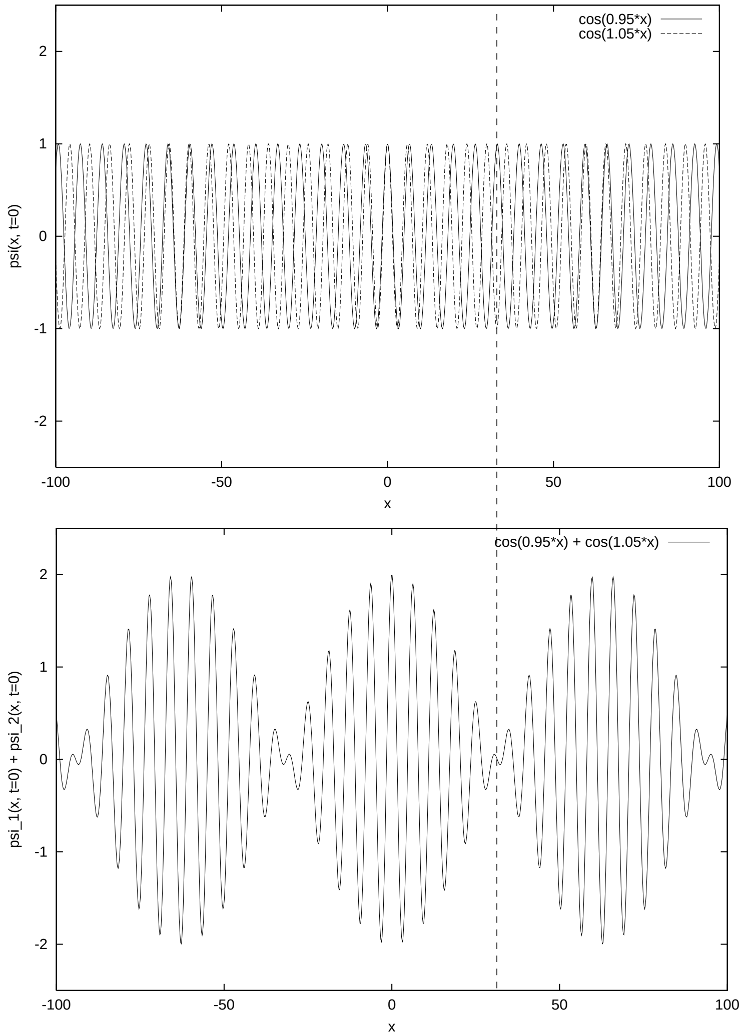

Figure 3: Two cosine waves with similar wavelengths and their interference pattern. The vertical dashed line marks the point where $1.05x = 0.95x + \pi$.

This reasoning may be rather imprecise (you might quibble about the definition of Δk or about factors of 2 or π), but the conclusion is simple and correct: the half-width Δx of the wavepacket is related to the half-width Δk of the spread of contributing wavevectors via

$$\Delta x \Delta k \gtrsim \frac{\pi}{2} \, .$$

Because of the qualitative nature of the derivation this inequality is not strict, but a strict inequality can be derived and differs only in the value of the constant on the right-hand side.

Since a wavepacket of size Δx travelling at speed v takes time $\Delta x/v$ to pass any point, a limit on the minimum size of the wavepacket is equivalent to a limit on the minimum duration. This accords with the discussion of short and long sounds at the beginning of this section.

Note that nothing has been said about the maximum size of the wavepacket. It is always possible to choose the phase shifts and amplitudes of the components such that they interfere constructively at any number of arbitrary places, so the maximum size is unbounded.

In the case of quantum mechanics, where De Broglie's equation says that the momentum p is equal to $\hbar k$, the above inequality translates into Heisenberg's uncertainty principle:

$$\Delta x \Delta p \gtrsim \frac{\hbar \pi}{2} \, .$$

The strict mathematical version of the uncertainty principle, which I'll be using in the lectures, is rather weaker:

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

Group Velocity

You should already know that the envelope of a "musical" wavepacket (that is, a wavepacket containing a narrow range of k vectors centred on the carrier wavevector k_c) travels at the group velocity. To help understand this result, let us return to the two-wave example discussed above.

Two-Wave Example

As t increases, the two travelling cosine waves ψ_1 and ψ_2 move to the right at the phase velocity ω/k. For light waves, the angular frequencies ω_1 and ω_2 are related to the wavevectors k_1 and k_2 via the dispersion relation $\omega = ck$. The phase velocities

$$v_1 \;=\; \frac{\omega_1}{k_1} \;=\; \frac{ck_1}{k_1} \;=\; c$$

and

$$v_2 \;=\; \frac{\omega_2}{k_2} \;=\; \frac{ck_2}{k_2} \;=\; c$$

are therefore both equal to c. Since the interference pattern of beats is just the sum of ψ_1 and ψ_2, both of which are moving at speed c, it too moves to the right at speed c. Apart from this constant motion, the shape of the interference pattern never changes.

For other kinds of waves, the dispersion relation is more complicated and v_1 and v_2 may differ. This makes it much harder to figure out how the interference pattern of beats moves and changes with time. In fact, the beat pattern moves at the group velocity $d\omega/dk$ rather than the phase velocity ω/k. For light waves, $d\omega/dk = \omega/k = c$ and so the group and phase velocities are the same. For De Broglie particle-waves, which have the dispersion relation $\omega = \hbar k^2/2m$, the group velocity

$$\frac{d\omega}{dk} = \frac{\hbar k}{m}$$

is twice the phase velocity

$$\frac{\omega}{k} = \frac{\hbar k}{2m}\ .$$

This means that the beat pattern, created by the interference of the two cosine waves, moves twice as fast as the waves themselves.

To see why the interference pattern moves at the group velocity, consider the regions where the two components of

$$\psi(x,t) = \cos(k_1 x - \omega_1 t) + \cos(k_2 x - \omega t)$$

interfere constructively. This happens where the arguments $k_1 x - \omega_1 t$ and $k_2 x - \omega_2 t$ of the two cosine functions differ by a multiple of 2π:

$$k_1 x - \omega_1 t = k_2 x - \omega_2 t + 2\pi n \qquad (n \text{ any integer})\ .$$

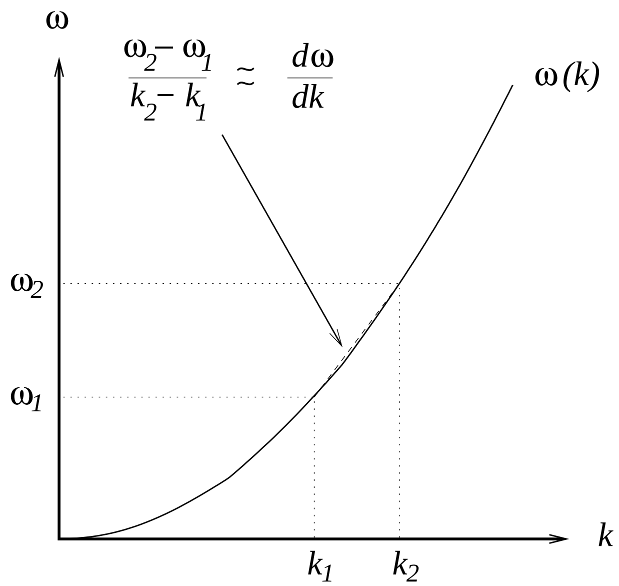

Figure 4: The slope $(\omega_2 - \omega_1)/(k_2 - k_1)$ of the (almost invisible) dashed line is approximately the same as the slope $d\omega/dk$ of the function $\omega(k)$.

For the $n = 0$ peak, the condition for constructive interference reduces to:

$$(k_2 - k_1)x = (\omega_2 - \omega_1)t \ .$$

When $t = 0$, the solution of this equation is $x = 0$ (in other words, the $n = 0$ peak is the broad peak in the middle of the lower panel in Figure 3). When $t > 0$, the position of the $n = 0$ peak is given by:

$$x = \frac{\omega_2 - \omega_1}{k_2 - k_1} t = \frac{\Delta\omega}{\Delta k} t \ .$$

The central peak of the interference pattern therefore moves at speed $\Delta\omega/\Delta k$.

If the wavelengths (and hence wavevectors and angular frequencies) of the two component waves are similar enough, the fraction $\Delta\omega/\Delta k$ is approximately equal to the derivative $d\omega/dk$ (see Figure 4). The interference pattern therefore moves at the group velocity:

$$v_g(k) = \frac{d\omega}{dk} \ .$$

Since Δk is assumed to be very small, it makes little difference whether the group velocity is evaluated at k_1 or k_2: $v_g(k_1) \approx v_g(k_2) \approx v_g((k_1 + k_2)/2)$. For aesthetic reasons, I prefer to use the average wavevector $(k_1 + k_2)/2$.

If the wavelengths of the two component waves differ by too much, the approximation $\Delta\omega/\Delta k \approx d\omega/dk$ may be poor. In this case, the velocity $\Delta\omega/\Delta k$ of the interference envelope will not be the same as the group velocity $d\omega/dk$.

General Case

Now consider a general wavepacket constructed by superposing many cosine waves. If the wavepacket is a "musical" one — in other words, if all the waves contributing to the superposition have similar wavelengths — it is possible to show that the interference envelope moves at the group velocity.

The proof uses the complex representation of a travelling wave introduced earlier in the course:

$$\psi(x,t) \;=\; a\cos(kx - \omega t + \phi) \;=\; \mathrm{Re}\left(Ae^{i(kx-\omega t)}\right) ,$$

where the constant $A = ae^{i\phi}$ is known as the complex amplitude. The complex representation of a wavepacket consisting of many travelling waves is:

$$\psi(x,t) = \sum_{n=1}^{N} A_n e^{i(k_n x - \omega_n t)} ,$$

where, as usual, the "Re" symbol has been omitted.

Since the wavepacket is musical, the wavevectors k_n are all very close to the carrier wavevector k_c:

$$k_n = k_c + \Delta k_n ,$$

where Δk_n is small. The angular frequency $\omega_n = \omega(k_n)$ may therefore be approximated using the first two terms of a Taylor series:

$$\omega_n \;=\; \omega(k_c + \Delta k_n) \;\approx\; \omega(k_c) + \left.\frac{d\omega}{dk}\right|_{k=k_c} \Delta k_n \;=\; \omega_c + v_g \Delta k_n ,$$

where $v_g = d\omega/dk|_{k=k_c}$. The expression for $\psi(x,t)$ then becomes:

$$\begin{aligned}\psi(x,t) &\approx \sum_{n=1}^{N} A_n e^{i[(k_c+\Delta k_n)x - (\omega_c + v_g \Delta k_n)t]} \\ &= \sum_{n=1}^{N} A_n e^{i(k_c x - \omega_c t) + i\Delta k_n (x - v_g t)}\end{aligned}$$

$$= \quad e^{i(k_c x - \omega_c t)} \sum_{n=1}^{N} A_n e^{i\Delta k_n (x - v_g t)} \ .$$

The exponential prefactor is the carrier wave with wavelength $\lambda_c = 2\pi/k_c$, while the summation gives the shape of the envelope. The important point is that the envelope is a function of $x - v_g t$ only:

$$\psi(x,t) \quad \approx \quad e^{i(k_c x - \omega_c t)} f(x - v_g t) \ .$$

This means that the envelope has the same shape [the shape of $f(x)$] at all times. As t increases, this frozen shape simply moves to the right at speed v_g.

The only approximation in the above derivation was the replacement of ω_n by the first two terms of a Taylor series. This approximation is exact if the dispersion relation is linear ($\omega = ck$, as for light) and good whenever the dispersion relation is close to linear over the range of wavevectors contributing to the wavepacket. If the dispersion relation is not quite linear, however, the neglected higher-order terms cause the wavepacket to smear out gradually as it moves along. The wider the spread of wavelengths in the wavepacket, the more rapidly this smearing (called dispersion) occurs.