Lecture 4 - Wavepackets

What's important:
- wavepackets in position and momentum
- propagation of wavepackets

Text: Gasiorowicz, Chap. 2

In the previous lecture, we derived the Fourier transform of a function $f(x)$:

$$f(x) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} A(k) \exp(ikx)\, dk. \qquad (1)$$

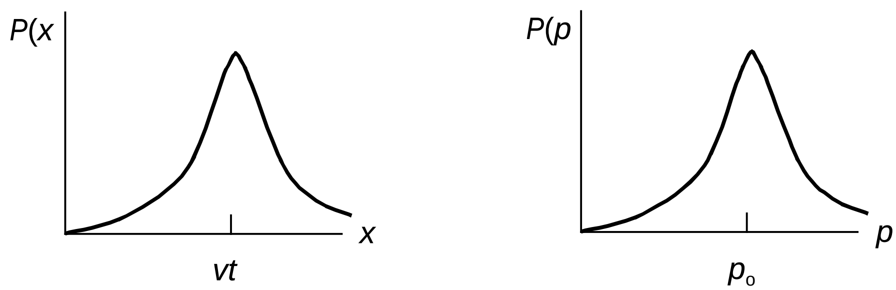
where

$$A(k) = (2\pi)^{-1/2} \int_{-\infty}^{+\infty} f(x) \exp(-ikx)\, dx. \qquad (2)$$

Here, $A(k)$ is a function of the continuous variable k, interpreted as a wavevector corresponding to the physical length x. Let's do a Fourier decomposition of a wavepacket, and then describe how the wavepacket propagates if k is treated as a momentum via $p = \hbar k$.

Wavepackets

In Lec. 2, we describe how the uncertainty principle leads to the idea that motion in quantum mechanics is probabilistic - the position and momentum of a particle are described by probability densities $P(x)$ and $P(p)$ that have a distribution around some mean value:



These functions look sort of Gaussian, as in $\exp(-\alpha k^2)$, where α reflects the width of the distribution. Let's *suppose* that the *WAVE AMPLITUDE* of a particle in k-space is actually Gaussian, with a form

$$g(k) = \exp(-\beta[k-k_o]^2), \qquad (3)$$

which is centered around $k = k_o$. Compared to Eq. (2), we will drop the factors of $(2\pi)^{1/2}$, as is done by Gasiorowicz; what interests us is the width of the distribution, not the normalization - in fact even with the missing $(2\pi)^{1/2}$, Eq. (3) is not normalized to unity. How does the amplitude in position behave if the amplitude in momentum is Gaussian?

We start by evaluating

$$f(x) = \int_{-\infty}^{+\infty} \exp(-\beta[k-k_o]^2) \exp(ikx)\, dk. \tag{4}$$

The first step in solving this integral is to combine the arguments of the exponentials

$$-\beta[k-k_o]^2 + ikx$$

then rewrite $K \equiv k-k_o$

$$-\beta K^2 + i\,(K+k_o)x.$$

Completing the square gives

$$\begin{aligned} -\beta K^2 + i\,(K+k_o)x &= -\beta K^2 + iKx + ik_ox \\ &= -\beta[K^2 + iKx/\beta - (ix/2\beta)^2] + \beta(ix/2\alpha)^2 + ik_ox \\ &= -\beta(K - ix/2\beta)^2 + \beta(ix/2\beta)^2 + ik_ox \\ &= -\beta(K - ix/2\beta)^2 - x^2/4\beta + ik_ox. \end{aligned}$$

Although this may be looking uglier by the minute, the integral itself is now solvable. Set

$$q \equiv K - ix/2\beta \qquad \text{and} \qquad dq = dK = dk.$$

so Eq. (4) becomes

$$f(x) = \exp(-x^2/4\beta) \bullet \exp(+ik_ox) \bullet \int_{-\infty}^{+\infty} \exp(-\beta q^2)\, dq, \tag{5}$$

where we have removed all the factors that don't depend on q from within the integral. Now, there is a subtle issue with making q complex, but the procedure is legal here, as students with a course on complex integration can verify. The numerical value of the integral is

$$\int_{-\infty}^{+\infty} \exp(-\beta q^2)\, dq = (1/\beta)^{1/2} \int_{-\infty}^{+\infty} \exp(-a^2)\, da = (1/\beta)^{1/2}\, S$$

where

$$\begin{aligned} S^2 &= \int_{-\infty}^{+\infty} \exp(-a^2)\, da \int_{-\infty}^{+\infty} \exp(-b^2)\, db = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \exp(-[a^2+b^2])\, da\, db \\ &= \int_0^{2\pi}\int_0^{\infty} \exp(-r^2)\; r\, dr\, d\theta \qquad \text{(switching to polar coords)} \\ &= 2\pi \bullet (1/2) \int_0^{\infty} \exp(-r^2)\, dr^2 \\ &= \pi \end{aligned}$$

or

$$S = \sqrt{\pi}.$$

Thus,

$$f(x) = \exp(-x^2/4\beta) \bullet \exp(+ik_ox)\, (\pi/\beta)^{1/2}. \tag{6}$$

In previous courses, one learned that the power of a wave is proportional to the square of its amplitude. Here, we will propose that the probability density of our wave is proportional to the square of $f(x)$, a precursor to introducing the wavefunction $\psi(x)$. From Eq. (6), then, the complex square of f is

$$|f(x)|^2 = (\pi/\beta) \exp(-x^2/2\beta) \qquad \text{(note the 2 from the square)} \tag{7}$$

What we have found so far, using $|f(x)|^2$ and $|g(k)|^2$:

- the distribution in position is Gaussian
- the distribution in wave vector is Gaussian.

We can determine the width of $|f(x)|^2$ by means of an integral, but let's avoid that by making the approximation that the width is equal to twice the value of x where $|f(x)|^2 = 1/e\ |f(0)|^2$. Thus,

$$\Delta x = 2 \bullet (2\beta)^{1/2}.$$

If we demand the same for the width in wave vector, we have

$$\Delta k = 2 / (2\beta)^{1/2}.$$

Taking the product

$$\Delta x \bullet \Delta k = 4. \quad (8)$$

Well, the 4 doesn't matter too much, the main thing is that the product of the widths is constant: as the distribution in k widens, the distribution in x shrinks, just what we want for Heisenberg's uncertainty principle.

OK, we've made some progress here. We introduced $f(x)$ and $g(k)$ as wave-like functions whose squares are proportional to probabilities. The widths of the distributions are inversely related, with a product equal to a constant. This is suggestive of a framework for treating quantum motion, but it's no proof.

Propagation of wave packets

Let's take our candidate wave-packets a little more seriously. Accepting them as the correct representations, we know the (one particle) probability distributions in position and wave-vector, but we don't know the joint probabilities (if a particle is at position x, what is the probability that it has a momentum p?). The fact that there is a distribution of momenta (through $p = \hbar k$) tells us that the wavepacket will spread out in space as time passes. That is, thinking of the distribution as representing an ensemble of particles occupying a region of x and p, the particles have a distribution of speeds even in one dimension, such that the faster ones will cover more ground in a given time than the slower ones. Let's determine how the spatial distribution evolves.

In first year, we show that a plane wave travelling to the right (positive x) is described by

$$\cos \text{ or } \sin\ (kx - \omega t)$$

where

$$k = 2\pi/\lambda \qquad \text{and} \qquad \omega = 2\pi/T,$$

and T = period, λ = wavelength. The words "plane wave" just mean that the wave has no y or z dependence. In these lectures, we've been using the complex representation exp(*ikx*) for a snapshot of a wave at fixed time, so our travelling plane-wave would be described as

$\exp(ikx - i\omega t)$.

Photon wavepackets

For particles travelling at the speed of light, we have

$$c = \lambda/T = (\lambda/2\pi) \bullet (2\pi/T) = \omega/k \qquad \text{or} \qquad \omega = kc. \tag{9}$$

Thus, our plane wave is

$\exp(ik[x - ct])$.

If we use these plane wave states, and repeat the previous calculations, we find that our position function $f(x)$ has become

$f(x,t) = f(x - ct)$.

In other words, it has the same functional form as before, but it's value at $x + ct$ is the same as the original value at x: the wave is travelling to the right. A wavepacket of photons, then does not change shape as it evolves.

Massive wavepackets

The simple relationship between c and ω is particular to photons. Let's see what happens for the de Brogile waves of massive particles, starting with the demand that

$$E = \omega\hbar \tag{10}$$

apply to massive particles as well as photons.

From the non-relativistic energy

$E = p^2/2m$,

this gives

$$\omega = p^2/2m\hbar = (\hbar/2m)k^2. \qquad \text{(non-relativistic)} \tag{11}$$

[This can be shown to be consistent with the de Broglie relation by the definition of the group velocity

$v_g = d\omega/dk = (\hbar/2m)2k = \hbar k/m$ from (11 + 13)

$v_g = p/m$ from definition

-> $p = \hbar k$]

In general, ω is not a linear function of k. It's useful to do a Taylor series expansion around k_o of the initial k-space distribution (say k_o is the central value), as in

$$\omega(k) = \omega(k_o) + (k-k_o)(d\omega/dk)_{ko} + (1/2)\bullet(k-k_o)^2(d^2\omega/dk^2)_{ko} + \ldots$$

which can be parametrized as

$$\omega(k) = \omega(k_o) + (k-k_o)\,v_g + ß(k-k_o)^2 + \ldots \qquad (12)$$

$$v_g = \text{group velocity} = (d\omega/dk)_{ko} \qquad ß = (d^2\omega/dk^2)_{ko}/2. \qquad (13)$$

(The definition of $ß$ in Gasiorowicz is out by a factor of two; first line in Eq. (2-15) is inconsistent). The entire calculation of $f(x, t)$ can be repeated as before, using the travelling wave expression

$$\exp(ikx - i\omega t)$$

with ω removed by Eq. (12). The math is sketched out in Gasiorowicz, and leads to

$$|f(x,t)|^2 = \left(\frac{\pi^2}{\alpha^2 + ß^2 t^2}\right)^{1/2} \exp[-\alpha(x - v_g t)^2 / 2(\alpha^2 + ß^2 t^2)]. \qquad (14)$$

Our previous expressions are regained when $v_g = c$ and $ß = 0$.

What do we see from the exponential?

1. The $x - v_g t$ term in the numerator shows that the peak of the distribution travels along at the group velocity v_g.
2. The denominator increases with time, meaning that the wavepacket is spreading: the factor $\sqrt{\alpha}$ found for the stationary wave becomes

$$(\alpha^2 + ß^2 t^2)^{1/2} = \sqrt{\alpha} \bullet (1 + ß^2 t^2/\alpha^2)^{1/2}. \qquad (15)$$