Gaussian Wave Packets

The general FOURIER EXPANSION IN PLANE WAVES is $\Psi(\vec{\mathbf{r}},t) = \int_{-\infty}^{\infty} a(\vec{\mathbf{k}}) e^{i(\vec{\mathbf{k}}\cdot\vec{\mathbf{r}}-\omega t)} d^3k$ where we must remember that ω is a *function of* $\vec{\mathbf{k}}$, not just a constant; the DISPERSION RELATION $\omega(\vec{\mathbf{k}})$ determines all the key physical properties of the wave such as PHASE VELOCITY $\vec{\mathbf{v}}_p \equiv \vec{\mathbf{k}}\omega/k^2$ and GROUP (PHYSICAL) VELOCITY $\vec{\mathbf{v}}_g \equiv \vec{\nabla}_k\, \omega$.

The picture is a lot simpler if we assume that *all* waves propagate along the $\hat{x}$ direction, giving the 1-dimensional version $\Psi(x,t) = \int_{-\infty}^{\infty} a(k) e^{i(kx-\omega t)} dk$ with $v_p = \omega/k$ and $v_g = d\omega/dk$.

The *Gaussian* distribution of wavenumbers

$$a(k) = \frac{A}{\sigma_k\sqrt{2\pi}} \exp\left[-\frac{(k-k_\circ)^2}{2\sigma_k^2}\right]$$

has a mean wavenumber $\langle k\rangle = k_\circ$ and a variance $\langle (k-\langle k\rangle)^2\rangle = \sigma_k^2$ (so that σ_k is the *standard deviation* of k).

$$\text{At } t=0\,,\text{ we have}\quad \Psi(x,0) \equiv \psi(x) = \frac{A}{\sigma_k\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\frac{(k-k_\circ)^2}{2\sigma_k^2}\right] e^{ikx} dk$$

$$\text{or}\quad \psi(x) = \frac{A e^{ik_\circ x}}{\sigma_k\sqrt{2\pi}} \int_{-\infty}^{\infty} \exp\left[-\frac{k'^2}{2\sigma_k^2}\right] e^{ik'x} dk' \quad \text{where} \quad k' \equiv k - k_\circ$$

If we now let $u \equiv \dfrac{k'}{\sqrt{2}\sigma_k}$ so that $dk' = \sqrt{2}\sigma_k du$, we have

$$\psi(x) = \frac{A e^{ik_\circ x}}{\sigma_k\sqrt{2\pi}} \cdot \sqrt{2}\sigma_k \int_{-\infty}^{\infty} e^{-u^2} \cdot e^{i\sqrt{2}\sigma_k x u} du = \frac{A}{\sqrt{\pi}} e^{ik_\circ x} \int_{-\infty}^{\infty} \exp\left[-\left(u^2 - i\sqrt{2}\sigma_k x u\right)\right] du.$$

Completing the square, $u^2 - i\sqrt{2}\sigma_k x u = \left(u - \dfrac{i\sigma_k}{\sqrt{2}} x\right)^2 + \dfrac{\sigma_k^2}{2} x^2$, giving

$$\psi(x) = \frac{A}{\sqrt{\pi}} \exp\left[-\frac{\sigma_k^2 x^2}{2}\right] e^{ik_\circ x} \int_{-\infty}^{\infty} e^{-z^2} dz \qquad \text{where} \qquad z \equiv u - \frac{i\sigma_k x}{\sqrt{2}}$$

The definite integral has the value $\sqrt{\pi}$ (look it up in a table of integrals!) giving

$$\psi(x) = A \exp\left[-\frac{\sigma_k^2 x^2}{2}\right] e^{ik_\circ x} \qquad \text{or} \qquad \psi(x) = A \exp\left[-\frac{x^2}{2\sigma_x^2}\right] e^{ik_\circ x} \qquad \text{where} \qquad \sigma_x = \frac{1}{\sigma_k}$$

That is, the *rms* width of the *wave packet* about its initial mean of $\langle x\rangle = 0$ is $\sqrt{\langle (x-\langle x\rangle)^2\rangle} = \sigma_x = 1/\sigma_k$ and the product of the x and k widths obeys the UNCERTAINTY RELATION $\sigma_x\sigma_k = 1$ at $t = 0$.

Normalization: The requirement that the particle be *somewhere* at $t = 0$ provides the numerical value of A: $\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1 = A^2 \int_{-\infty}^{\infty} \exp\left[-\frac{x^2}{\sigma_x^2}\right] dx = A^2 \sigma_x \int_{-\infty}^{\infty} e^{-u^2} du$ where $u \equiv x/\sigma_x$. Again the definite integral equals $\sqrt{\pi}$, giving $1 = A^2 \sigma_x \sqrt{\pi}$ or $A = \sqrt{\frac{1}{\sigma_x \sqrt{\pi}}} = \sqrt{\frac{\sigma_k}{\sqrt{\pi}}}$. We have now fully described $\psi(x) \equiv \Psi(x, 0)$.

Dispersion: *What happens at later times?* Each plane-wave *component* of $\Psi(x, t)$ has a different k and therefore progapates at a different *velocity* $v = p/m = \hbar k/m = d\omega/dk = v_g$. Thus they all move away from $x = 0$ at a different rate and become spread out or *dispersed* [hence the name "DISPERSION RELATION" for $\omega(k)$] relative to their *average* position [the centre of the wave packet] at $\langle x(t) \rangle = \left(\frac{k_\circ}{m}\right) t$.

The width of the wave packet, σ_x, therefore increases with time from its minimum value $\sigma_x(0)$ at $t = 0$. The time dependence can be calculated with some effort (not shown here); the result is

$$\sigma_x(t) = \sqrt{\sigma_x^2(0) + \left[\frac{\hbar t}{2m\sigma_x(0)}\right]^2}.$$

The normalization constant A will *decrease* with time (as the spatial extent of the wave packet increases) in order to maintain $\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$. Thus the probability of finding the particle within dx of its mean position $\langle x(t) \rangle$ steadily decreases with time as the wave packet disperses.

Examples: It is instructive to estimate the *rate* of dispersion (*i.e.* how fast the wave packet spreads out) for a few simple cases:

- First consider an electron that is initially confined to a region of a size $\sigma_x(0) = 0.1$ *nm* (*i.e.* roughly atomic dimensions) in a gaussian wave packet. For simplicity we will let $k_\circ = 0$ — that is, the electron is (on average) at rest. If the electron is *free* (as we have assumed throughout this treatment) then its wave packet will expand to $\sqrt{2}$ times its initial size in a time $t_2 = \frac{2m}{\hbar} \sigma_x^2(0) = 1.72 \times 10^{-15}$ *s*.
- If the same electron is confined much more loosely to a region of a size $\sigma_x(0) = 1$ μm, the time required for it to disperse until $\sigma_x(t) = \sqrt{2}\sigma_x(0)$ is 10^8 times longer: $t_2 = 17.2$ *ns*.
- The same electron initially confined to a 1 *mm* sized wave packet will take 0.0172 *s* to disperse to a wave packet 1.414 *mm* in size; and so on.
- A one-gram marble localized to within 0.1 *mm* will delocalize spontaneously (the physical meaning of dispersion) to 0.1414 *mm* only after $t_2 = 1.89 \times 10^{24}$ *s* — that is, 6×10^{16} *years!*