Evolution of a Wave Packet

A Gaussian wave packet $\psi(x,t)$ spreads out in time because of the dispersive nature of the diffusion equation. We can see this in broad terms by looking as usual at a plane wave (Fourier mode) of wavenumber k and angular frequency ω

$$\psi \;\sim\; e^{ikx-i\omega t}$$

and asking what relation between ω and k (the so-called dispersion relation) is imposed by the equation. As an aside, we note that, for the wave equation

$$\frac{\partial^2\psi}{\partial t^2} \;=\; c^2\,\frac{\partial^2\psi}{\partial x^2},$$

substituting the above expression for ψ yields the familiar expression

$$\omega^2 \;=\; c^2k^2,$$

so the plane wave propagates with speed $c = \omega/k$.

For the Schrodinger equation (or the diffusion equation), we have (for a free particle)

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

Looking again at a plane wave solution we now find

$$i\hbar(-i\omega) \;=\; -\,\frac{\hbar^2}{2m}(-k^2),$$

or

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

Thus different waves move at different speeds and the wave packet must change shape as time goes on.

We can understand how this works in more detail by decomposing our Gaussian wave packet $\psi(x,t)$ into momentum space—i.e. by Fourier transforming it in terms of momentum p or wavenumber $k = p/\hbar$. Let's start with a normalized wave function of the "minimum" initial form just described, with

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

where the leading factor simply normalizes $\int|\psi|^2 = 1$. Note that we have set $\bar{x} = 0$ and $\bar{p} = 0$ for convenience, so this wavefunction represents a particle at the origin with no net momentum.

This is not a pure momentum eigenmode, but we can express it in momentum space in terms of $\tilde{\psi}(k,0)$, where

$$\begin{aligned}\tilde{\psi}(k,0) \;&=\; \int_{-\infty}^{\infty}\psi(x)e^{-ikx}\,dx \\ &=\; e^{-2\Delta x^2k^2}. \end{aligned} \tag{1}$$

Incidentally, we can see here that the "width" of $|\psi(x)|^2$ is $\sigma_x = \sqrt{2}\Delta x$, while the width of $|\tilde{\psi}|^2$ is $\sigma_k = 1/(2\sqrt{2}\Delta x)$, so $\sigma_x\sigma_k = \frac{1}{2}$, as stated earlier.

The transformed Schrodinger equation is

$$i\hbar\frac{\partial\tilde{\psi}}{\partial t} \;=\; \frac{\hbar^2k^2}{2m},$$

with solution

$$\tilde{\psi} \;=\; \tilde{\psi}_0\, e^{-i\hbar k^2 t/2m} \;=\; \tilde{\psi}_0\, e^{-iEt/\hbar}$$

where $E = p^2/2m = \hbar^2k^2/2m$. Thus for each mode, the solution to the time-dependent Schrodinger equation is easy to write down:

$$\begin{aligned}\tilde{\psi}(k,t) \;&=\; \tilde{\psi}(k,0)\, e^{-i\hbar k^2 t/2m} \\ &=\; e^{-2\Delta x^2 k^2[1+i\hbar t/(2m\Delta x^2)]}\end{aligned}$$

Without going into too much more algebra, comparing with Eq.1 we can see that the width of $\psi(x,t)$ is increasing with time. Taking the absolute value and squaring, we find that the effective Δx governing the width of $|\psi|^2$ scales as

$$\Delta x^2(t) \;=\; \Delta x^2\left(1+\frac{\hbar^2t^2}{4m\Delta x^4}\right).$$