Problem: Evolution of a free Gaussian wavepacket

Consider a free particle which is described at $t = 0$ by the normalized Gaussian wave function

$$\Psi(x,0) \;=\; \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} \quad .$$

The normalization factor is easy to obtain. We wish to find its time evolution. How does one do this ? Remember the recipe in quantum mechanics. We expand the given wave function in terms of the energy eigenfunctions and we know how individual energy eigenfunctions evolve. We then reconstruct the wave function at a later time t by superposing the parts with appropriate phase factors. For a free particle $H = p^2/(2m)$ and therefore, momentum eigenfunctions are also energy eigenfunctions. So it is the mathematics of Fourier transforms!

It is straightforward to find $\Phi(k,0)$ the Fourier transform of $\Psi(x,0)$:

$$\Psi(x,0) \;=\; \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \Phi(k,0)\, e^{ikx} \quad .$$

Recall that the Fourier transform of a Gaussian is a Gaussian.

$$\phi(k) \;\equiv\; \Phi(k,0) \;=\; \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, \Psi(x,0)\, e^{-ikx} \tag{1.1}$$

$$\;=\; \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \int_{-\infty}^{\infty} dx\; e^{-ikx}\, e^{-ax^2} \;=\; \left(\frac{1}{2\pi a}\right)^{1/4} e^{-\frac{k^2}{4a}} \tag{1.2}$$

What this says is that the Gaussian spatial wave function is a superposition of different momenta with the probability of finding the momentum between k_1 and $k_1 + dk$ being proportional to $\exp(-k_1^2/(2a))\, dk$.

So the initial wave function is a superposition of different plane waves with different coefficients (usually called amplitudes). Note that $\exp ikx$ for each real k is also an eigenfunction of the Hamiltonian with eigenvalue $\boxed{E_k \;=\; \frac{\hbar^2 k^2}{2m}}$. Therefore, we know that $\exp(ikx)$ evolves in time with a time dependence given by $\boxed{e^{-iE_k t/\hbar}}$. So the time-evolved state, $\Psi(x,t)$, is given by

$$\Psi(x,t) \;=\; \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \phi(k)\, e^{ikx}\, e^{-iE_k t/\hbar} \tag{1.3}$$

$$\;=\; \left(\frac{1}{2\pi a}\right)^{1/4} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, e^{-\frac{k^2}{4a}}\, e^{-iE_k t/\hbar}\, e^{ikx} \tag{1.4}$$

where we know E_k and this integral has to be done.

The exponential has an argument given by

$$-\frac{k^2}{4a}\,[1 + \frac{2i\hbar a t}{m}] \;=\; -\,\frac{bk^2}{2} \;\text{ where }\; b \;=\; \frac{1}{2a}\left(1 + \frac{2i\hbar a t}{m}\right) \quad .$$

Thus the integral to be done is

$$\left(\frac{1}{2\pi a}\right)^{1/4} \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}} \; e^{-bk^2/2} \, e^{ikx}$$

and this can be done in the usual way in spite of the fact that b is complex since the integral is well-defined. We obtain, using

$$\int_{-\infty}^{\infty} dk \, e^{-bk^2/2} \, e^{ikx} \;=\; \sqrt{\frac{2\pi}{b}} \, e^{-\frac{x^2}{2b}} \;, \tag{1.5}$$

$$\text{the result} \quad \Psi(x,t) \;=\; \left(\frac{1}{2\pi a}\right)^{1/4} \sqrt{\frac{1}{b}} \, e^{-\frac{x^2}{2b}} \tag{1.6}$$

$$\;=\; \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1+\frac{2i\hbar a t}{m}}} \, \exp[-\frac{ax^2}{(1+\frac{2i\hbar a t}{m})}] \;. \tag{1.7}$$

The probability density is given by (after a wee bit of algebra)

$$|\Psi(x,t)|^2 \;=\; \sqrt{\frac{2a}{\pi}} \frac{1}{\sqrt{1+(\frac{2\hbar a t}{m})^2}} \, e^{-\frac{2ax^2}{1+(\frac{2\hbar a t}{m})^2}} \tag{1.8}$$

from which we can read off

$$\langle x^2 \rangle \;=\; \frac{1}{4a}\left[1+\left(\frac{2\hbar a t}{m}\right)^2\right] \;. \tag{1.9}$$

Note that the initial width $\frac{1}{4a}$ increases quadratically as a function of time.

To understand this result it is useful to rewrite it. We note that since $< x >= 0$ we have the initial $< x^2 >$ is $1/(4a)$. Let us call this $\sigma_0^2 = 1/(4a)$, in a great notational leap forward. So the width at time t is given by (chasing the factors of a and replacing them by $\sigma_0^2/2$)

$$\langle x^2 \rangle_t \;\equiv\; \sigma_x^2(t) \;=\; \sigma_0^2 \;+\; \frac{\hbar^2 t^2}{4m^2\sigma_0^2} \;. \tag{1.10}$$

Now we note that the uncertainty in the momentum can be read off from the wave function in k-space. Since $\phi(k)$ is Gaussian we find

$$\langle k^2 \rangle \;=\; a \;\; \text{and hence} \;\; \sigma_p^2 \;=\; \hbar^2 a \;=\; \frac{\hbar^2}{4\sigma_0^2}$$

where we have rewritten a in terms of σ_0 and used the de Broglie relation.[1]

$$\text{Therefore,} \quad \sigma_x^2(t) \;=\; \sigma_0^2 \;+\; \frac{\sigma_p^2 t^2}{m^2} \;. \tag{1.11}$$

[1] Why can the initial wave function be called a *minimum uncertainty wave packet*? How does the momentum uncertainty change as a function of time ? Why ?

So the initial uncertainty in the position increases with an extra part which can be thought of as follows: $\sigma_p t/m$ is the distance traveled by a classical particle with momentum equal to the uncertainty σ_p in a time t. So for $t << \sigma_0/(\sigma_p/m)$ the width remains unchanged.

Given an arbitrary initial wave function $\Psi(x,0)$ for a free particle we can find $\Psi(x,t)$. First find its decomposition in terms of $\phi(k)$:[2]

$$\Psi(x,0) = \int_{-\infty}^{\infty} \frac{dx}{\sqrt{2\pi}}\, \phi(k)\, e^{ikx} .$$

Then each plane wave, an eigenfunction of the free particle of the Hamiltonian with eigenvalue E_k, evolves in time and at time t picks up a phase factor $e^{-iE_k t/\hbar}$. Therefore we have

$$\Psi(x,t) = \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, \phi(k)\, e^{ikx}\, e^{-iE_k t/\hbar} \tag{1.12}$$

$$= \int_{-\infty}^{\infty} \frac{dk}{\sqrt{2\pi}}\, e^{ikx}\, e^{-iE_k t/\hbar} \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}}\, e^{-iky}\Psi(y,0) \quad \text{replacing} \quad \phi(k) \tag{1.13}$$

$$= \int_{-\infty}^{\infty} dy \left[\int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ik(x-y)}\, e^{-iE_k t/\hbar} \right] \Psi[y,0] \tag{1.14}$$

$$= \int_{-\infty}^{\infty} dy\, G(x,t;y,0)\, \Psi[y,0] \tag{1.15}$$

where we have defined the corresponding Green's function for the Schrödinger equation:

$$G(x,t;y,0) \equiv \int_{-\infty}^{\infty} dy \left[\int_{-\infty}^{\infty} \frac{dk}{2\pi}\, e^{ik(x-y)}\, e^{-iE_k t/\hbar} \right] .$$

Note that given the function $\Psi(y,0)$ (y is just a dummy variable), G tells you how to propagate the system in time and obtain the function $\Psi(x,t)$ at time t. G is known as the **free-particle propagator**. It is also called the Feynman propagator for a non-relativistic free particle. Performing the integral we find the explicit expression

$$G(x,t;y,0) = \sqrt{\frac{m}{2\pi i\hbar t}}\, e^{i\,\frac{m(x-y)^2}{2\hbar t}}$$

for $t > 0$. As $t \to 0$ this goes over to a delta function as one can check. Finding the Green's function for other problems such as the quantum harmonic oscillator is somewhat tedious. (See R. P. Feynman and A. R. Hibbs, "Quantum Mechanics and Path Integrals", unfortunately, poorly proof-read.)

[2] $\phi(k)$ can be found as usual by the inverse Fourier transform:

$$\phi(k) = \int_{-\infty}^{\infty} \frac{dy}{\sqrt{2\pi}}\, \Psi(y,0)\, e^{-iky} .$$