

FREE PARTICLE: GAUSSIAN WAVE PACKET

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.22.

While analyzing the free particle, we saw that we could construct a normalizable combination of stationary states by writing

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} e^{-i\hbar k^2 t/2m} dk \quad (1)$$

Given the initial wave function, we can find $\phi(k)$ via Plancherel's theorem:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} dx \quad (2)$$

The integral 1 cannot usually be done in closed form, but one case where it can is if the initial wave function is a Gaussian, of the form

$$\Psi(x,0) = A e^{-ax^2} \quad (3)$$

To find A, we normalize:

$$A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = 1 \quad (4)$$

The integral comes out to $\sqrt{\pi/2a}$ from which we get

$$A = \left(\frac{2a}{\pi}\right)^{1/4} \quad (5)$$

Finding $\Psi(x,t)$ requires finding $\phi(k)$ via equation 2. So we get (using Maple to do the integral):

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \int_{-\infty}^{\infty} e^{-ax^2 - ikx} dx \quad (6)$$

$$= \left(\frac{1}{2\pi a}\right)^{1/4} e^{-k^2/4a} \quad (7)$$

We can now use 1 again using Maple to do the integral:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} e^{-i\hbar k^2 t/2m} dk \quad (8)$$

$$= \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi a} \right)^{1/4} \int_{-\infty}^{\infty} e^{-k^2/4a} e^{ikx} e^{-i\hbar k^2 t/2m} dk \quad (9)$$

$$= \left(\frac{2a}{\pi} \right)^{1/4} \frac{e^{-ax^2/(1+2i\hbar at/m)}}{\sqrt{1+2i\hbar at/m}} \quad (10)$$

where Maple was used for the integral.

Calculating $|\Psi(x,t)|^2$ can be done using Maple, but it seems to require a bit of help. First we write out the complex conjugate:

$$\Psi^*(x,t) = \left(\frac{2a}{\pi} \right)^{1/4} \frac{e^{-ax^2/(1-2i\hbar at/m)}}{\sqrt{1-2i\hbar at/m}} \quad (11)$$

Then we calculate $\Psi^*\Psi$ using the Maple command `simplify(evalc(Psi*Psi))` assuming positive and we get

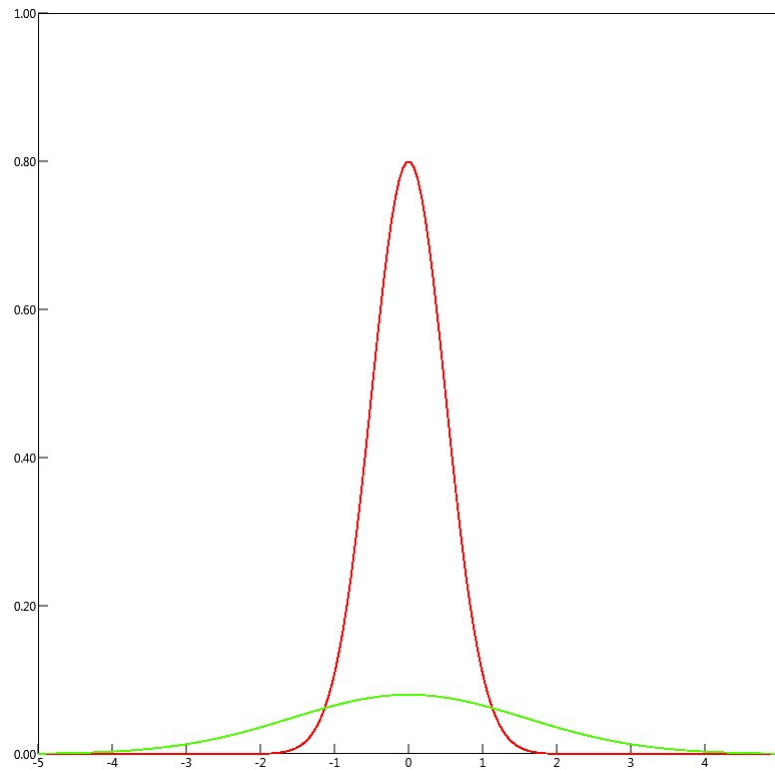
$$|\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}} \frac{e^{-2ax^2/[1+(2\hbar at/m)^2]}}{\sqrt{1+(2\hbar at/m)^2}} \quad (12)$$

$$= \sqrt{\frac{2}{\pi}} w e^{-2w^2 x^2} \quad (13)$$

with

$$w \equiv \left(\frac{a}{1+(2\hbar at/m)^2} \right)^{1/2} \quad (14)$$

At $t = 0$, $w = \sqrt{a}$, so $|\Psi(x,t)|^2 = \sqrt{2a/\pi} e^{-2ax^2}$ which is correct. The wave packet at $t = 0$ is therefore a Gaussian centred at $x = 0$. As t increases, w gets smaller but the centre of the Gaussian does not move from $x = 0$ so the packet spreads out. A couple of plots show this behaviour. We've set $a = 1$ in both plots. In the red plot $t = 0$ so $w = 1$ and in the green plot t is larger, at a value such that $w = 0.1$.



We can get the mean values of position and momentum by integration, although it takes a bit of work. By symmetry, $\langle x \rangle = \langle p \rangle = 0$. To get the other two average values, we use integration with Maple.

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\Psi(x,t)|^2 dx \quad (15)$$

$$= \frac{1}{4w^2} \quad (16)$$

$$= \frac{1 + (2\hbar at/m)^2}{4a} \quad (17)$$

This shows that the wave function spreads out with time. At $t = 0$ $\langle x^2 \rangle = 1/4a$, but it then increases quadratically with t .

Calculating $\langle p^2 \rangle$ starts with:

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \Psi^* \frac{\partial^2}{\partial x^2} \Psi dx \quad (18)$$

This can be evaluated with the Maple command `simplify(evalc(int(-h^2*simplify(evalc(psixtconj*(d/dx$2))), x = -infinity .. infinity))) assuming positive` where `psixtconj` and `psixt` are the Maple expressions for Ψ^* and Ψ respectively. The result is:

$$\langle p^2 \rangle = a\hbar^2 \quad (19)$$

The uncertainty principle thus becomes

$$\sigma_x \sigma_p = \sqrt{\langle x^2 \rangle \langle p^2 \rangle} \quad (20)$$

$$= \frac{\hbar}{2} \sqrt{1 + (2\hbar a t / m)^2} \quad (21)$$

The system has the least uncertainty at $t = 0$. Uncertainty increases with time as the wave packet spreads out.

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