

## 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

$$(0.1) \quad \Psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} e^{-i\hbar k^2 t / 2m} dk$$

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

$$(0.2) \quad \phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x, 0) e^{-ikx} dx$$

The integral 0.1 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

$$(0.3) \quad \Psi(x, 0) = A e^{-ax^2}$$

To find  $A$ , we normalize:

$$(0.4) \quad A^2 \int_{-\infty}^{\infty} e^{-2ax^2} dx = 1$$

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

$$(0.5) \quad A = \left( \frac{2a}{\pi} \right)^{1/4}$$

Finding  $\Psi(x, t)$  requires finding  $\phi(k)$  via equation 0.2. So we get (using Maple to do the integral):

$$(0.6) \quad \phi(k) = \frac{1}{\sqrt{2\pi}} \left(\frac{2a}{\pi}\right)^{1/4} \int_{-\infty}^{\infty} e^{-ax^2 - ikx} dx$$

$$(0.7) \quad = \left(\frac{1}{2\pi a}\right)^{1/4} e^{-k^2/4a}$$

We can now use 0.1 again using Maple to do the integral:

$$(0.8) \quad \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} e^{-i\hbar k^2 t/2m} dk$$

$$(0.9) \quad = \frac{1}{\sqrt{2\pi}} \left(\frac{1}{2\pi a}\right)^{1/4} \int_{-\infty}^{\infty} e^{-k^2/4a} e^{ikx} e^{-i\hbar k^2 t/2m} dk$$

$$(0.10) \quad = \left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/(1+2i\hbar at/m)}}{\sqrt{1+2i\hbar at/m}}$$

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:

$$(0.11) \quad \Psi^*(x,t) = \left(\frac{2a}{\pi}\right)^{1/4} \frac{e^{-ax^2/(1-2i\hbar at/m)}}{\sqrt{1-2i\hbar at/m}}$$

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

$$(0.12) \quad |\Psi(x,t)|^2 = \sqrt{\frac{2a}{\pi}} \frac{e^{-2ax^2/[1+(2\hbar at/m)^2]}}{\sqrt{1+(2\hbar at/m)^2}}$$

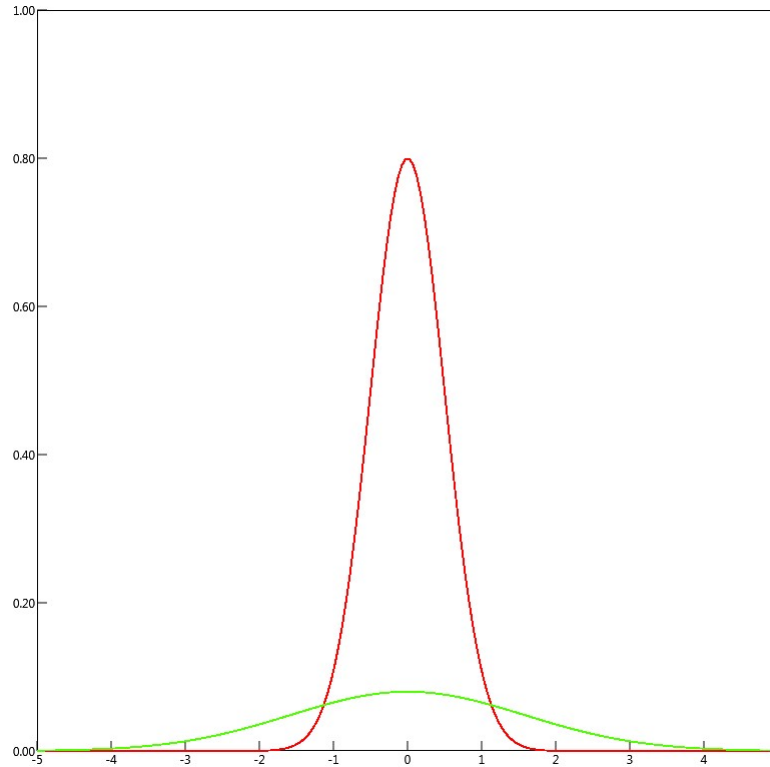
$$(0.13) \quad = \sqrt{\frac{2}{\pi}} w e^{-2w^2 x^2}$$

with

$$(0.14) \quad w \equiv \left(\frac{a}{1+(2\hbar at/m)^2}\right)^{1/2}$$

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.

$$(0.15) \quad \langle x^2 \rangle = \int_{-\infty}^{\infty} x^2 |\Psi(x,t)|^2 dx$$

$$(0.16) \quad = \frac{1}{4w^2}$$

$$(0.17) \quad = \frac{1 + (2\hbar at/m)^2}{4a}$$

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:

$$(0.18) \quad \langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} \Psi^* \frac{\partial^2}{\partial x^2} \Psi dx$$

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  $\Psi^*$  and  $\Psi$  respectively. The result is:

$$(0.19) \quad \langle p^2 \rangle = a\hbar^2$$

The uncertainty principle thus becomes

$$(0.20) \quad \sigma_x \sigma_p = \sqrt{\langle x^2 \rangle \langle p^2 \rangle}$$

$$(0.21) \quad = \frac{\hbar}{2} \sqrt{1 + (2\hbar a t / m)^2}$$

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

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