**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

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

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

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

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

$$\Psi(x,0)=Ae^{-ax^2} \tag{3}$$

To find $A$, we normalize:

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

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

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

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

$$\begin{aligned}\phi(k) &= \frac{1}{\sqrt{2\pi}}\left(\frac{2a}{\pi}\right)^{1/4}\int_{-\infty}^{\infty}e^{-ax^2-ikx}dx &(6)\\ &= \left(\frac{1}{2\pi a}\right)^{1/4}e^{-k^2/4a} &(7)\end{aligned}$$

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

$$\begin{aligned}
\Psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{ikx}e^{-i\hbar k^2t/2m}dk & (8)\\
&= \frac{1}{\sqrt{2\pi}}\left(\frac{1}{2\pi a}\right)^{1/4}\int_{-\infty}^{\infty}e^{-k^2/4a}e^{ikx}e^{-i\hbar k^2t/2m}dk & (9)\\
&= \left(\frac{2a}{\pi}\right)^{1/4}\frac{e^{-ax^2/(1+2i\hbar at/m)}}{\sqrt{1+2i\hbar at/m}} & (10)
\end{aligned}$$

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:

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

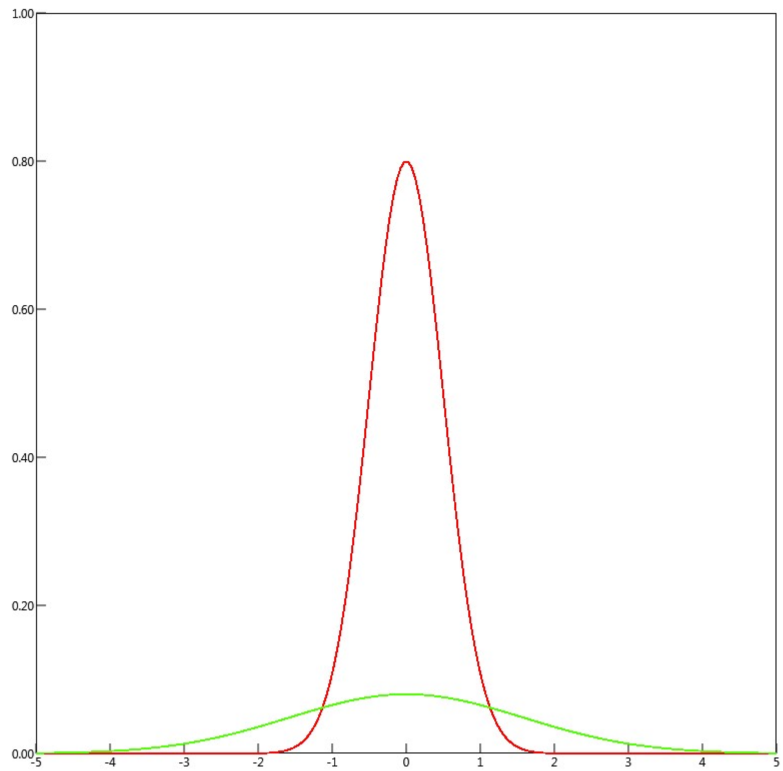
Then we calculate $\Psi^*\Psi$ using the Maple command *simplify(evalc(*$\Psi^*\Psi$*)) assuming positive* and we get

$$\begin{aligned}
|\Psi(x,t)|^2 &= \sqrt{\frac{2a}{\pi}}\frac{e^{-2ax^2/\left[1+(2\hbar at/m)^2\right]}}{\sqrt{1+(2\hbar at/m)^2}} & (12)\\
&= \sqrt{\frac{2}{\pi}}we^{-2w^2x^2} & (13)
\end{aligned}$$

with

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

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.

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

$$= \frac{1}{4w^2} \tag{16}$$

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

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:

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

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

$$\langle p^2 \rangle = a\hbar^2 \tag{19}$$

The uncertainty principle thus becomes

$$\sigma_x \sigma_p = \sqrt{\langle x^2 \rangle \langle p^2 \rangle} \tag{20}$$

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

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

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