FREE PARTICLE AS GAUSSIAN WAVE PACKET

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The general solution of the time-independent Schrödinger equation in one dimension can be written in terms of a propagator U as

$$\psi(x,t)=\int dx'\,U\left(x,x',t-t_0\right)\psi\left(x',t_0\right) \tag{1}$$

To use this solution, we need to specify the initial state $\psi(x',t_0)$ at time t_0, and we also need to know the actual form of U, which depends on the hamiltonian for the problem. In the case of the free particle (where there is no potential energy term in the hamiltonian), U is

$$U\left(x,x',t-t_0\right)=\sqrt{\frac{m}{2\pi i\hbar\,(t-t_0)}}e^{i(x-x')^2m/2\hbar(t-t_0)} \tag{2}$$

The solution of 1 therefore reduces to specifying $\psi(x',t_0)$. In the following, to keep things relatively simple, we'll take $t_0=0$. Then the propagator is

$$U\left(x,x',t\right)=\sqrt{\frac{m}{2\pi i\hbar t}}e^{i(x-x')^2m/2\hbar t} \tag{3}$$

To model a particle starting at the origin, a sensible choice for $\psi(x,0)$ is some function that peaks at the origin and falls off fairly rapidly on either side. Most books that study the free particle treat the case where the particle starts life as a Gaussian function, of the form

$$\psi(x,0)=Ae^{-ax^2} \tag{4}$$

Since $|\psi(x,0)|^2$ is the probability density, we need to ensure that its integral over all space is 1, so we need to normalize ψ by finding A. That is, we require

$$A^2\int_{-\infty}^{\infty}e^{-2ax^2}dx=1 \tag{5}$$

The integral is a standard Gaussian integral which you can look up, or do with Maple. We have

$$\int_{-\infty}^{\infty} e^{-2ax^2}dx = \sqrt{\frac{2\pi}{a}} \tag{6}$$

so we must have

$$\begin{aligned} A &= \left(\frac{2a}{\pi}\right)^{1/4} \\ \psi(x,0) &= \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2} \end{aligned} \tag{7}$$

The wave function is then

$$\psi(x,t) = \sqrt{\frac{m}{2\pi i\hbar t}}\left(\frac{2a}{\pi}\right)^{1/4}\int_{-\infty}^{\infty} dx'\; e^{i(x-x')^2 m/2\hbar t}e^{-ax'^2} \tag{8}$$

We can do the integral using Maple, with the result (after cancelling a few terms common to numerator and denominator):

$$\psi(x,t) = \left(\frac{2a}{\pi}\right)^{1/4}\sqrt{\frac{-im}{2a\hbar t - im}}\exp\left[-\frac{iamx^2}{im-2a\hbar t}\right] \tag{9}$$

We need to clean this up a bit to get the answer typically found in books. Multiply the fraction in the square root by $\frac{i/m}{i/m}$ to get

$$\psi(x,t) = \left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1+2ia\hbar t/m}}\exp\left[-\frac{iamx^2}{im-2a\hbar t}\right] \tag{10}$$

Finally, multiply the exponent by $\frac{-i/m}{-i/m}$ to get the final result:

$$\psi(x,t) = \left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1+2ia\hbar t/m}}\exp\left[-\frac{ax^2}{1+2ia\hbar t/m}\right] \tag{11}$$

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:

$$\psi^*(x,t) = \left(\frac{2a}{\pi}\right)^{1/4}\frac{e^{-ax^2/(1-2i\hbar at/m)}}{\sqrt{1-2i\hbar at/m}} \tag{12}$$

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

$$
\begin{aligned}
|\psi(x,t)|^2 &= \sqrt{\frac{2a}{\pi}}\frac{e^{-2ax^2/\left[1+(2\hbar at/m)^2\right]}}{\sqrt{1+(2\hbar at/m)^2}} && (13)\\
&= \sqrt{\frac{2}{\pi}}we^{-2w^2x^2} && (14)
\end{aligned}
$$

with

$$w \equiv \left(\frac{a}{1+(2\hbar at/m)^2}\right)^{1/2} \tag{15}$$

At $t=0$, $w=\sqrt{a}$, so $|\psi(x,t)|^2 = \sqrt{2a/\pi}e^{-2ax^2}$ which is correct (by comparing with 7). 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. Fig. 1 shows $|\psi(x,t)|^2$ for 3 values of w, showing how the wave packets spreads as t increases (and thus w decreases).

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.

$$
\begin{aligned}
\langle x^2\rangle &= \int_{-\infty}^{\infty} x^2|\psi(x,t)|^2 dx && (16)\\
&= \frac{1}{4w^2} && (17)\\
&= \frac{1+(2\hbar at/m)^2}{4a} && (18)
\end{aligned}
$$

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:

$$\langle p^2\rangle = -\hbar^2\int_{-\infty}^{\infty}\psi^*\frac{\partial^2}{\partial x^2}\psi dx \tag{19}$$

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

$$\langle p^2\rangle = a\hbar^2 \tag{20}$$

The uncertainty principle thus becomes

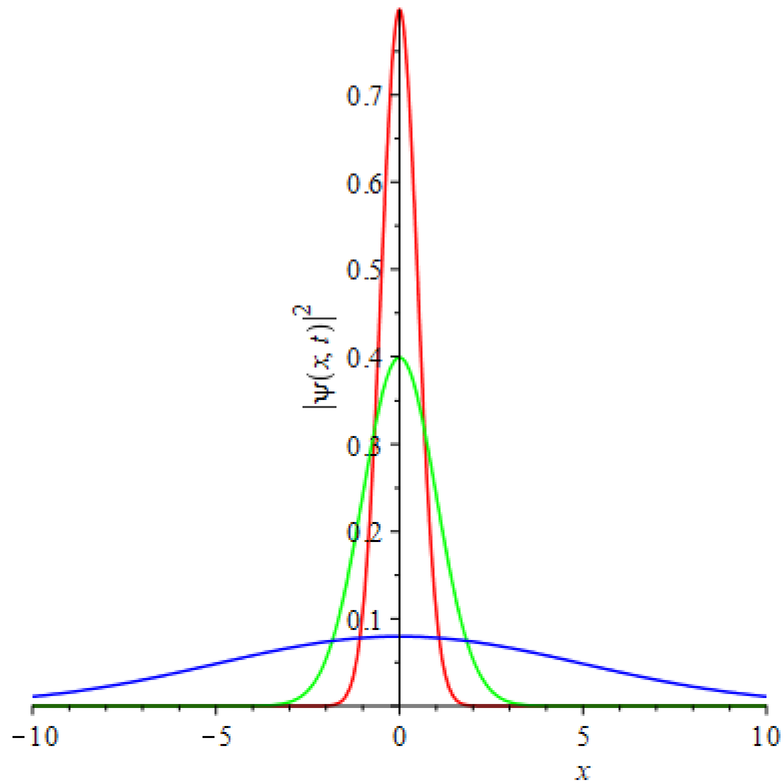

FIGURE 1. Plots of $|\Psi(x,t)|^2$ versus x for $w = 1$ (red), $w = 0.5$ (green) and $w = 0.1$ (blue).

$$\sigma_x \sigma_p = \sqrt{\langle x^2 \rangle \langle p^2 \rangle} \tag{21}$$

$$= \frac{\hbar}{2}\sqrt{1 + (2\hbar a t/m)^2} \tag{22}$$

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

REFERENCES

(1) Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press, Chapter 5.
(2) Berman, Paul R. (2018), *Introductory Quantum Mechanics*, Springer, Chapter 3.

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