FREE PARTICLE AS MOVING GAUSSIAN WAVE PACKET

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Previously, we looked at the free particle as a stationary Gaussian wave packet. We used the free particle propagator which is, for $t_0 = 0$:

$$U\left(x,x',t\right) = \sqrt{\frac{m}{2\pi i\hbar t}}e^{i(x-x')^2 m/2\hbar t} \tag{1}$$

With this propagator and the initial state $\psi\left(x',0\right)$ of the wave function, we can find the wave function at future times with the formula

$$\psi\left(x,t\right) = \int dx'\, U\left(x,x',t\right)\psi\left(x',0\right) \tag{2}$$

The static wave packet has the initial condition

$$\psi(x',0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax'^2} \tag{3}$$

where the constant $\left(\frac{2a}{\pi}\right)^{1/4}$ ensures that the wave function is normalized. The parameter a describes the initial spread of the Gaussian function.

To introduce some motion into the wave packet, we can use the initial state

$$\psi(x',0) = \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax'^2} e^{ip_0 x'/\hbar} \tag{4}$$

where p_0 is the initial momentum, so the particle moves with speed

$$v_0 = \frac{p_0}{m} \tag{5}$$

Since the extra term $e^{ip_0 x'/\hbar}$ has a purely imaginary exponent, the normalization is unaffected.

To work out the wave function we 'just' have to plug 1 and 4 into 2 and work out the integral. I have tried this several ways and cannot reproduce the wave functions quoted in Shankar and Berman, but perhaps a perceptive reader can spot where I have gone wrong.

The integral we need to do is

$$\psi(x,t)=\sqrt{\frac{m}{2\pi i\hbar t}}\left(\frac{2a}{\pi}\right)^{1/4}\int dx'\ e^{i(x-x')^2m/2\hbar t}e^{-ax'^2}e^{ip_0x'/\hbar} \tag{6}$$

We can add up the exponents, expand the brackets and collect terms to give a quadratic in x' to give for the exponent:

$$\text{exponent}=\left(-a+\frac{im}{2\hbar t}\right)x'^2+\frac{i}{\hbar}\left(p_0-\frac{mx}{t}\right)x'+i\frac{mx^2}{2\hbar t} \tag{7}$$

Thus the integral is

$$\int_{-\infty}^{\infty}dx'\ e^{-Ax'^2+Bx+C} \tag{8}$$

with

$$\begin{aligned}A&\equiv a-\frac{im}{2\hbar t}\\ B&\equiv\frac{i}{\hbar}\left(p_0-\frac{mx}{t}\right)\\ C&\equiv i\frac{mx^2}{2\hbar t}\end{aligned} \tag{9}$$

This is a standard Gaussian integral, which has the value (tabulated, or use Maple):

$$\int_{-\infty}^{\infty}dx'\ e^{-Ax'^2+Bx'+C}=\sqrt{\frac{\pi}{A}}e^{B^2/4A+C} \tag{10}$$

The exponent comes out to (after simplifying a bit):

$$\frac{B^2}{4A}+C=\frac{(mx-p_0t)^2}{2\hbar t\,(im-2a\hbar t)}+i\frac{mx^2}{2\hbar t} \tag{11}$$

$$=\frac{(x-p_0t/m)^2}{2\hbar t\,(im-2a\hbar t)/m^2}+i\frac{mx^2}{2\hbar t} \tag{12}$$

The constant in front comes out to

$$\sqrt{\frac{m}{2\pi i\hbar t}}\left(\frac{2a}{\pi}\right)^{1/4}\sqrt{\frac{\pi}{A}}=\left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1-2ia\hbar t/m}} \tag{13}$$

Thus the wave function is

$$\psi(x,t)=\left(\frac{2a}{\pi}\right)^{1/4}\frac{1}{\sqrt{1-2ia\hbar t/m}}\exp\left[\frac{(x-p_0t/m)^2}{2\hbar t(im-2a\hbar t)/m^2}+i\frac{mx^2}{2\hbar t}\right] \tag{14}$$

We can check a few things to see if this makes sense. The probability density is (again, I'm using Maple for the calculations):

$$|\psi(x,t)|^2=\sqrt{\frac{2a}{\pi\left(1+(2\hbar at/m)^2\right)}}\exp\left[\frac{-2(x-p_0t/m)^2a}{1+(2\hbar at/m)^2}\right] \tag{15}$$

Using Maple, we can verify that

$$\int_{-\infty}^{\infty}dx\ |\psi(x,t)|^2=1 \tag{16}$$

which is encouraging.

We can now calculate a few properties of the wave packet. We have

$$\langle x\rangle=\int_{-\infty}^{\infty}dx\ \psi^*(x,t)\,x\psi(x,t)=\frac{p_0t}{m}=v_0t \tag{17}$$

which shows that the mean position of the packet moves at a constant speed v_0.

For the momentum, we have

$$\langle p\rangle=\frac{\hbar}{i}\int_{-\infty}^{\infty}dx\ \psi^*(x,t)\frac{\partial}{\partial x}[\psi(x,t)]=p_0 \tag{18}$$

In other words, the momentum stays constant with time.

How about the variances? We have

$$\left\langle x^2\right\rangle=\int_{-\infty}^{\infty}dx\ \psi^*(x,t)\,x^2\psi(x,t) \tag{19}$$

$$=\frac{1+\left[(2\hbar at)^2+4ap_0^2t^2\right]/m^2}{4a} \tag{20}$$

Comparing this with the result we had for the stationary packet, which is

$$\left\langle x^2\right\rangle=\frac{1+(2\hbar at/m)^2}{4a} \tag{21}$$

we see that the formulas agree for $p_0=0$. Having an extra term involving p_0 causes $\left\langle x^2\right\rangle$ to increase faster with time.

For the momentum, we have

$$\left\langle p^2\right\rangle = -\hbar^2\int_{-\infty}^{\infty}dx\;\psi^*(x,t)\frac{\partial^2}{\partial x^2}[\psi(x,t)] \tag{22}$$
$$= a\hbar^2+p_0^2 \tag{23}$$

which again reduces to the stationary case with $p_0=0$.

The uncertainty is then

$$(\Delta x)^2(\Delta p)^2 = \left(\left\langle x^2\right\rangle-\langle x\rangle^2\right)\left(\left\langle p^2\right\rangle-\langle p\rangle^2\right) \tag{24}$$
$$= \frac{\hbar^2}{4}\left(1+(2\hbar at/m)^2\right) \tag{25}$$

so the uncertainty is the square root of this, or

$$(\Delta x)(\Delta p) = \frac{\hbar}{2}\sqrt{1+(2\hbar at/m)^2} \tag{26}$$

which is the same as in the stationary case.

Thus the travelling Gaussian wave packet behaves just like the stationary one, except that it moves with speed v_0.

Returning to 14, the reason I'm uncertain about this result is that the books I've looked in have a term like

$$e^{ip_0(x-p_0t/m)/\hbar} \tag{27}$$

in place of the $\exp\left[i\frac{mx^2}{2\hbar t}\right]$ term in 14. Try as I might, I cannot see where this term comes from. Given that all the properties of position and momentum appear correct with my solution, I'm inclined to think that I have got it right, but please do leave a comment if you can see anything wrong.

References

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

Comments

From hugin; 18 Mar 2021, 11:44.

Hi, and thank you for these notes. Two comments:

a) The extra term comparing 20 to 21 is just the contribution from the wavepacket center motion: ${p_0}^2t^2/m^2$. This is an artifact of the wavepacket's motion relative to the coordinate system. So instead of your comment after

21, that a moving wavepacket spreads faster, I think a more correct interpretation would be that exp$((x^2–p_0t/m))$ = (the non-moving variance). In other words, the moving Gaussian spreads just as rapidly as the non-moving Gaussian, but in 20 looks different because it picks up the wavepacket motion relative to the coordinate system. By the way, one often introduces a symbol for 20, e.g. $a^2(t)$. This simplified expressions like 14 quite a bit, making them more readily interpretable.

b) Eq. 14 is indeed correct, and you can transform it into an expression containing 27 by expanding and then re-completing the square to collect all x^2 terms inside one parenthesis in the exponent of 14. I agree it's not an easy square-completion, but it checks out. A way to obtain a result with 27 directly from calculation is to do inverse Fourier transforming the momentum-space wavepacket, where the time evolution is diagonal. (See e.g. https://quantummechanics.ucsd.edu/ph130a/130_notes/node83.html).