

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 $t_0 = 0$:

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

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

$$\psi(x, t) = \int dx' U(x, x', t) \psi(x', 0) \quad (2)$$

The static wave packet has the initial condition

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

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

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

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

$$v_0 = \frac{p_0}{m} \quad (5)$$

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

$$\psi(x, t) = \sqrt{\frac{m}{2\pi i \hbar t}} \left(\frac{2a}{\pi}\right)^{1/4} \int dx' e^{i(x-x')^2 m/2\hbar t} e^{-ax'^2} e^{ip_0 x'/\hbar} \quad (6)$$

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

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

Thus the integral is

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

with

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

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

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

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

$$\frac{B^2}{4A} + C = \frac{(mx - p_0 t)^2}{2\hbar t (im - 2a\hbar t)} + i \frac{mx^2}{2\hbar t} \quad (11)$$

$$= \frac{(x - p_0 t/m)^2}{2\hbar t (im - 2a\hbar t)/m^2} + i \frac{mx^2}{2\hbar t} \quad (12)$$

The constant in front comes out to

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

Thus the wave function is

$$\psi(x, t) = \left(\frac{2a}{\pi}\right)^{1/4} \frac{1}{\sqrt{1 - 2ia\hbar t/m}} \exp\left[\frac{(x - p_0 t/m)^2}{2\hbar t(im - 2a\hbar t)/m^2} + i\frac{mx^2}{2\hbar t}\right] \quad (14)$$

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

$$|\psi(x, t)|^2 = \sqrt{\frac{2a}{\pi(1 + (2\hbar at/m)^2)}} \exp\left[\frac{-2(x - p_0 t/m)^2 a}{1 + (2\hbar at/m)^2}\right] \quad (15)$$

Using Maple, we can verify that

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

which is encouraging.

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

$$\langle x \rangle = \int_{-\infty}^{\infty} dx \psi^*(x, t) x \psi(x, t) = \frac{p_0 t}{m} = v_0 t \quad (17)$$

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

For the momentum, we have

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

In other words, the momentum stays constant with time.

How about the variances? We have

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

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

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

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

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

For the momentum, we have

$$\langle p^2 \rangle = -\hbar^2 \int_{-\infty}^{\infty} dx \psi^*(x, t) \frac{\partial^2}{\partial x^2} [\psi(x, t)] \quad (22)$$

$$= a\hbar^2 + p_0^2 \quad (23)$$

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

The uncertainty is then

$$(\Delta x)^2 (\Delta p)^2 = \left(\langle x^2 \rangle - \langle x \rangle^2 \right) \left(\langle p^2 \rangle - \langle p \rangle^2 \right) \quad (24)$$

$$= \frac{\hbar^2}{4} \left(1 + (2\hbar at/m)^2 \right) \quad (25)$$

so the uncertainty is the square root of this, or

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

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

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

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.