# EXERCISE 18
# Free-particle Gaussian wave packet

The general expression for the wave function of a free particle is given by

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) \exp\left[ik\left(x - \frac{\hbar k}{2m}t\right)\right] dk \,.$$

Suppose the function $\phi(k)$ has a Gaussian form:

$$\phi(k) = \frac{\sqrt{\sigma}}{\pi^{1/4}} \exp\left[-\frac{\sigma^2}{2}\left(k - \frac{p}{\hbar}\right)^2\right] .$$

Here, $p$ and $\sigma > 0$ are real parameters.

1. Substitute $\phi(k)$ into the general expression for $\Psi(x,t)$ and evaluate the $k$-integral to demonstrate that

   $$\Psi(x,t) = \frac{1}{\pi^{1/4}\sqrt{\alpha\sigma}} \exp\left[-\frac{1}{2\alpha\sigma^2}\left(x - \frac{pt}{m}\right)^2 + i\frac{px}{\hbar} - i\frac{p^2 t}{2\hbar m}\right] ,$$

   where

   $$\alpha = 1 + i\frac{\hbar t}{m\sigma^2} \,.$$

2. Verify that $\Psi(x,t)$ is normalized to unity.

3. Calculate the expectation values of the particle's position and momentum, $\langle x\rangle$ and $\langle p\rangle$.

4. Calculate the corresponding uncertainties, $\Delta x$ and $\Delta p$. Explicitly confirm that the product of the uncertainties is consistent with the Heisenberg uncertainty principle.

# Solution

1. Substituting $\phi(k)$ into the general expression for $\Psi(x,t)$, we have

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} \underbrace{\frac{\sqrt{\sigma}}{\pi^{1/4}}\exp\left[-\frac{\sigma^2}{2}\left(k-\frac{p}{\hbar}\right)^2\right]}_{\phi(k)} \exp\left[ik\left(x-\frac{\hbar k}{2m}t\right)\right]\,dk \\ &= \frac{1}{\pi^{1/4}}\sqrt{\frac{\sigma}{2\pi}}\int_{-\infty}^{+\infty}\exp\underbrace{\left[-\frac{\sigma^2}{2}\left(k-\frac{p}{\hbar}\right)^2 + ik\left(x-\frac{\hbar k}{2m}t\right)\right]}_{Z}\,dx\,.\end{aligned}$$

The argument of the exponential in the last expression can be rewritten as

$$\begin{aligned}Z &= -\frac{\sigma^2}{2}\left(k^2-\frac{2p}{\hbar}k+\frac{p^2}{\hbar^2}\right)+ikx-i\frac{\hbar t}{2m}k^2 \\ &= -\frac{\sigma^2}{2}\underbrace{\left(1+\frac{\hbar t}{m\sigma^2}\right)}_{\alpha}k^2+\left(\frac{\sigma^2 p}{\hbar}+ix\right)k-\frac{\sigma^2p^2}{2\hbar^2}\,.\end{aligned}$$

Consequently,

$$\Psi(x,t) = \frac{1}{\pi^{1/4}}\sqrt{\frac{\sigma}{2\pi}}\int_{-\infty}^{+\infty}\exp\left[-\frac{\alpha\sigma^2}{2}k^2+\left(\frac{\sigma^2p}{\hbar}+ix\right)k-\frac{\sigma^2p^2}{2\hbar^2}\right]dx\,.$$

Using the integral

$$\int_{-\infty}^{+\infty}e^{-ax^2+bx}\,dx=\sqrt{\frac{\pi}{a}}\,e^{b^2/4a} \qquad (\operatorname{Re}a>0)\,,$$

we get

$$\begin{aligned}\Psi(x,t) &= \frac{1}{\pi^{1/4}}\sqrt{\frac{\sigma}{2\pi}}\sqrt{\frac{2\pi}{\alpha\sigma^2}}\exp\left[\frac{\left(\frac{\sigma^2p}{\hbar}+ix\right)^2}{2\alpha\sigma^2}-\frac{\sigma^2p^2}{2\hbar^2}\right] \\ &= \frac{1}{\pi^{1/4}\sqrt{\alpha\sigma}}\exp\underbrace{\left[-\frac{1}{2\alpha\sigma^2}\left(x-i\frac{\sigma^2p}{\hbar}\right)^2-\frac{\sigma^2p^2}{2\hbar^2}\right]}_{W}\,. \qquad (1)\end{aligned}$$

The argument of the exponential function can be rewritten as

$$\begin{aligned}
W &= -\frac{1}{2\alpha\sigma^2}\left(x-\frac{pt}{m}+\frac{pt}{m}-i\frac{\sigma^2 p}{\hbar}\right)^2-\frac{\sigma^2p^2}{2\hbar^2}\\
&= -\frac{1}{2\alpha\sigma^2}\left[x-\frac{pt}{m}-i\frac{\sigma^2 p}{\hbar}\underbrace{\left(1+i\frac{\hbar t}{m\sigma^2}\right)}_{\alpha}\right]^2-\frac{\sigma^2p^2}{2\hbar^2}\\
&= -\frac{1}{2\alpha\sigma^2}\left(x-\frac{pt}{m}-i\frac{\alpha\sigma^2 p}{\hbar}\right)^2-\frac{\sigma^2p^2}{2\hbar^2}\\
&= -\frac{1}{2\alpha\sigma^2}\left\{\left(x-\frac{pt}{m}\right)^2-2\left(x-\frac{pt}{m}\right)i\frac{\alpha\sigma^2 p}{\hbar}-\frac{\alpha^2\sigma^4p^2}{\hbar^2}\right\}-\frac{\sigma^2p^2}{2\hbar^2}\\
&= -\frac{1}{2\alpha\sigma^2}\left(x-\frac{pt}{m}\right)^2+i\left(x-\frac{pt}{m}\right)\frac{p}{\hbar}+\frac{\alpha\sigma^2p^2}{2\hbar^2}-\frac{\sigma^2p^2}{2\hbar^2}\\
&= -\frac{1}{2\alpha\sigma^2}\left(x-\frac{pt}{m}\right)^2+i\frac{px}{\hbar}-i\frac{p^2t}{m\hbar}+\underbrace{(\alpha-1)}_{i\hbar t/m\sigma^2}\frac{\sigma^2p^2}{2\hbar^2}\\
&= -\frac{1}{2\alpha\sigma^2}\left(x-\frac{pt}{m}\right)^2+i\frac{px}{\hbar}-i\frac{p^2t}{m\hbar}+i\frac{\hbar t}{m\sigma^2}\frac{\sigma^2p^2}{2\hbar^2}\\
&= -\frac{1}{2\alpha\sigma^2}\left(x-\frac{pt}{m}\right)^2+i\frac{px}{\hbar}-i\frac{p^2t}{2m\hbar}\,.
\end{aligned}$$

Finally, substituting $W$ into Eq. (1), we arrive at the desired expression for the particle's wave function:

$$\boxed{\Psi(x,t)=\frac{1}{\pi^{1/4}\sqrt{\alpha\sigma}}\exp\left[-\frac{1}{2\alpha\sigma^2}\left(x-\frac{pt}{m}\right)^2+i\frac{px}{\hbar}-i\frac{p^2t}{2\hbar m}\right]}$$

2. The probability density of the particle is given by

$$\begin{aligned}
|\Psi(x,t)|^2 &= \Psi^*(x,t)\Psi(x,t)\\
&= \frac{1}{\sigma\sqrt{\pi\alpha^*\alpha}}\exp\left[-\frac{1}{2\sigma^2}\left(\frac{1}{\alpha}+\frac{1}{\alpha^*}\right)\left(x-\frac{pt}{m}\right)^2\right]\\
&= \frac{1}{\sqrt{\pi}|\alpha|\sigma}\exp\left[-\frac{\alpha+\alpha^*}{2|\alpha|^2\sigma^2}\left(x-\frac{pt}{m}\right)^2\right]\,.
\end{aligned}$$

Since

$$\alpha+\alpha* = 2\,,$$

we have

$$|\Psi(x,t)|^2 = \frac{1}{\sqrt{\pi}|\alpha|\sigma} \exp\left[-\frac{1}{|\alpha|^2\sigma^2}\left(x - \frac{pt}{m}\right)^2\right]. \tag{2}$$

Then, the normalization integral reads

$$\begin{aligned}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx &= \frac{1}{\sqrt{\pi}|\alpha|\sigma}\int_{-\infty}^{+\infty} \exp\left[-\frac{1}{|\alpha|^2\sigma^2}\left(x - \frac{pt}{m}\right)^2\right] dx \\ &= \frac{1}{\sqrt{\pi}|\alpha|\sigma}\sqrt{\pi|\alpha|^2\sigma^2} \\ &= 1\,.\end{aligned}$$

Therefore, the wave function is indeed properly normalized.

3. The probability density, Eq. (2), is symmetric about $x = pt/m$. Therefore, the expectation value of the particle's position is given by (see EXERCISE 3)

$$\boxed{\langle x\rangle = \frac{pt}{m}}$$

The expectation value of the particle's momentum can be calculated as follows. Since

$$\frac{\partial\Psi(x,t)}{\partial x} = \left[-\frac{1}{\alpha\sigma^2}\left(x - \frac{pt}{m}\right) + i\frac{p}{\hbar}\right]\Psi(x,t)\,,$$

we have

$$\begin{aligned}\langle p\rangle &= -i\hbar\int_{-\infty}^{+\infty} \Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial x}\, dx \\ &= -i\hbar\int_{-\infty}^{+\infty} \Psi^*(x,t)\left[-\frac{1}{\alpha\sigma^2}\left(x - \frac{pt}{m}\right) + i\frac{p}{\hbar}\right]\Psi(x,t) \\ &= \frac{i\hbar}{\alpha\sigma^2}\int_{-\infty}^{+\infty}\left(x - \frac{pt}{m}\right)|\Psi(x,t)|^2\, dx + p\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx\,.\end{aligned}$$

The first integral in the last expression vanishes, as the integrand is an odd (antisymmetric) function of $x - pt/\hbar$. The second integral equals one in accordance with the normalization condition satisfied by $\Psi$. Therefore,

$$\boxed{\langle p\rangle = p}$$

An alternative (and quicker!) way to arrive at the same conclusion is to use the definition of the mean momentum:

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} = m\frac{d}{dt}\left(\frac{pt}{m}\right) = p\,.$$

4. The uncertainty in position, $\Delta x$, is calculated as follows:

$$\begin{aligned}(\Delta x) &= \int_{-\infty}^{+\infty} \Psi^*(x,t)\,(x-\langle x\rangle)^2\,\Psi(x,t)\,dx \\ &= \int_{-\infty}^{+\infty} \left(x-\frac{pt}{m}\right)^2 |\Psi(x,t)|^2\,dx \\ &= \int_{-\infty}^{+\infty} \left(x-\frac{pt}{m}\right)^2 \frac{1}{\sqrt{\pi}|\alpha|\sigma} \exp\left[-\frac{1}{|\alpha|^2\sigma^2}\left(x-\frac{pt}{m}\right)^2\right] dx\,.\end{aligned}$$

Changing the integration variable to

$$y = \frac{1}{|\alpha|\sigma}\left(x-\frac{pt}{m}\right)\,,$$

we get

$$(\Delta x)^2 = \frac{|\alpha|^2\sigma^2}{\sqrt{\pi}} \underbrace{\int_{-\infty}^{+\infty} y^2 e^{-y^2}\,dx}_{\sqrt{\pi}/2} = \frac{|\alpha|^2\sigma^2}{2}\,.$$

Taking into account that

$$|\alpha|^2 = \left|1+i\frac{\hbar t}{m\sigma^2}\right|^2 = 1+\left(\frac{\hbar t}{m\sigma^2}\right)^2\,,$$

we obtain

$$\boxed{\Delta x = \frac{\sigma}{\sqrt{2}}\sqrt{1+\left(\frac{\hbar t}{m\sigma^2}\right)^2}}$$

To calculate the uncertainty in momentum, $\Delta p$, we start from the definition:

$$\begin{aligned}(\Delta p)^2 &= \int_{-\infty}^{+\infty} \Psi^*(x,t)\,(\hat{p}-\langle p\rangle)^2\,\Psi(x,t)\,dx \\ &= \int_{-\infty}^{+\infty} \Psi^*(x,t)\left(-i\hbar\frac{\partial}{\partial x}-p\right)^2 \Psi(x,t)\,dx\,.\end{aligned}$$

Then,

$$\begin{aligned}\left(-i\hbar\frac{\partial}{\partial x}-p\right)\Psi &= -i\hbar\frac{\partial\Psi}{\partial x}-p\Psi \\ &= -i\hbar\left[-\frac{1}{\alpha\sigma^2}\left(x-\frac{pt}{m}\right)+i\frac{p}{\hbar}\right]\Psi-p\Psi \\ &= \frac{i\hbar}{\alpha\sigma^2}\left(x-\frac{pt}{m}\right)\Psi\,,\end{aligned}$$

and

$$\begin{aligned}
\left(-i\hbar\frac{\partial}{\partial x}-p\right)^2\Psi &= \left(-i\hbar\frac{\partial}{\partial x}-p\right)\underbrace{\left(-i\hbar\frac{\partial}{\partial x}-p\right)\Psi}_{\text{calculated above}} \\
&= \left(-i\hbar\frac{\partial}{\partial x}-p\right)\frac{i\hbar}{\alpha\sigma^2}\left(x-\frac{pt}{m}\right)\Psi \\
&= \frac{i\hbar}{\alpha\sigma^2}\left\{-i\hbar\frac{\partial}{\partial x}\left(x-\frac{pt}{m}\right)\Psi - p\left(x-\frac{pt}{m}\right)\Psi\right\} \\
&= \frac{i\hbar}{\alpha\sigma^2}\left\{-i\hbar\Psi - i\hbar\left(x-\frac{pt}{m}\right)\frac{\partial\Psi}{\partial x} - p\left(x-\frac{pt}{m}\right)\Psi\right\} \\
&= \frac{i\hbar}{\alpha\sigma^2}\left\{-i\hbar\Psi + \left(x-\frac{pt}{m}\right)\underbrace{\left(-i\hbar\frac{\partial}{\partial x}-p\right)\Psi}_{\text{calculated above}}\right\} \\
&= \frac{i\hbar}{\alpha\sigma^2}\left\{-i\hbar\Psi + \left(x-\frac{pt}{m}\right)\frac{i\hbar}{\alpha\sigma^2}\left(x-\frac{pt}{m}\right)\Psi\right\} \\
&= \frac{\hbar^2}{\alpha\sigma^2}\Psi - \frac{\hbar^2}{\alpha^2\sigma^4}\left(x-\frac{pt}{m}\right)^2\Psi\,.
\end{aligned}$$

Hence,

$$\begin{aligned}
(\Delta p)^2 &= \int_{-\infty}^{+\infty}\Psi^*\left(-i\hbar\frac{\partial}{\partial x}-p\right)^2\Psi\,dx \\
&= \frac{\hbar^2}{\alpha\sigma^2}\underbrace{\int_{-\infty}^{+\infty}|\Psi|^2\,dx}_{1} - \frac{\hbar^2}{\alpha^2\sigma^4}\underbrace{\int_{-\infty}^{+\infty}\left(x-\frac{pt}{m}\right)^2|\Psi|^2\,dx}_{(\Delta x)^2} \\
&= \frac{\hbar^2}{\alpha\sigma^2} - \frac{\hbar^2}{\alpha^2\sigma^4}\frac{|\alpha|^2\sigma^2}{2} \\
&= \frac{2-\alpha^*}{\alpha}\frac{\hbar^2}{2\sigma^2}\,.
\end{aligned}$$

Finally, since

$$2-\alpha^* = \alpha\,,$$

we arrive at

$$\boxed{\Delta p = \frac{\hbar}{\sqrt{2}\sigma}}$$

The product of the uncertainties in position and momentum is no smaller than

Heisenberg's threshold, $\hbar/2$. Indeed,

$$\Delta x \Delta p = \frac{\sigma}{\sqrt{2}}\sqrt{1+\left(\frac{\hbar t}{m\sigma^2}\right)^2}\,\frac{\hbar}{\sqrt{2}\sigma} = \frac{\hbar}{2}\sqrt{1+\left(\frac{\hbar t}{m\sigma^2}\right)^2} \geq \frac{\hbar}{2}\,.$$

At $t = 0$, our Gaussian wave packet represents a minimal-uncertainty state for which $\Delta x \Delta p = \hbar/2$.