The Gaussian Wavepacket

A useful integral

First, verify the "completed" square:

$$-a\left[x-\frac{b}{2a}\right]^2+\frac{b^2}{4a}=-a\left[x^2-\frac{b}{a}x+\frac{b^2}{4a^2}\right]+\frac{b^2}{4a}=-ax^2+bx.$$

Now use this expression in the integral

$$\begin{aligned}
\int_{-\infty}^{+\infty} e^{-ax^2+bx}\,dx &= \int_{-\infty}^{+\infty} e^{-a[x-b/(2a)]^2+b^2/(4a)}\,dx \\
&= e^{b^2/(4a)}\int_{-\infty}^{+\infty} e^{-a[x-b/(2a)]^2}\,dx \\
&\quad \text{change variable to } y=x-b/(2a)\text{, giving} \ldots \\
&= e^{b^2/(4a)}\int_{-\infty}^{+\infty} e^{-ay^2}\,dy \\
&\quad \text{change variable again to } u=\sqrt{a}y\text{, giving} \ldots \\
&= e^{b^2/(4a)}\frac{1}{\sqrt{a}}\int_{-\infty}^{+\infty} e^{-u^2}\,du \\
&\quad \text{recognize the given integral, giving} \ldots \\
&= \sqrt{\frac{\pi}{a}}e^{b^2/(4a)}. \qquad (1)
\end{aligned}$$

⟦*Grading:* 2 points for verifying the completed square, 2 points for coming up with the change of variable, 6 points for evaluating the integral. Any different correct strategy earns full credit.⟧

A somewhat less useful integral

Integrate by parts using

$$\begin{aligned}
u &= x & dv &= xe^{-x^2}\,dx \\
du &= dx & v &= -\tfrac{1}{2}e^{-x^2}
\end{aligned}$$

whence

$$\begin{aligned}
\int_{-\infty}^{+\infty} x^2e^{-x^2}\,dx &= \int_{-\infty}^{+\infty} x(xe^{-x^2})\,dx \\
&= -\tfrac{1}{2}\,xe^{-x^2}\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} -\tfrac{1}{2}e^{-x^2}\,dx \\
&= 0-0+\tfrac{1}{2}\int_{-\infty}^{+\infty} e^{-x^2}\,dx \\
&= \frac{\sqrt{\pi}}{2}. \qquad (2)
\end{aligned}$$

⟦*Grading:* 10 points. Any different correct strategy, for example parametric differentiation from the "useful integral" (1), earns full credit.⟧

Static properties of a Gaussian wavepacket

a. Normalization:

$$\begin{aligned}
\psi_0(x) &= \frac{A}{\sqrt{\sigma}} e^{-x^2/\sigma^2} e^{ip_0 x/\hbar} \\
|\psi_0(x)|^2 &= \frac{A^2}{\sigma} e^{-2x^2/\sigma^2} \qquad (3)\\
1 &= \int_{-\infty}^{+\infty} |\psi_0(x)|^2\,dx = \frac{A^2}{\sigma}\int_{-\infty}^{+\infty} e^{-2x^2/\sigma^2}\,dx = \frac{A^2}{\sigma}\sqrt{\frac{\pi\sigma^2}{2}} = A^2\sqrt{\frac{\pi}{2}}
\end{aligned}$$

so

$$A = \sqrt[4]{\frac{2}{\pi}}. \qquad (4)$$

b. Mean and indeterminacy in x:

$$\langle \hat{x} \rangle = \int_{-\infty}^{+\infty} x|\psi_0(x)|^2\,dx = \frac{A^2}{\sigma}\int_{-\infty}^{+\infty} xe^{-2x^2/\sigma^2}\,dx = 0 \quad \text{because integrand is odd.}$$

$$\begin{aligned}
\langle \hat{x}^2 \rangle &= \int_{-\infty}^{+\infty} x^2|\psi_0(x)|^2\,dx \\
&= \frac{A^2}{\sigma}\int_{-\infty}^{+\infty} x^2 e^{-2x^2/\sigma^2}\,dx \\
&\quad \text{change variable to } u = \sqrt{2}x/\sigma, \text{ giving } \ldots \\
&= \frac{A^2}{\sigma}\left(\frac{\sigma}{\sqrt{2}}\right)^3 \int_{-\infty}^{+\infty} u^2 e^{-u^2}\,du \\
&\quad \text{use ``a somewhat less useful integral'' (2), giving } \ldots \\
&= \frac{A^2}{\sigma}\left(\frac{\sigma}{\sqrt{2}}\right)^3 \frac{\sqrt{\pi}}{2} = \frac{\sigma^2}{4}.
\end{aligned}$$

And

$$(\Delta x)^2 = \langle \hat{x}^2 \rangle - \langle \hat{x} \rangle^2 = \langle \hat{x}^2 \rangle,$$

so

$$\Delta x = \sigma/2. \qquad (5)$$

c. Momentum representation of the wavefunction:

$$\begin{aligned}
\tilde{\psi}_0(p) &= \frac{1}{\sqrt{2\pi\hbar}}\int_{-\infty}^{+\infty} e^{-ipx/\hbar}\psi_0(x)\,dx \\
&= \frac{1}{\sqrt{2\pi\hbar}}\frac{A}{\sqrt{\sigma}}\int_{-\infty}^{+\infty} e^{-x^2/\sigma^2} e^{i(p_0-p)x/\hbar}\,dx.
\end{aligned}$$

Now use the "useful integral" (1) with $a = 1/\sigma^2$ and $b = i(p_0 - p)/\hbar$. Note that, as required, $\Re e\{a\} > 0$.

$$\begin{aligned}
\tilde{\psi}_0(p) &= \frac{1}{\sqrt{2\pi\hbar}}\frac{A}{\sqrt{\sigma}}\sqrt{\pi\sigma^2}\, e^{[-(p_0-p)^2/\hbar^2]/[4/\sigma^2]} \\
&= A\sqrt{\frac{\sigma}{2\hbar}} e^{-(p-p_0)^2\sigma^2/4\hbar^2}. \qquad (6)
\end{aligned}$$

d. Mean and indeterminacy in p:

$$|\tilde{\psi}_0(p)|^2 = \frac{A^2\sigma}{2\hbar} e^{-(p-p_0)^2\sigma^2/2\hbar^2}.$$

It's clear from inspection that this probability density is centered on p_0, and hence that $\langle\hat{p}\rangle = p_0$. If you feel compelled to produce a more algorithmic proof, then simply evaluate $\langle\hat{p} - p_0\rangle$, which is easily seen to vanish, to prove that $\langle\hat{p}\rangle = p_0$.

$$\begin{aligned}
(\Delta p)^2 &= \langle(\hat{p} - p_0)^2\rangle \\
&= \frac{A^2\sigma}{2\hbar} \int_{-\infty}^{+\infty} (p-p_0)^2 e^{-(p-p_0)^2\sigma^2/2\hbar^2}\, dp \\
& \quad \text{change variable to } u = (p-p_0)\sigma/\sqrt{2}\hbar, \text{ giving } \ldots \\
&= \frac{A^2\sigma}{2\hbar}\left(\frac{\sqrt{2}\hbar}{\sigma}\right)^3 \int_{-\infty}^{+\infty} u^2 e^{-u^2}\, du \\
&= \frac{A^2\sigma}{2\hbar}\left(\frac{\sqrt{2}\hbar}{\sigma}\right)^3 \frac{\sqrt{\pi}}{2} = \frac{\hbar^2}{\sigma^2}.
\end{aligned}$$

So

$$\Delta p = \frac{\hbar}{\sigma}. \tag{7}$$

⟦Once the momentum representation (6) is in hand, then these calculations are considerably easier than evaluating things like

$$\langle\hat{p}\rangle = \int_{-\infty}^{+\infty} \psi_0^*(x)\left[-i\hbar\frac{\partial\psi_0(x)}{\partial x}\right] dx. \quad ⟧$$

e. $\Delta x \Delta p = \hbar/2$ . . . this is a minimum indeterminacy wavepacket.

⟦*Grading:* 2 points each for **(a)** and **(b)**, 3 points each for **(c)** and **(d)**, zip for **(e)**.⟧

Force-free time evolution of a Gaussian wavepacket

a. From the time development of energy eigenstates,

$$\tilde{\psi}(p,t) = e^{-(i/\hbar)E(p)t}\, \tilde{\psi}_0(p),$$

where $E(p) = p^2/2m$. While from the properties of momentum wavefunctions,

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{+ipx/\hbar}\, \tilde{\psi}(p)\, dp.$$

Putting these together,

$$\begin{aligned}
\psi(x,t) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{i(px-E(p)t)/\hbar}\, \tilde{\psi}_0(p)\, dp \\
&= \frac{1}{\sqrt{2\pi\hbar}} A\sqrt{\frac{\sigma}{2\hbar}} \int_{-\infty}^{+\infty} e^{i(px-E(p)t)/\hbar} e^{-(p-p_0)^2\sigma^2/4\hbar^2}\, dp \\
&= \frac{A}{\hbar}\sqrt{\frac{\sigma}{4\pi}} \int_{-\infty}^{+\infty} e^{i(px-E(p)t)/\hbar} e^{-(p-p_0)^2\sigma^2/4\hbar^2}\, dp.
\end{aligned}$$

Use

$$\begin{aligned} p' &= p - p_0 \\ px - E(p)t &= (p' + p_0)x - \frac{1}{2m}(p' + p_0)^2 t \\ &= -p'^2 \frac{t}{2m} + p'\left(x - \frac{p_0}{m}t\right) + p_0 x - E(p_0)t \end{aligned}$$

to find

$$\begin{aligned} &\psi(x,t) \\ = \;& \frac{A}{\hbar}\sqrt{\frac{\sigma}{4\pi}} e^{i(p_0 x - E(p_0)t)/\hbar} \int_{-\infty}^{+\infty} \exp\left\{ i \left[-p'^2 \frac{t}{2m} + p'\left(x - \frac{p_0}{m}t\right)\right] \frac{1}{\hbar} \right\} e^{-p'^2\sigma^2/4\hbar^2}\, dp' \\ = \;& \frac{A}{\hbar}\sqrt{\frac{\sigma}{4\pi}} e^{i(p_0 x - E(p_0)t)/\hbar} \int_{-\infty}^{+\infty} \exp\left\{ -p'^2 \left(\frac{\sigma^2}{4\hbar^2} + i\frac{t}{2m\hbar} \right) + i\frac{p'}{\hbar}\left(x - \frac{p_0}{m}t\right) \right\} dp' \\ = \;& \frac{A}{\hbar}\sqrt{\frac{\sigma}{4\pi}} e^{i(p_0 x - E(p_0)t)/\hbar} \int_{-\infty}^{+\infty} \exp\left\{ -\frac{p'^2}{\hbar^2} \left(\frac{\sigma^2}{4} + i\frac{\hbar t}{2m} \right) + i\frac{p'}{\hbar}\left(x - \frac{p_0}{m}t\right) \right\} dp', \end{aligned}$$

which suggests the change of variable $k = p'/\hbar$ giving

$$\psi(x,t) = A\sqrt{\frac{\sigma}{4\pi}} e^{i(p_0 x - E(p_0)t)/\hbar} \int_{-\infty}^{+\infty} \exp\left\{ -k^2 \left(\frac{\sigma^2}{4} + i\frac{\hbar t}{2m} \right) + ik\left(x - \frac{p_0}{m}t\right) \right\} dk. \tag{8}$$

b. Within the curly brackets toward the right we recognize the quantity

$$x - \frac{p_0}{m}t,$$

which plucks our force-free motion heartstrings by reminding us of classical equations like

$$x(t) = \frac{p_0}{m}t.$$

But the quantity within the curly brackets toward the left doesn't pluck any heartstring of mine. Define the dimensionless quantity

$$\beta = 1 + i\frac{2\hbar}{\sigma^2 m}t$$

so the equation is

$$\psi(x,t) \;=\; A\sqrt{\frac{\sigma}{4\pi}} e^{i(p_0 x - E(p_0)t)/\hbar} \int_{-\infty}^{+\infty} \exp\left\{ -\frac{k^2\sigma^2\beta}{4} + ik\left(x - \frac{p_0}{m}t\right) \right\} dk.$$

Now use the "useful integral" (1) with $x = k$, $a = \sigma^2\beta/4$, and $b = i[x - (p_0/m)t]$. Note that, as required, $\Re e\{a\} = \sigma^2/4 > 0$.

$$\begin{aligned} \psi(x,t) &= A\sqrt{\frac{\sigma}{4\pi}} e^{i(p_0 x - E(p_0)t)/\hbar} \sqrt{\frac{4\pi}{\sigma^2\beta}} e^{-(x - \frac{p_0}{m}t)^2/\sigma^2\beta} \\ &= A\frac{1}{\sqrt{\sigma\beta}} e^{i(p_0 x - E(p_0)t)/\hbar} e^{-(x - \frac{p_0}{m}t)^2/\sigma^2\beta} \end{aligned} \tag{9}$$

c. We seek $|\psi(x,t)|^2 = \psi^*(x,t)\psi(x,t)$. Start off by computing, for $z = e^{-r/\beta}$, where r is real and β complex,

$$\begin{aligned}
|z|^2 &= z^* z = e^{-r/\beta} e^{-r/\beta^*} \\
&= \exp\left\{ -r\left(\frac{1}{\beta} + \frac{1}{\beta^*} \right) \right\} \\
&= \exp\left\{ -r\left(\frac{\beta^* + \beta}{\beta^* \beta} \right) \right\} \\
&= \exp\left\{ -r\left(\frac{2\Re e\{\beta\}}{|\beta|^2} \right) \right\}.
\end{aligned}$$

Thus

$$|\psi(x,t)|^2 = \frac{A^2}{\sigma\sqrt{\beta^*\beta}} \exp\left\{ -\left(x - \frac{p_0}{m}t \right)^2 \frac{1}{\sigma^2} \left(\frac{2\Re e\{\beta\}}{|\beta|^2} \right) \right\}.$$

But

$$|\beta|^2 = 1 + \left(\frac{2\hbar}{\sigma^2 m} t \right)^2 \qquad \text{and} \qquad \Re e\{\beta\} = 1$$

so

$$|\psi(x,t)|^2 = \frac{A^2}{\sigma|\beta|} e^{-2(x - \frac{p_0}{m}t)^2/\sigma^2|\beta|^2}. \tag{10}$$

This expression has exactly the same Gaussian form as $|\psi_0(x)|^2$, equation (3), except that

$$x \to x - \frac{p_0}{m}t \qquad \text{and} \qquad \sigma \to \sigma|\beta|,$$

where

$$|\beta| = \sqrt{1 + \left(\frac{2\hbar}{\sigma^2 m} t \right)^2}.$$

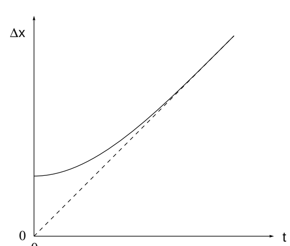
Thus the probability density remains always a Gaussian, but it is centered on

$$\langle \hat{x} \rangle_t = \frac{p_0}{m} t \tag{11}$$

and has position indeterminacy

$$(\Delta x)_t = \frac{\sigma}{2} \sqrt{1 + \left(\frac{2\hbar}{\sigma^2 m} t \right)^2}. \tag{12}$$

The center of the wavepacket moves exactly like a classical particle, but the indeterminacy spreads out.



⟦*Grading:* 3 points for **(a)**, 4 points for **(b)**, 3 points for **(c)**.⟧