The Gaussian Wavepacket

A useful integral

First, verify the "completed" square:

$$-\left(\frac{u\alpha}{\sqrt{2}} - i\frac{y}{\sqrt{2}\alpha}\right)^2 - \frac{y^2}{2\alpha^2} = -\left[\frac{u^2\alpha^2}{2} - 2\frac{u\alpha}{\sqrt{2}}\,i\frac{y}{\sqrt{2}\alpha} - \frac{y^2}{2\alpha^2}\right] - \frac{y^2}{2\alpha^2} = -\frac{u^2\alpha^2}{2} + iuy.$$

⟦*Technical note:* To assure convergence of the integral, we must have $\Re e\{\alpha^2\} > 0$. When we select a square root of α^2, we will always take one with $\Re e\{\alpha\} > 0$.⟧

$$\int_{-\infty}^{+\infty} \exp\left\{-\frac{u^2\alpha^2}{2} + iuy\right\} du = \exp\left\{-\frac{y^2}{2\alpha^2}\right\} \int_{-\infty}^{+\infty} \exp\left\{-\left(\frac{u\alpha}{\sqrt{2}} - i\frac{y}{\sqrt{2}\alpha}\right)^2\right\} du$$

Now change variable to

$$x = \left(\frac{u\alpha}{\sqrt{2}} - i\frac{y}{\sqrt{2}\alpha}\right),$$

giving

$$\begin{aligned}
\int_{-\infty}^{+\infty} \exp\left\{-\frac{u^2\alpha^2}{2} + iuy\right\} du &= e^{-y^2/2\alpha^2} \int_{-\infty}^{+\infty} e^{-x^2} \left(\frac{\sqrt{2}}{\alpha}\,dx\right) \\
&= \frac{\sqrt{2\pi}}{\alpha} e^{-y^2/2\alpha^2}. \qquad (1)
\end{aligned}$$

A somewhat less useful integral

$$\begin{aligned}
\int_{-\infty}^{+\infty} x^2 e^{-x^2}\,dx &= 2\int_0^\infty x^2 e^{-x^2}\,dx \\
&= 2\int_0^\infty x(xe^{-x^2})\,dx.
\end{aligned}$$

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

$$\begin{aligned}
\int_{-\infty}^{+\infty} x^2 e^{-x^2}\,dx &= 2\int_0^\infty x(xe^{-x^2})\,dx \\
&= 2\left[-\tfrac{1}{2}\,xe^{-x^2}\Big|_0^\infty - \int_0^\infty -\tfrac{1}{2}e^{-x^2}\,dx\right] \\
&= 2\left[0 - 0 + \tfrac{1}{2}\int_0^\infty e^{-x^2}\,dx\right] \\
&= \frac{\sqrt{\pi}}{2}. \qquad (2)
\end{aligned}$$

Static properties of a Gaussian wavepacket

a. Normalization:

$$\psi(x;0) = \frac{A}{\sqrt{\sigma}} e^{-x^2/2\sigma^2} e^{i(p_0/\hbar)x} \tag{3}$$

$$|\psi(x;0)|^2 = \frac{A^2}{\sigma} e^{-x^2/\sigma^2} \tag{4}$$

$$1 = \int_{-\infty}^{+\infty} |\psi(x;0)|^2\, dx = A^2 \int_{-\infty}^{+\infty} e^{-x^2/\sigma^2} \frac{dx}{\sigma} = A^2\sqrt{\pi} \qquad \text{so...}$$

$$A = \frac{1}{\sqrt[4]{\pi}}. \tag{5}$$

b. Mean and indeterminacy in x:

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

$$\begin{aligned}
\langle \hat{x}^2 \rangle &= \int_{-\infty}^{+\infty} x^2|\psi(x;0)|^2\, dx \\
&= \frac{A^2}{\sigma} \int_{-\infty}^{+\infty} x^2 e^{-x^2/\sigma^2}\, dx \qquad [\![\text{Use substitution } u = x/\sigma\ldots]\!] \\
&= A^2\sigma^2 \int_{-\infty}^{+\infty} u^2 e^{-u^2}\, du \qquad [\![\text{Use "A somewhat less useful integral" (2)}\ldots]\!] \\
&= A^2\sigma^2 \frac{\sqrt{\pi}}{2} = \frac{1}{\sqrt{\pi}}\sigma^2 \frac{\sqrt{\pi}}{2} = \frac{\sigma^2}{2}.
\end{aligned}$$

And

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

so

$$\Delta x = \sigma/\sqrt{2}. \tag{6}$$

c. Momentum representation of the wavefunction:

$$\begin{aligned}
\tilde{\psi}(p;0) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{-i(p/\hbar)x} \psi(x;0)\, dx \\
&= \frac{1}{\sqrt{2\pi\hbar}} \frac{A}{\sqrt{\sigma}} \int_{-\infty}^{+\infty} e^{-x^2/2\sigma^2} e^{i((p_0-p)/\hbar)x}\, dx.
\end{aligned}$$

Now use the "useful integral" (1) with $u = x$, $\alpha = 1/\sigma$, and $y = (p_0 - p)/\hbar$. Note that, as required, $\Re e\{\alpha\} > 0$.

$$\begin{aligned}
\tilde{\psi}(p;0) &= \frac{1}{\sqrt{2\pi\hbar}} \frac{A}{\sqrt{\sigma}} \frac{\sqrt{2\pi}}{1/\sigma} e^{-(p_0-p)^2\sigma^2/2\hbar^2} \\
&= A\sqrt{\frac{\sigma}{\hbar}} e^{-(p-p_0)^2\sigma^2/2\hbar^2}.
\end{aligned} \tag{7}$$

d. Mean and indeterminacy in p:

$$|\tilde{\psi}(p;0)|^2 = \frac{A^2\sigma}{\hbar} e^{-(p-p_0)^2\sigma^2/\hbar^2}.$$

It's clear from inspection that this probability density is centered on p_0, and hence that $\langle p \rangle = p_0$. 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 $\langle p \rangle = p_0$.

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

So

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

[[Once the momentum representation (7) is in hand, then these calculations are considerably easier than evaluating things like

$$\langle \hat{p} \rangle = \int_{-\infty}^{+\infty} \psi^*(x;0) \left(-i\hbar \frac{\partial \psi(x;0)}{\partial x} \right) dx. \quad]\!]$$

Force-free motion of a Gaussian wavepacket

a. From the time development of energy eigenstates,

$$\tilde{\psi}(p;t) = e^{-(i/\hbar)E(p)t}\tilde{\psi}(p;0).$$

While from the properties of momentum wavefunctions,

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

Putting these together,

$$\begin{aligned}
\psi(x;t) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} e^{i(px - E(p)t)/\hbar} \tilde{\psi}(p;0)\, dp \\
&= \frac{1}{\sqrt{2\pi\hbar}} A \sqrt{\frac{\sigma}{\hbar}} \int_{-\infty}^{+\infty} e^{i(px-E(p)t)/\hbar} e^{-(p-p_0)^2\sigma^2/2\hbar^2}\, dp.
\end{aligned}$$

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 get

$$\begin{aligned}
\psi(x;t) &= \frac{A}{\sqrt{2\pi\hbar}}\sqrt{\frac{\sigma}{\hbar}}e^{i(p_0x-E(p_0)t)/\hbar}\int_{-\infty}^{+\infty}\exp\left\{i\left(-p'^2\frac{t}{2m}+p'\left(x-\frac{p_0}{m}t\right)\right)\frac{1}{\hbar}\right\}e^{-p'^2\sigma^2/2\hbar^2}\,dp' \\
&= \frac{A}{\sqrt{2\pi\hbar}}\sqrt{\frac{\sigma}{\hbar}}e^{i(p_0x-E(p_0)t)/\hbar}\int_{-\infty}^{+\infty}\exp\left\{-p'^2\left(\frac{\sigma^2}{2\hbar^2}+i\frac{t}{2m\hbar}\right)\right\}\exp\left\{i\frac{p'}{\hbar}\left(x-\frac{p_0}{m}t\right)\right\}\,dp' \\
&= \frac{A}{\sqrt{2\pi\hbar}}\sqrt{\frac{\sigma}{\hbar}}e^{i(p_0x-E(p_0)t)/\hbar}\int_{-\infty}^{+\infty}\exp\left\{-\frac{p'^2}{2\hbar^2}\left(\sigma^2+i\frac{t\hbar}{m}\right)\right\}\exp\left\{i\frac{p'}{\hbar}\left(x-\frac{p_0}{m}t\right)\right\}\,dp',
\end{aligned}$$

which suggests the substitution $k = p'/\hbar$ giving

$$\psi(x;t) = A\sqrt{\frac{\sigma}{2\pi}}e^{i(p_0x-E(p_0)t)/\hbar}\int_{-\infty}^{+\infty}\exp\left\{-\frac{k^2}{2}\left(\sigma^2+i\frac{t\hbar}{m}\right)\right\}\exp\left\{ik\left(x-\frac{p_0}{m}t\right)\right\}\,dk.$$

b. 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 part the multiplies the k^2 doesn't pluck any heartstring of mine. Write the dimensionless quantity

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

so the equation is

$$\psi(x;t) = A\sqrt{\frac{\sigma}{2\pi}}e^{i(p_0x-E(p_0)t)/\hbar}\int_{-\infty}^{+\infty}\exp\left\{-\frac{k^2\sigma^2\beta}{2}\right\}\exp\left\{ik\left(x-\frac{p_0}{m}t\right)\right\}\,dk.$$

The integral here is the "useful integral" (1) with $u = k$, $\alpha = \sigma\sqrt{\beta}$, and $y = x - (p_0/m)t$. Note that, as required, $\Re e\{\alpha^2\} = \sigma^2 > 0$. Using that integral, we get

$$\begin{aligned}
\psi(x;t) &= A\sqrt{\frac{\sigma}{2\pi}}e^{i(p_0x-E(p_0)t)/\hbar}\frac{\sqrt{2\pi}}{\sigma\sqrt{\beta}}e^{-(x-\frac{p_0}{m}t)^2/2\sigma^2\beta} \\
&= A\frac{1}{\sqrt{\sigma\beta}}e^{i(p_0x-E(p_0)t)/\hbar}e^{-(x-\frac{p_0}{m}t)^2/2\sigma^2\beta}. \qquad (8)
\end{aligned}$$

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,

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

Thus

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

But

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

so

$$|\psi(x;t)|^2 = \frac{1}{\sqrt{\pi}\sigma|\beta|} e^{-(x-\frac{p_0}{m}t)^2/\sigma^2|\beta|^2}. \tag{9}$$

This expression has exactly the same Gaussian form as $|\psi(x;0)|^2$, equation (4), except that

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

where

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

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

$$\langle \hat{x} \rangle_t = \frac{p_0}{m}t \tag{10}$$

and has position uncertainty

$$(\Delta x)_t = \frac{\sigma}{\sqrt{2}}\sqrt{1 + \left(\frac{\hbar}{m\sigma^2}t\right)^2}. \tag{11}$$

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