Gaussian Integrals and Gaussian Wave Packets

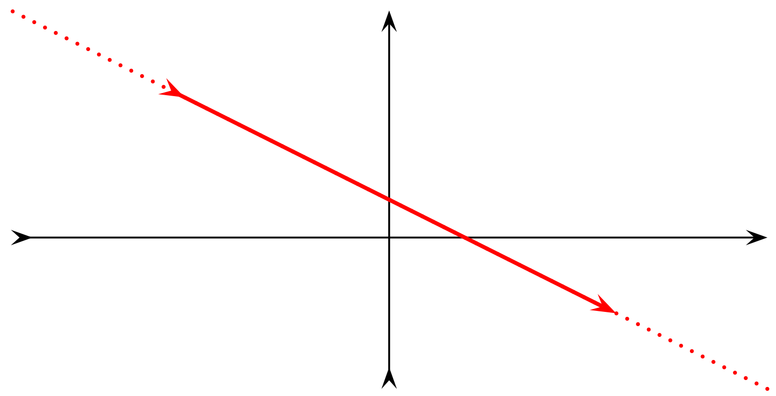
First, a **Theorem:** For any complex α with a positive real part and for any complex β,

$$I = \int_{-\infty}^{+\infty} dx \, \exp\bigl(-\alpha(x+\beta)^2\bigr) = \sqrt{\frac{\pi}{\alpha}}. \qquad (1)$$

Proof: changing integration variable from x to $y = \sqrt{\alpha}(x+\beta)$, we get

$$I = \int_\Gamma \frac{dy}{\sqrt{\alpha}} \exp(-y^2) \qquad (2)$$

where the integral is over a tilted line in the complex plane,



(3)

The tilt angle of this line is $-\frac{1}{2}\arg(\alpha)$, so for $\mathrm{Re}\,\alpha > 0$ this angle is between $-45°$ and $+45°$, hence $\exp(-y^2) \to 0$ at both asymptotic ends of the line.

In complex analysis, the contour integrals of analytic functions are invariant under contour deformations as long as the contour does not cross any singularities of the integral and the end points — if any — stay in the same place. The integrand of (2) is analytic and does not have any singularities at finite y, so we may deform the contour any way we like as long as its ends stay at complex infinity. Or rather, the ends stay at infinity and the directions in which they approach ∞ stays within 45° degrees of the real axis so that the integrand diminishes rather than blows up. In particular, we may tilt the red line (3) and move it back to the real axis, thus

$$I \;=\; \frac{1}{\sqrt{\alpha}} \int\limits_{\substack{\text{real}\\\text{axis}}} dy\, \exp(-y^2) \;=\; \frac{1}{\sqrt{\alpha}} \times \sqrt{\pi}. \tag{4}$$

Quod erat demonstrandum.

Now let's apply this theorem to the *Gaussian wave packets* and their Fourier transforms. For simplicity, let's work in one space dimension where a Gaussian wave packet has form

$$\Psi(x) \;=\; \Psi_0 \times e^{ik_0x} \times \exp\bigl(-\tfrac{1}{2}A(x-x_0)^2\bigr). \tag{5}$$

Usually, A is a real and positive parameter related to the packet's width Δx, or more accurately root-mean-square deviation of x from the packet's center x_0 as weighed by $|\Psi(x)|^2$:

$$\int |\Psi|^2\, dx \;=\; |\Psi_0|^2 \int \exp(-A(x-x_0)^2\, dx \;=\; |\Psi_0|^2 \times \sqrt{\frac{\pi}{A}}\,, \tag{6}$$

$$\int |(x-x_0^2) \times \Psi|^2\, dx \;=\; |\Psi_0|^2 \int (x-x_0)^2 \exp(-A(x-x_0)^2\, dx \;=\; |\Psi_0|^2 \times \frac{\sqrt{\pi}}{2A^{3/2}}\,, \tag{7}$$

$$\text{hence} \quad (\Delta x)^2 \;\stackrel{\text{def}}{=}\; \frac{\int (x-x_0)^2 \times |\Psi|^2 dx}{\int |\Psi|^2 dx} \;=\; \frac{1}{2A}\,, \tag{8}$$

so the packet's width is

$$\Delta x \;=\; \frac{1}{\sqrt{2A}}\,. \tag{9}$$

However, sometimes people use Gaussian wave packets with complex A, which is OK as long as $\operatorname{Re} A > 0$; in this case,

$$\int |\Psi|^2\, dx \;=\; |\Psi_0|^2 \int \exp\bigl(-\operatorname{Re}(A) \times (x-x_0)^2\bigr)\, dx \;=\; |\Psi_0|^2 \times \sqrt{\frac{\pi}{\operatorname{Re}(A)}}\,, \tag{10}$$

$$\int |(x - x_0^2) \times \Psi|^2 \, dx \;=\; |\Psi_0|^2 \int (x - x_0)^2 \exp\bigl(-\operatorname{Re}(A) \times (x - x_0)^2\bigr) \, dx \;=\; |\Psi_0|^2 \times \frac{\sqrt{\pi}}{2(\operatorname{Re}(A))^{3/2}}, \tag{11}$$

$$\text{hence} \quad (\Delta x)^2 \;\stackrel{\text{def}}{=}\; \frac{\int (x - x_0)^2 \times |\Psi|^2 dx}{\int |\Psi|^2 dx} \;=\; \frac{1}{2\operatorname{Re}(A)}, \tag{12}$$

so the packet's width is

$$\Delta x \;=\; \frac{1}{\sqrt{2\operatorname{Re}(A)}}. \tag{13}$$

Next, consider the Fourier transform of a wave packet

$$\tilde{\Psi}(k) \;=\; \int dx \, e^{-ikx} \, \Psi(x), \qquad \Psi(x) \;=\; \int \frac{dk}{2\pi} \, e^{+ikx} \, \tilde{\Psi}(k). \tag{14}$$

For the Gaussian wave packet (5), this Fourier transform becomes

$$\begin{aligned} \tilde{\Psi}(k) \;&=\; \int dx \, e^{-ikx} \times \Psi_0 e^{ik_0 x} \times \exp\bigl(-\tfrac{1}{2}A(x - x_0)^2\bigr) \\ &=\; \Psi_0 \int dx \, \exp\Bigl(-\tfrac{1}{2}A(x - x_0)^2 \;+\; i(k_0 - k)x\Bigr) \end{aligned} \tag{15}$$

where the net exponent amounts to

$$\begin{aligned} -\tfrac{1}{2}A(x - x_0)^2 \;+\; i(k_0 - k)x \;&=\; -\tfrac{1}{2}A(x - x_0)^2 \;+\; i(k_0 - k)(x - x_0) \;+\; i(k_0 - k)x_0 \\ &=\; -\frac{A}{2}\left((x - x_0) \;+\; i\frac{(k_0 - k)}{A}\right)^2 \;-\; \frac{(k_0 - k)^2}{2A} \;+\; i(k_0 - k)x_0 \end{aligned} \tag{16}$$

where the last two terms do not depend on x while the first term has the form of $-\alpha(x + \beta)^2$ for $\alpha = \frac{1}{2}A$ and $\beta = -x_0 + i(k_0 - k)/A$. Consequently,

$$\begin{aligned} \tilde{\Psi}(k) \;&=\; \Psi_0 \int dx \left(-\frac{A}{2}\left(x - x_0 + \frac{i(k_0 - k)}{A}\right)^2 \;-\; \frac{(k_0 - k)^2}{2A} \;+\; i(k_0 - k)x_0\right) \\ &=\; \Psi_0 \exp\left(-\frac{(k_0 - k)^2}{2A}\right) \exp\bigl(ix_0(k_0 - k)\bigr) \times \int dx \, \exp\left(-\frac{A}{2}\left(x - x_0 + \frac{i(k_0 - k)}{A}\right)^2\right) \\ &=\; \Psi_0 \exp\left(-\frac{(k_0 - k)^2}{2A}\right) \exp\bigl(ix_0(k_0 - k)\bigr) \times \sqrt{\frac{2\pi}{A}}, \end{aligned} \tag{17}$$

or

$$\tilde{\Psi}(k) = \left[\sqrt{\frac{2\pi}{A}}\, e^{ik_0x_0}\,\Psi_0\right] \times e^{-ix_0k} \times \exp\left(-\frac{(k-k_0)^2}{2A}\right). \tag{18}$$

Thus, *the Fourier transform of a Gaussian wave packet in x space is itself a Gaussian wave packet in k space*. Moreover, the width parameters of the two Gaussian packets are related as

$$A_k = \frac{1}{A_x}, \tag{19}$$

hence

$$(\Delta k)^2 = \frac{1}{2\,\mathrm{Re}\,A_k} = \frac{1}{2\,\mathrm{Re}(1/A_x)}. \tag{20}$$

Consequently, the product of the x-space and the k-space widths of the same packet amounts to

$$\frac{1}{(\Delta x)^2} \times \frac{1}{(\Delta k)^2} = 2\,\mathrm{Re}(A) \times 2\,\mathrm{Re}(1/A) = \frac{4(\mathrm{Re}\,A)^2}{|A|^2}, \tag{21}$$

$$\Downarrow$$

$$\Delta x \times \Delta k = \frac{1}{2}\,\frac{|A|}{\mathrm{Re}\,A}, \tag{22}$$

which means:

$$\text{for a real } A, \quad \Delta x \times \Delta k = \frac{1}{2},$$
$$\text{but for a complex } A, \quad \Delta x \times \Delta k > \frac{1}{2}.$$