GAUSSIAN

①

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \qquad \mu = 0$$

$$f(x) = \frac{I_0}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2}$$

$$\int_{-\infty}^{\infty} dx\, f(x) = \frac{I_0}{\sigma\sqrt{2\pi}} \underbrace{\int_{-\infty}^{\infty} e^{-x^2/2\sigma^2} dx}_{\cancel{\sqrt{\pi}/\sqrt{2\sigma^2}}\quad \sqrt{\pi 2\sigma^2}} = I_0 \quad \checkmark$$

FOURIER TRANFORM

$$F(k) = \int_{-\infty}^{\infty} f(x)\, e^{-2\pi i k x} dx$$

$$F(k) = \frac{I_0}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-x^2/2\sigma^2 - 2\pi i k x}$$

$$= \frac{I_0}{\sigma\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, e^{-\left(\frac{x^2}{2\sigma^2} + 2\pi i k x\right)} = \frac{I_0}{\cancel{\sigma\sqrt{2\pi}}} \sqrt{\cancel{\pi 2\sigma^2}} \cdot$$

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

$$a = \frac{1}{2\sigma^2} \qquad b = 2\pi i k$$

$$b^2 = -4\pi^2 k^2$$

$$\cdot\, e^{-4\pi^2 k^2 \cancel{2}\sigma^2/\cancel{4}2} = I_0\, e^{-2\pi^2 k^2 \sigma^2}$$

$$F(k) = I_0\, e^{-2\pi^2 k^2 \sigma^2}$$

(2)

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2}$$

$$\longrightarrow F(k) = I_0 \, e^{-2\pi^2 k^2 \sigma^2}$$

Now check for delta function

$$f(x) = I_0 \, \delta(x) \qquad \int_{-\infty}^{\infty} f(x) = I_0$$

$$F(k) = \int_{-\infty}^{\infty} e^{-2\pi i k x} I_0 \, \delta(x) = I_0$$

Also, note that

$$\lim_{\sigma \to 0} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2} = \delta(x)$$

which also holds at the level of Fourier transform

$$F_{GAUSS}(k) = I_0 \, e^{-2\pi^2 k^2 \sigma^2}$$

$$\lim_{\sigma \to 0} F_{GAUSS}(k) = I_0 = F_{DELTA}(k)$$

So one can go from gaussians to delta function via smooth limit of setting variance to zero

Now for inverse Fourier

$$\mathcal{F}^{-1}[F(k)] = \int_{\mathbb{R}^n} e^{2\pi i x k} F(k)\, dk$$

note that $F(k)$ must be an integrable function

- no poles

Let's check for a Gaussian

$$F_{GAUSS}(k) = I_0\, e^{-2\pi^2 k^2 \sigma^2}$$

$$f(x) = \mathcal{F}^{-1}[F(k)] = \int_{-\infty}^{\infty} I_0\, e^{-2\pi^2 k^2 \sigma^2}\, e^{2\pi i x k}\, dx$$

$$= I_0 \int_{-\infty}^{\infty} d\cancel{k}\, e^{-(2\pi^2\sigma^2 k^2 - 2\pi i x k)}$$

$$= I_0 \sqrt{\cancel{\pi}/2\cancel{\pi}^2\sigma^2}\; e^{(-\cancel{2}\cancel{\pi} i x)^2 / \cancel{4}\, 2\cancel{\pi}^2\sigma^2}$$

$$f(x) = I_0 \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-x^2/2\sigma^2} \checkmark$$

So analytically things work fine

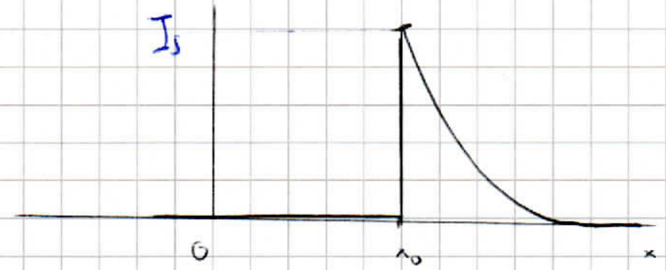
→ What about numerically?

NOW FOR SPECIMEN SIGNAL

$$I_{SAMPLE}(x) = I_s \, e^{-ax} \, u(x)$$

$$u(x) = \begin{cases} 0 & x < 0 \\ 1 & x \geq 0 \end{cases}$$

$$I_{SAMPLE}(x) = \begin{cases} I_s \, e^{-a(x-x_s)} \, u(x-x_s) & x \geq x_s \\ 0 & x \leq x_s \end{cases}$$



$$f_{SPEC}(x) = I_s \, e^{-a(x-x_s)} \, u(x-x_s) \qquad x \geq x_s$$

COMPUTE FOURIER TRANSFORM

$$F_{SAMPLE}(k) = \int_{-\infty}^{\infty} dx \, e^{-2\pi i k x} f_{SPEC}(x)$$

$$F_{SAMPLE}(k) = I_s \int_{x_0}^{\infty} dx \, e^{-2\pi i k x - a(x-x_s)}$$

$$= I_s \int_{x_0}^{\infty} dx \, e^{-x(a+2\pi i k)} e^{a x_s}$$

$$= I_s \, e^{a x_s} \int_{x_0}^{\infty} dx \, e^{-x(a+2\pi i k)}$$

$$F_{kSAMPLE}(k) = I_S e^{a x_S} \underbrace{\int_{x_S}^{\infty} dx \, e^{-x(a+2\pi i k)}}$$ (5)

$$\frac{-1}{a+2\pi i k} e^{-x(a+2\pi i k)} \Big|_{x_S}^{\infty}$$

$$\frac{1}{a+2\pi i k} e^{-x_S(a+2\pi i k)}$$

$$F_{kSAMPLE}(k) = \frac{1}{a+2\pi i k} e^{-2\pi i k x_S}$$

SIGNAL + BACKGROUND

$$I_{TOT}(x) = \frac{I_0}{\sigma\sqrt{2\pi}} e^{-x^2/2\sigma^2} + I_S e^{-a(x-x_S)} u(x-x_S)$$

$$\boxed{F_{TOT}(k) = I_0 e^{-2\pi^2 k^2 \sigma^2} + \frac{1}{a+2\pi i k} e^{-2\pi i k x_S}}$$

Analytical Fourier transform

EGERTON

FOURIER TRANSFORM TURNS CONVOLUTIONS INTO PRODUCTS

$$(f \otimes g)(x) = \int_{-\infty}^{\infty} f(x') g(x-x') \, dx' = \int_{-\infty}^{\infty} f(x-x') g(x') \, dx'$$

$$\mathcal{F}\left[(f \otimes g)\right] = F_f(k) \, F_g(k)$$

TEHEOTERITAL SINGLE SCATTERING $\longrightarrow I_{S1, TH}$

EXPERIMENTAL " "

$$I_{S1, EXP}(x) = \int_{-\infty}^{\infty} I(x') \, I_{ZLP}(x'-x) \, dx$$

$$\boxed{j(k) = z(k) \, e^{s(k)/I_0}}$$

$$I_{ZLP}(x) = I_0 \, R(x)$$

$$z(k) = \int_{-\infty}^{\infty} dx \, e^{-2\pi i kx} \, I_{ZLP}(x)$$

$$s(k) = \int_{-\infty}^{\infty} dx \, e^{-2\pi i kx} \, I_{1S, TH}(x)$$

$$j(k) = \int_{-\infty}^{\infty} dx \, e^{-2\pi i kx} \, I_{1S, EXP}$$

IN OUR TOY MODEL

$$f(k) = I_0 e^{-2\pi^2 k^2 \sigma^2} \times \mathrm{Exp}\left(\frac{e^{-2\pi i k x_s}}{I_0 (a + 2\pi i k)} \right)$$

NOT CORRECT! → DEPENDING ON IF WE CONSIDER

LET'S CONSIDER ONLY SINGLE SCATTERING

$$I_{1S,\,EXP} = \int_{-\infty}^{\infty} R(\Delta E - \Delta E')\, I_{1S,\,TH}(\Delta E')\, d\Delta E'$$

$$I_{1S,\,TH}(\Delta E) = I_S\, e^{-a(x - x_S)}\, U(x - x_S)$$

$$I_{1S,\,EXP} = \int_{-\infty}^{\infty} dx\, \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(\Delta E - \Delta E')^2}{2\sigma^2}}\, I_S\, e^{-a(x - x_S)}\, U(x - x)$$

$$I_{1S,\,EXP}(\Delta E) = \int_{x_S}^{\infty} \frac{I_S}{\sqrt{2\pi\sigma^2}}\, d\Delta E'\, e^{-\frac{(\Delta E - \Delta E')^2}{2\sigma^2}}\, e^{-a(x - x_S)}$$

$$I_{1S,\,EXP}(\Delta E) = \frac{I_S}{\sqrt{2\pi\sigma^2}} \int_{x_S}^{\infty} d\Delta E'\, e^{-\frac{\Delta E^2 - 2\Delta E \Delta E' + \Delta E'^2}{2\sigma^2}}\, e^{-a(\Delta E' - \Delta E_S)}$$

$$= \frac{I_S}{\sqrt{2\pi\sigma^2}} \int_{E_S}^{\infty} e^{-\frac{\Delta E^2}{2\sigma^2} + a E_S}\, d\Delta E'\, e^{-\Delta E'^2/2\sigma^2 + \Delta E'\left(-a + \frac{2\Delta E}{2\sigma^2}\right)}$$

$$I_{1S,EXP}(\Delta E) = \frac{I_s}{\sqrt{2\pi\sigma^2}} e^{-\Delta E^2/2\sigma^2 + a E_s} \times$$

$$\times \int_{E_s}^{\infty} d\Delta E' \, e^{-\Delta E'^2/2\sigma^2 + \Delta E'\left(-a + \Delta E/\sigma^2\right)}$$

$B = 2\sigma^2$ $\quad C = \left(-a + \Delta E/\sigma^2\right)$

$A = E_s$

$$\int_A^{\infty} dx \, e^{-x^2/B + xC} = \frac{\sqrt{\pi B}}{2} e^{BC^2/4} \left[\mathrm{ERF}\left(\frac{BC - 2A}{2\sqrt{B}}\right) + 1 \right]$$

$$\boxed{I_{1S,EXP}(\Delta E) = \frac{I_s}{\sqrt{2\pi\sigma^2}} e^{-\Delta E^2/2\sigma^2 + a E_s} \times \frac{\sqrt{2\pi\sigma^2}}{2} e^{\frac{2\sigma^2}{4}\left(\Delta E/\sigma^2 - a\right)^2} \left(\mathrm{ERF}\left(\frac{2\sigma^2\left(-a + \Delta E/\sigma^2\right) - 2E_s}{2\sqrt{2}\,\sigma} \right) + 1 \right)}$$

Note that in the limit $\sigma \to \infty$

$$R(\Delta E) \to \delta(\Delta E)$$

and we expect $I_{1S,EXP}(\Delta E) \to I_{1S,TH}(\Delta E)$

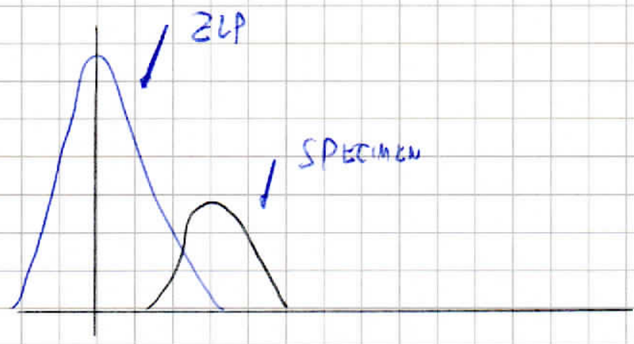
$$= I_s \, e^{-\cancel{(x - x_s)}\,(\Delta E - E_s)} \, \upsilon(\Delta E - E_s)$$

$$I_{1S,EXP}(\Delta E) = \frac{I_S}{2}\, e^{-\Delta E^2/2\sigma^2 + a E_S + \frac{\sigma^2}{2}\left(\Delta E/\sigma^2 - a\right)^2} \times$$

$$\times \left(\mathrm{Erf}\left(\frac{\sigma^2\left(-a + \Delta E/\sigma^2\right) - E_S}{\sqrt{2}\,\sigma} \right) + 1 \right)$$

ONE SHOULD CHECK LIMIT

[ALSO FOR OTHER FUNCTIONS FOR SPECIMEN]



$$I_{ZLP}(\Delta E) = \frac{I_0}{\sqrt{2\pi\sigma^2}}\, e^{-\Delta E^2/2\sigma^2}$$

$$\cancel{I_{SPEC}} \quad I_{1S,TH} = \frac{I_S}{\sqrt{2\pi\sigma_S^2}}\, e^{-\frac{(\Delta E - E_S)^2}{2\sigma_S^2}}$$

$$I_{1S,EXP}(\Delta E) = \int_{-\infty}^{\infty} d\Delta E' \, \frac{\cancel{I_0}}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(\Delta E - \Delta E')^2}{2\sigma^2}} \times$$

$$I_S/\sqrt{2\pi\sigma_S^2}\; e^{-\frac{(\Delta E' - E_S)^2}{2\sigma_S^2}}$$

$$I_{1S,EXP}(\Delta E) = \frac{\cancel{I_0}\, I_S}{2\pi\, \sigma\, \sigma_S} \int_{-\infty}^{\infty} d\Delta E'\, e^{-\frac{(\Delta E - \Delta E')^2}{2\sigma^2} - \frac{(\Delta E' - E_S)^2}{2\sigma_S^2}}$$ 10

$d_1 = \Delta E \qquad d_2 = E_S$

$s_1 = \sigma_1 \qquad s_2 = \sigma_S$

$$= \frac{\cancel{\sqrt{2\pi}}\, \cancel{\sigma\sigma_S}}{\sqrt{2\pi}\sqrt{\sigma^2 + \sigma_S^2}} \times e^{-\frac{(\Delta E - E_S)^2}{2(\sigma^2 + \sigma_S^2)}} \times \frac{\cancel{I_0}\, I_S}{\cancel{2\pi}\, \cancel{\sigma\sigma_S}}$$

$$\boxed{I_{1S,EXP}(\Delta E) = \frac{I_S}{\sqrt{2\pi(\sigma^2 + \sigma_S^2)}}\, e^{-\frac{(\Delta E - E_S)^2}{2(\sigma^2 + \sigma_S^2)}}}$$

Note right limit $\sigma \to 0$

$$I_{S,EXP} \longrightarrow \frac{I_S}{\sqrt{2\pi\sigma_S^2}}\, e^{-\frac{(\Delta E - E_S)^2}{2\sigma_S^2}} = I_{1S,TH}$$

QED

GAUSSIANS PERFECT FOR TOY MODEL

$$I_{TOT}(\Delta E) = \frac{I_0}{\sqrt{2\pi\sigma^2}}\, e^{-\Delta E^2/2\sigma^2} + \frac{I_S}{\sqrt{2\pi\sigma_S^2}}\, e^{-\frac{(\Delta E - E_S)^2}{2\sigma_S^2}}$$

$$\mathcal{F}\left[I_{1S,TH}\right] = \int_{-\infty}^{\infty} dx\, e^{-2\pi i k x}\, \frac{I_S}{\sqrt{2\pi\sigma_S^2}}\, e^{-\frac{(\Delta E - E_S)^2}{2\sigma_S^2}}$$

$$= \frac{I_S}{\sqrt{2\pi\sigma_S^2}}\, e^{-E_S^2/2\sigma_S^2} \int_{-\infty}^{\infty} dx\, e^{-x^2/2\sigma_S^2 + 2xE_S/2\sigma_S^2 - 2\pi i k x}$$

$$\int_{-\infty}^{\infty} dx\, e^{-x^2/2\sigma_s^2 + x(\cancel{2}E_s/\sigma_s^2 - 2\pi i k)}$$

$$a = 2\sigma_s^2 \qquad b = E_s/\sigma_s^2 - 2\pi i k$$

$$= \sqrt{\pi}\sqrt{2\sigma_s^2}\, e^{\cancel{2}\sigma_s^2/4\left(E_s/\sigma_s^2 - 2\pi i k\right)^2}$$

$$= \sqrt{2\pi\sigma_s^2}\, e^{\sigma_s^{\cancel{4}}/\cancel{2}\left(E_s^2/\cancel{2}\sigma_s^4 - \cancel{2}E_s/\sigma_s^{\cancel{2}}\, 2\pi i k - \cancel{4}\pi^2 k^2 \sigma_s^2\right)}$$

$$= I_s\, e^{-2\pi^2 k^2 \sigma_s^2 - 2E_s \pi i k}$$

$$\boxed{\mathcal{F}\left[I_{s,TH}\right] = I_s\, e^{-2\pi^2 k^2 \sigma_s^2 - 2E_s \pi i k}}$$

All integrals can be computed analytically