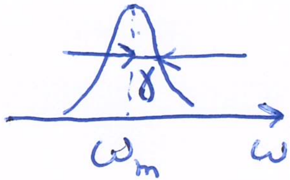
SMOOTHING SPECTRA BY LEAST-SQUARES FITS

$$F(\omega) = \frac{S}{\pi} \frac{\gamma}{(\omega - \omega_m)^2 + \gamma^2}$$



$$F^{-1}(\omega) = \frac{\pi}{S\gamma}\left[\omega^2 - 2\omega_m\omega + \omega_m^2 + \gamma^2\right] =$$

$$= \frac{\pi}{S\gamma}\omega^2 - \frac{2\pi\omega_m}{S\gamma}\omega + \frac{\pi(\omega_m^2 + \gamma^2)}{S\gamma}$$

We could try to minimize the sum, <u>but</u> the values will be too large

$\Rightarrow$ the use of the <u>reduced</u> and <u>centered</u> variable instead of ω

I Hypothesis 1

$$x = \frac{\omega - \omega_m}{\omega_m}$$

$$\hookrightarrow \omega = x\omega_m + \omega_m = \omega_m(1+x)$$

$$F^{-1}(x) = \frac{\pi\omega_m^2}{S\gamma}(1+x)^2 - \frac{2\pi\omega_m^2}{S\gamma}(1+x) + \frac{\pi(\omega_m^2+\gamma^2)}{S\gamma} =$$

$$= \cdots =$$

$$= \underbrace{\frac{\pi\omega_m^2}{S\gamma}}_{\equiv a_2} x^2 + \underbrace{\frac{\pi\gamma}{S}}_{\equiv a_0} = a_2 x^2 + a_0$$

$$E(a_2, a_0) = \sum_{i=1}^{N} w_i (a_2 x_i^2 + a_0 - y_i)^2$$

$$\begin{cases} \left(E(a_2, a_0)\right)'_{a_2} = \sum_{i=1}^{N} w_i \, 2 (a_2 x_i^2 + a_0 - y_i) x_i^2 = 0 \\ \left(E(a_2, a_0)\right)'_{a_0} = \sum_{i=1}^{N} w_i \, 2 (a_2 x_i^2 + a_0 - y_i) = 0 \end{cases}$$

$$\begin{cases} a_2 \sum w_i x_i^4 + a_0 \sum w_i x_i^2 = \sum w_i y_i x_i^2 \\ a_2 \sum w_i x_i^2 + a_0 \sum w_i = \sum w_i y_i \end{cases}$$

We devide each equation by N, which gives us the mean values:

$$\begin{cases} a_2 \langle x^4 \rangle + a_0 \langle x^2 \rangle = \langle y x^2 \rangle \\ a_2 \langle x^2 \rangle + a_0 \langle 1 \rangle = \langle y \rangle \end{cases}$$

This system of equations can be written in matrix notation: 4

$$\underbrace{\begin{pmatrix} \langle x^4 \rangle & \langle x^2 \rangle \\ \langle x^2 \rangle & \langle 1 \rangle \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a_2 \\ a_0 \end{pmatrix}}_{X} = \underbrace{\begin{pmatrix} \langle yx^2 \rangle \\ \langle y \rangle \end{pmatrix}}_{B}$$

and we obtain:

$$a_2 = \frac{\begin{vmatrix} \langle yx^2 \rangle & \langle x^2 \rangle \\ \langle y \rangle & \langle 1 \rangle \end{vmatrix}}{\begin{vmatrix} \langle x^4 \rangle & \langle x^2 \rangle \\ \langle x^2 \rangle & \langle 1 \rangle \end{vmatrix}} = \dots$$

your calculations ...

$$a_0 = \frac{\begin{vmatrix} \langle x^4 \rangle & \langle yx^2 \rangle \\ \langle x^2 \rangle & \langle y \rangle \end{vmatrix}}{\begin{vmatrix} \langle x^4 \rangle & \langle x^2 \rangle \\ \langle x^2 \rangle & \langle 1 \rangle \end{vmatrix}} = \dots$$

We get:

$$a_0 = \frac{\langle yx^2\rangle\langle x^2\rangle - \langle y\rangle\langle x^4\rangle}{\langle x^2\rangle^2 - \langle x^4\rangle\langle 1\rangle}$$

and

$$a_2 = \frac{\langle y\rangle\langle x^2\rangle - \langle yx^2\rangle\langle 1\rangle}{\langle x^2\rangle^2 - \langle x^4\rangle\langle 1\rangle}$$

So, we need to calculate:

$\langle x^2\rangle$, $\langle x^4\rangle$, $\langle y\rangle$, $\langle yx^2\rangle$ and $\langle 1\rangle$.

After that, with a_0 and a_2 we can obtain γ and S (we know ω_m).

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$$\begin{cases} a_2 = \dfrac{\pi \omega_m^2}{S\gamma} \\[2ex] a_0 = \dfrac{\pi \gamma}{S} \end{cases} \Rightarrow \begin{cases} S\gamma = \dfrac{\pi \omega_m^2}{a_2} & (1) \\[2ex] \dfrac{\gamma}{S} = \dfrac{a_0}{\pi} & (2) \end{cases}$$

We multiply (1) by (2):

$$\cancel{S}\gamma \cdot \frac{\gamma}{\cancel{S}} = \frac{\cancel{\pi}\omega_m^2}{a_2} \cdot \frac{a_0}{\cancel{\pi}}$$

$$\gamma^2 = \frac{a_0}{a_2}\omega_m^2$$

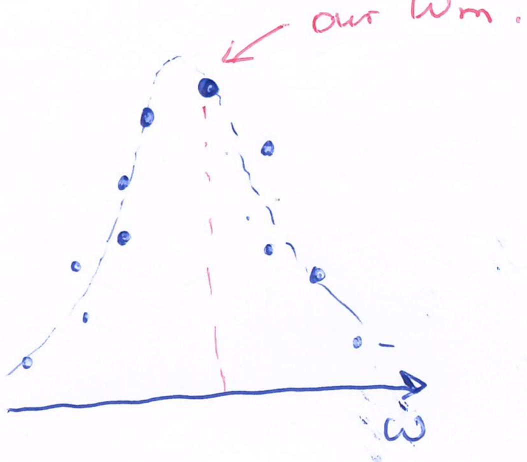
$$\boxed{\gamma = \sqrt{\frac{a_0}{a_2}}\,\omega_m}$$

On the other hand, from (1) we have:

$$S = \frac{\pi \omega_m^2}{a_2 \gamma} = \frac{\pi \omega_m^{\cancel{2}}}{a_2} \cdot \frac{\sqrt{a_2}}{\sqrt{a_0}\,\cancel{\omega_m}} = \frac{\pi \omega_m}{\sqrt{a_0 a_2}}$$

$$\boxed{S = \frac{\pi \omega_m}{\sqrt{a_0 a_2}}}$$

Problem:



II Hypothesis 2

(to be used for Practical Work)

$$x = \frac{\omega - \bar{\omega}}{\sqrt{\overline{\omega^2} - \bar{\omega}^2}} \equiv \frac{\omega - \bar{\omega}}{\sigma}$$

$\bar{\omega}$ – mean (not-weigted!) value

σ – RMS

$\hookrightarrow \omega = \sigma x + \bar{\omega}$

$$F^{-1}(x) = \frac{\pi}{S\gamma}\omega^2 - \frac{2\pi\omega_m}{S\gamma}\omega + \frac{\pi(\omega_m^2 + \gamma^2)}{S\gamma} =$$

$= \ldots$ your calculations $=$

$$F^{-1}(x) = \cdots =$$

$$= \underbrace{\frac{\pi\sigma^2}{S\gamma}}_{= a_2} x^2 + \underbrace{\frac{2\pi\sigma}{S\gamma}\left(\bar{\omega} - \omega_m\right)}_{= a_1} x + \underbrace{\frac{\pi}{S\gamma}\left[\gamma^2 + \left(\bar{\omega} - \omega_m\right)^2\right]^2}_{= a_0}$$

Next, we should minimize the coefficients:

$$E(a_0, a_1, a_2) = \sum_{i=1}^{N} w_i \left(a_2 x_i^2 + a_1 x_i + a_0 - y_i\right)^2$$

Note: y_i will be taken as the inverse of the experimental intensities $F_{exp\,i}$ i.e. $y_i \equiv \left(F_{exp\,i}\right)^{-1}$

$$\begin{cases} E'_{a_0} = 0 \\ E'_{a_1} = 0 \\ E'_{a_2} = 0 \end{cases} \longrightarrow \begin{cases} \sum_{i=1}^{N} w_i \, 2(a_2 x_i^2 + a_1 x_i + a_0 - y_i) = 0 \\ \sum_{i=1}^{N} w_i \, 2(a_2 x_i^2 + a_1 x_i + a_0 - y_i) x_i = 0 \\ \sum_{i=1}^{N} w_i \, 2(a_2 x_i^2 + a_1 x_i + a_0 - y_i) x_i^2 = 0 \end{cases}$$

Your calculations

...

$$\begin{cases} a_2\sum w_i x_i^2 + a_1\sum w_i x_i + a_0\sum w_i = \sum w_i y_i \\ a_2\sum w_i x_i^3 + a_1\sum w_i x_i^2 + a_0\sum w_i x_i = \sum w_i y_i x_i \\ a_2\sum w_i x_i^4 + a_1\sum w_i x_i^3 + a_0\sum w_i x_i^2 = \sum w_i y_i x_i^2 \end{cases}$$

In matrix form, putting a_0 first:

$$\underbrace{\begin{pmatrix} \sum w_i & \sum w_i x_i & \sum w_i x_i^2 \\ \sum w_i x_i & \sum w_i x_i^2 & \sum w_i x_i^3 \\ \sum w_i x_i^2 & \sum w_i x_i^3 & \sum w_i x_i^4 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix}}_{X} = \underbrace{\begin{pmatrix} \sum w_i y_i \\ \sum w_i y_i x_i \\ \sum w_i y_i x_i^2 \end{pmatrix}}_{B}$$

After division by N:

$$\begin{pmatrix} \langle 1 \rangle & \langle x \rangle & \langle x^2 \rangle \\ \langle x \rangle & \langle x^2 \rangle & \langle x^3 \rangle \\ \langle x^2 \rangle & \langle x^3 \rangle & \langle x^4 \rangle \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} \langle y \rangle \\ \langle xy \rangle \\ \langle x^2 y \rangle \end{pmatrix}$$

Your calculations to get

a_0

a_1

a_2

$$a_0 = \frac{\begin{vmatrix} \langle y\rangle & \langle x\rangle & \langle x^2\rangle \\ \langle xy\rangle & \langle x^2\rangle & \langle x^3\rangle \\ \langle x^2y\rangle & \langle x^3\rangle & \langle x^4\rangle \end{vmatrix}}{\begin{vmatrix} \langle 1\rangle & \langle x\rangle & \langle x^2\rangle \\ \langle x\rangle & \langle x^2\rangle & \langle x^3\rangle \\ \langle x^2\rangle & \langle x^3\rangle & \langle x^4\rangle \end{vmatrix}} =$$

$$= \frac{\langle y\rangle\langle x^2\rangle\langle x^4\rangle + \langle xy\rangle\langle x^3\rangle\langle x^2\rangle + \langle x\rangle\langle x^3\rangle\langle x^2y\rangle - \langle x^2y\rangle\langle x^2\rangle^2 - \langle y\rangle\langle x^3\rangle^2 - \langle x\rangle\langle xy\rangle\langle x^4\rangle}{\langle 1\rangle\langle x^2\rangle\langle x^4\rangle + 2\langle x\rangle\langle x^2\rangle\langle x^3\rangle - \langle x^2\rangle^3 - \langle 1\rangle\langle x^3\rangle^2 - \langle x\rangle^2\langle x^4\rangle}$$

$$a_1 = \frac{\begin{vmatrix} \langle 1\rangle & \langle y\rangle & \langle x^2\rangle \\ \langle x\rangle & \langle xy\rangle & \langle x^3\rangle \\ \langle x^2\rangle & \langle x^2 y\rangle & \langle x^4\rangle \end{vmatrix}}{\begin{vmatrix} \langle 1\rangle & \langle x\rangle & \langle x^2\rangle \\ \langle x\rangle & \langle x^2\rangle & \langle x^3\rangle \\ \langle x^2\rangle & \langle x^3\rangle & \langle x^4\rangle \end{vmatrix}} =$$

$$= \frac{\langle 1\rangle\langle xy\rangle\langle x^4\rangle + \langle x^2\rangle\langle x^3\rangle\langle y\rangle + \langle x\rangle\langle x^2\rangle\langle x^2 y\rangle - \langle x^2\rangle^2\langle xy\rangle - \langle x\rangle\langle x^4\rangle\langle y\rangle - \langle 1\rangle\langle x^3\rangle\langle x^2 y\rangle}{\quad}$$

$$a_2 = \frac{\begin{vmatrix} \langle 1\rangle & \langle x\rangle & \langle y\rangle \\ \langle x\rangle & \langle x^2\rangle & \langle xy\rangle \\ \langle x^2\rangle & \langle x^3\rangle & \langle x^2 y\rangle \end{vmatrix}}{\begin{vmatrix} \langle 1\rangle & \langle x\rangle & \langle x^2\rangle \\ \langle x\rangle & \langle x^2\rangle & \langle x^3\rangle \\ \langle x^2\rangle & \langle x^3\rangle & \langle x^4\rangle \end{vmatrix}} =$$

$$= \frac{\langle 1\rangle\langle x^2\rangle\langle x^2 y\rangle + \langle x\rangle\langle x^3\rangle\langle y\rangle + \langle x\rangle\langle x^2\rangle\langle xy\rangle - \langle x^2\rangle^2\langle y\rangle - \langle x\rangle^2\langle x^2 y\rangle - \langle 1\rangle\langle x^3\rangle\langle xy\rangle}{}$$

As soon as we have

$a_0, a_1, a_2,$

we can come back to

S, γ, ω_m

your calculations
to express
S, γ, ω_m in function of $a_0, a_1, a_2 \dots$

$$\begin{cases} a_2 = \dfrac{\pi\sigma^2}{S\gamma} & (*) \\[2ex] a_1 = \dfrac{2\pi\sigma}{S\gamma}(\bar{\omega}-\omega_m) & (**) \\[2ex] a_0 = \dfrac{\pi\gamma^2}{S\gamma} + \dfrac{\pi}{S\gamma}(\bar{\omega}-\omega_m)^2 & (***) \end{cases}$$

$$(*) \rightarrow \frac{\pi}{S\gamma} = \frac{a_2}{\sigma^2}$$

inserting this in $(**)$ we get

$$a_1 = 2\cancel{\sigma}\cdot\frac{a_2}{\sigma^{\cancel{2}}}(\bar{\omega}-\omega_m)$$

$$\boxed{\omega_m = \bar{\omega} - \frac{\sigma a_1}{2a_2}}$$ and we insert it in $(***)$:

$$a_0 = \frac{a_2}{\sigma^2}\gamma^2 + \frac{a_2}{\sigma^2}\left(\frac{a_1\sigma}{2a_2}\right)^2 =$$

$$= \frac{a_2\gamma^2}{\sigma^2} + \frac{a_1^2}{4a_2}$$

and we can express γ:

$$\frac{a_2}{\sigma^2}\gamma^2 = a_0 - \frac{a_1^2}{4a_2}$$

$$a_2\gamma^2 = a_0\sigma^2 - \frac{a_1^2}{4a_2}\sigma^2$$

$$\gamma^2 = \frac{a_0}{a_2}\sigma^2 - \frac{a_1^2}{4a_2^2}\sigma^2 = \sigma^2\left(\frac{a_0}{a_2} - \frac{a_1^2}{4a_2^2}\right)$$

So that

$$\boxed{\gamma = \sigma \sqrt{\frac{a_0}{a_2} - \frac{a_1^2}{4a_2^2}}}$$

Further, we replace γ in $\frac{\pi}{S\gamma} = \frac{a_2}{\sigma^2}$

to get S:

$$S = \frac{\pi\sigma^2}{a_2 \gamma} = \frac{\pi\sigma^{\cancel{2}}}{a_2 \cancel{\sigma} \sqrt{\frac{a_0}{a_2} - \frac{a_1^2}{4a_2^2}}} = \frac{\pi\sigma}{\sqrt{a_0 a_2 - a_1^2/4}}$$

$$\boxed{S = \frac{\pi\sigma}{\sqrt{a_0 a_2 - \frac{a_1^2}{4}}}}$$