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MUSRFIT plug-in for simple β -NMR resonance line shapes

This library contains useful functions to fit NMR and β -NMR line shapes. The functional form of the powder averages was taken from M. Mehring, Principles of High Resolution NMR in Solids (Springer 1983). The `libLineProfile` library currently contains the following functions:

LineGauss

$$A(f) = e^{-\frac{(f-f_0)^2}{2\sigma^2}} \quad (1)$$

Gaussian line shape around f_0 with width σ and height 1.

MUSRFIT theory line: `userFcn libLineProfile LineGauss 1 2`

Parameters: f_0, σ .

LineLaplace

$$A(f) = e^{-\frac{|f-f_0|}{\sigma}} \quad (2)$$

Laplaceian line shape around f_0 with width σ and height 1.

MUSRFIT theory line: `userFcn libLineProfile LineLaplace 1 2`

Parameters: f_0, σ .

LineLorentzian

$$A(f) = \frac{\sigma^2}{4(f-f_0)^2 + \sigma^2} \quad (3)$$

Lorentzian line shape around f_0 with width σ and height 1.

MUSRFIT theory line: `userFcn libLineProfile LineLorentzian 1 2`

Parameters: f_0, σ .

LineSkewLorentzian

$$A(f) = \frac{\sigma * \sigma_a}{4(f-f_0)^2 + \sigma_a^2}, \quad \sigma_a = \frac{2\sigma}{1 + e^{a(f-f_0)}} \quad (4)$$

Skewed Lorentzian line shape around f_0 with width σ , height 1 and skewness parameter a .

MUSRFIT theory line: `userFcn libLineProfile LineSkewLorentzian 1 2 3`

Parameters: f_0, σ, a .

LineSkewLorentzian2

$$A(f) = \begin{cases} \frac{\sigma_1^2}{4(f-f_0)^2 + \sigma_1^2}, & f < f_0 \\ \frac{\sigma_2^2}{4(f-f_0)^2 + \sigma_2^2}, & f > f_0 \end{cases} \quad (5)$$

Skewed Lorentzian line shape around f_0 with height 1 and widths σ_1 , and σ_2 .

MUSRFIT theory line: `userFcn libLineProfile LineSkewLorentzian2 1 2 3`

Parameters: f_0, σ_1, σ_2 .

PowderLineAxialLor

$$A(f) = I_{ax}(f) \circledast \left(\frac{\sigma^2}{4f^2 + \sigma^2} \right) \quad (6)$$

Powder average of a axially symmetric interaction, convoluted with a Lorentzian.

$$I_{ax}(f) = \begin{cases} \frac{1}{2\sqrt{(f_{\parallel}-f_{\perp})(f-f_{\perp})}} & f \in (f_{\perp}, f_{\parallel}) \cup (f_{\parallel}, f_{\perp}) \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

The maximal height of the curve is normalized to ~ 1 .

MUSRFIT theory line: `userFcn libLineProfile PowderLineAxialLor 1 2 3`

Parameters: $f_{\parallel}, f_{\perp}, \sigma$.

PowderLineAxialGss

$$A(f) = I_{ax}(f) \circledast \left(e^{-\frac{(f-f_0)^2}{2\sigma^2}} \right) \quad (8)$$

Powder average of a axially symmetric interaction (Eq. 7), convoluted with a Gaussian. The maximal height of the curve is normalized to ~ 1 .

MUSRFIT theory line: `userFcn libLineProfile PowderLineAxialGss 1 2 3`

Parameters: $f_{\parallel}, f_{\perp}, \sigma$.

PowderLineAsymLor

$$A(f) = I(f) \circledast \left(\frac{\sigma^2}{4f^2 + \sigma^2} \right) \quad (9)$$

Powder average of a asymmetric interaction, convoluted with a Lorentzian. Assume without loss of generality that $f_1 < f_2 < f_3$, then

$$I(f) = \begin{cases} \frac{K(m)}{\pi\sqrt{(f-f_1)(f_3-f_2)}}, & f_3 \geq f > f_2 \\ \frac{K(m)}{\pi\sqrt{(f_3-f)(f_2-f_1)}}, & f_2 > f \geq f_1 \\ 0 & \text{otherwise} \end{cases} \quad (10)$$

$$m = \begin{cases} \frac{(f_2-f_1)(f_3-f)}{(f_3-f_2)(f-f_1)}, & f_3 \geq f > f_2 \\ \frac{(f-f_1)(f_3-f_2)}{(f_3-f)(f_2-f_1)}, & f_2 > f \geq f_1 \end{cases} \quad (11)$$

$$K(m) = \int_0^{\pi/2} \frac{d\varphi}{\sqrt{1-m^2 \sin^2 \varphi}}, \quad (12)$$

where $K(m)$ is the complete elliptic integral of the first kind. Note that $f_1 < f_2 < f_3$ is not required by the code. The maximal height of the curve is normalized to ~ 1 .

MUSRFIT theory line: `userFcn libLineProfile PowderLineAsymLor 1 2 3 4`

Parameters: f_1, f_2, f_3, σ .

PowderLineAsymGss

$$A(f) = I(f) \circledast \left(e^{-\frac{(f-f_0)^2}{2\sigma^2}} \right) \quad (13)$$

Powder average of a asymmetric interaction (Eq. 10-12), convoluted with a Gaussian. The maximal height of the curve is normalized to ~ 1 .

MUSRFIT theory line: `userFcn libLineProfile PowderLineAsymGss 1 2 3 4`

Parameters: f_1, f_2, f_3, σ .