PAUL SCHERRER INSTITUT

Memorandum

Date: August 17, 2018

From: J. A. Krieger
E-Mail: jonas.krieger@psi.ch

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

$$A(f) = e^{-\frac{4\ln 2 (f-f_0)^2}{\sigma^2}} \tag{1}$$

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

$$A(f) = e^{-2\ln 2 \left|\frac{f-f_0}{\sigma}\right|} \tag{2}$$

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

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

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

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

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

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

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

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

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

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

The maximal height of the curve is normalized to $\sim$1.

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

Parameters: $f_\parallel$, $f_\perp$, σ.

PowderLineAxialGss

$$A(f) = I_{\mathrm{ax}}(f) \circledast \left(e^{-\frac{4\ln 2 (f-f_0)^2}{\sigma^2}}\right) \tag{8}$$

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

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

Parameters: $f_\parallel$, $f_\perp$, σ.

PowderLineAsymLor

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

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

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

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

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

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 $\sim$1.

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

Parameters: f_1, f_2,f_3, σ.

PowderLineAsymGss

$$A(f) = I(f) \circledast \left(e^{-\frac{4\ln 2 (f-f_0)^2}{\sigma^2}}\right) \tag{13}$$

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

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

Parameters: f_1, f_2,f_3, σ.