

Qensh fitting routine.

Function name: *Fit3_sqw_se_in_w_conv_par_lor*

Summary: This function performs the fit of the experimental data to a sum of a stretched exponential and a Lorentzian line.

NB: In the case $\beta=1$, the stretched exponential reduces to a Lorentzian.

Details: data are fitted to the following $S(Q, \omega)$:

$$S(Q, \omega) = S_{core}(Q, \omega') \otimes R(\omega) + Background(\omega) + \alpha \cdot S_{Buffer}(Q, \omega)$$

where

$$S_{core}(Q, \omega') = I_{El} \cdot \delta(\omega') + \left[\frac{I_{SE}}{2\pi} \int \exp\left(-\left(\frac{t}{\tau_{SE}}\right)^\beta \cos(\omega' t)\right) + \frac{I_B}{2\pi} \frac{\Gamma_L + 1/\tau_{SE}}{(\Gamma_L + 1/\tau_{SE})^2 + \omega'^2} \right] \cdot \exp\left(\frac{\omega'}{k_B T}\right)$$

and $\omega' = \omega - \omega_0$

and $Background(\omega) = \frac{bckd(\omega_{max}) - bckd(\omega_{min})}{\omega_{max} - \omega_{min}} \cdot (\omega - \omega_{max}) + bckd(\omega_{max})$

Param. #	symbol used in Eq. above	name	unit
0	ω_0	Elastic Peak Shift	meV
1		Resolution Shift	meV
2		Buffer Shift	meV
3	T	Sample Temperature	K
4	α	weighting factor for Buffer or substrate subtraction	
5	$bckd(\omega_{min})$	Background level at ω_{min}	A.U.
6	$bckd(\omega_{max})$	Background level at ω_{max}	A.U.
7	I_{el}	Elastic Peak Intensity	A.U.
8	I_{SE}	Stretched Exponential Intensity	A.U.
9	$1/\tau_{SE}$	Stretched Exponential correlation time	meV

10	β	Stretching exponent	
11	I_B	Lorentzian Intensity	A.U.
12	Γ_L	Lorentzian HWHM	meV

Note: Only the parameters highlighted in yellow should be used.