Qensh fitting routine.

Function name: *Fit3_sqw_aniso_diff_in_w_lor*

Summary: This function performs the fit of the experimental data to a sum of a stretched exponential and a Lorentzian line. This function is designed to fit "powder averaged" data for with a local anisotropy is suspected.

Details: data are fitted to the following S(Q,ω):

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

where

$$S_{core}(Q,\omega') = I_{El}.\delta(\omega') + \left[\frac{I_1}{2\pi} \int_0^{\pi} \frac{\Gamma_{//} \cos^2(\theta) + \Gamma_{perp} \sin^2(\theta)}{\left(\Gamma_{//} \cos^2(\theta) + \Gamma_{perp} \sin^2(\theta)\right)^2 + \omega'^2} d\theta + \frac{I_B}{2\pi} \frac{\Gamma_L}{\Gamma_L^2 + \omega'^2} \right] . \exp\left(\frac{\omega'}{k_B T} \right)$$

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

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

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(ω_{min})	Background level at ω_{min}	A.U.
6	bckd(ω_{max})	Background level at ω_{max}	A.U.
7	I_{el}	Elastic Peak Intensity	A.U.
8	I_1	Stretched Exponential Intensity	A.U.
9	$\Gamma_{//}$	HWHM due to the	meV

		“parallel” component of the dynamics	
10	Γ_{perp}	HWHM due to the “perpendicular” component of the dynamics	meV
11	I_B	Lorentzian Intensity	A.U.
12	Γ_L	Lorentzian HWHM	meV

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