Qensh fitting routine.

Function name: *fit3_sqw_gaussian_lor*

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

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

$$S_{core}(Q,\omega') = I_{El}.\delta(\omega') + \left[\frac{I_G}{\sqrt{2\pi}.HWHM_G} \exp\left(-\frac{1}{2}\left(\frac{\omega'}{HWHM_G} \right)^2 \right) + \frac{I_B}{2\pi} \frac{\Gamma_L}{\Gamma_L^2 + \omega'^2} \right] . \exp\left(\frac{\omega'}{k_B T} \right)$$

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

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

NB: The Gaussian standard deviation is σ_G=HVWM$_G$/sqrt(2*ln(2)) .

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_G	Gaussian Intensity	A.U.
9	HWHM$_G$	Gaussian HWHM	meV
10	I_B	Lorentzian Intensity	A.U.

11	Γ_L	Lorentzian HWHM	meV

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