

requirements on a QENS fitting GUI

(Reflection and extension to Shangamitra's and Miguel's suggestions. Blue like in Miguel's case nice to have options)

Content:

- it should be possible to subtract a (fitted) flat background from the resolution function (e.g. click box).
- not only a measured but also a fitted resolution function should be usable, which should be any user function, similarly to a fit model
- it should be possible to compare the fit results from different models, maybe as adding new fit module, as below.
- not only the data and fit but below also the residuals should be plotted
- fit functions:
 - It is nice to have a library, but more important to have a large freedom for user defined functions, partially based on predefined functions, but also allowing for e.g. integral, convolution, custom parameter restrictions (e.g. I , $(1-I)$), full python capability. Some examples could teach the syntax.
 - I would sort the library functions according to dimensionality.
 - Possibility for powder average
- Fitting data sets with different resolution should take into account that sensitivity of fit parameters differ. I'm not sure if it comes automatically... E.g. narrow component is not resolved in the low resolution data set.
- Binning for plot and binning for fit should be handled separately.
- Not equidistant binning should be available.
- Join data of e.g. different Temperatures as a new dimension.
- There IS a need for different fitting range for different spectra.
- Masking can include fit range, but should go beyond.

Appearance (just a trial, certainly improvable):

- A menu tab should be used, it will not be possible to put everything on one surface.
- Contents of the manu tabs should be able to open in a subwindow if meaningful, e.g. for defining the fit function.
- The user should be able to save customised appearance, since an optimal GUI depends on person and case.
- Menupoints:
 - ➔ General
 - Load / Save Project
 - Undo
 - New fit (→ new tabs: Fit function 2, Parameters 2, maybe even Fit setting 2)
 - ➔ Window
 - Show / hide options

- Load / Save Appearance
 - Plot parameters (or parameter derivatives, e.g. FWHM (Q^2) or $I_1 + I_2 \dots$, or EISF), also more than one on the same plot or to evaluate the results, χ^2 included
 - Plot data (and fit)
 - ➔ Data Input
 - Select data
 - Select resolution
 - ➔ Input manipulation
 - Rebin
 - Mask
 - Restore
 - Flat background from the resolution
 - ➔ Fit function
 - ➔ Fit setting
 - ➔ Parameters (handling → pop-up window, saving, loading)
 - ➔ Output
 - Data
 - Data + fit
- By default, the following could appear in the main window (as resizable subwindows):
- graphical fit result (with zooming, log, selective plot possibilities)
 - fit parameters