Data Analysis

We will use DAVE Mslice to plan for experiments, visualize and analyze the data.

Steps:

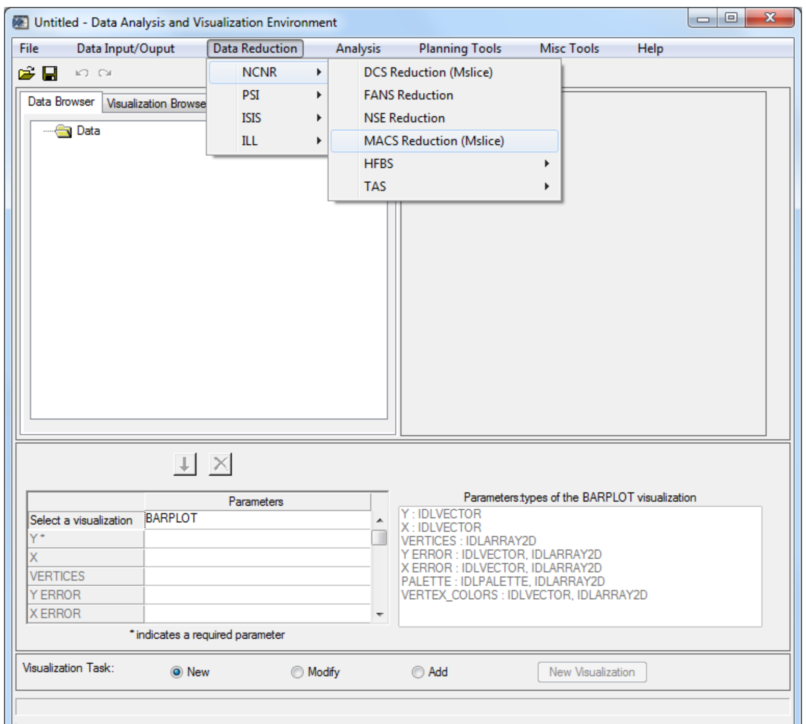
- Start DAVE. Use Mslice for experiment planning.
- Load and plot constant E data.
- Load data and plot H vs E dispersion slice.
- Figure out J and overplot the dispersion curve.
- Plot χ''T vs $\hbar\omega/k_B T$ at $\tilde{q}=\pi$(H=0.5).
- Fit to the scaling function.

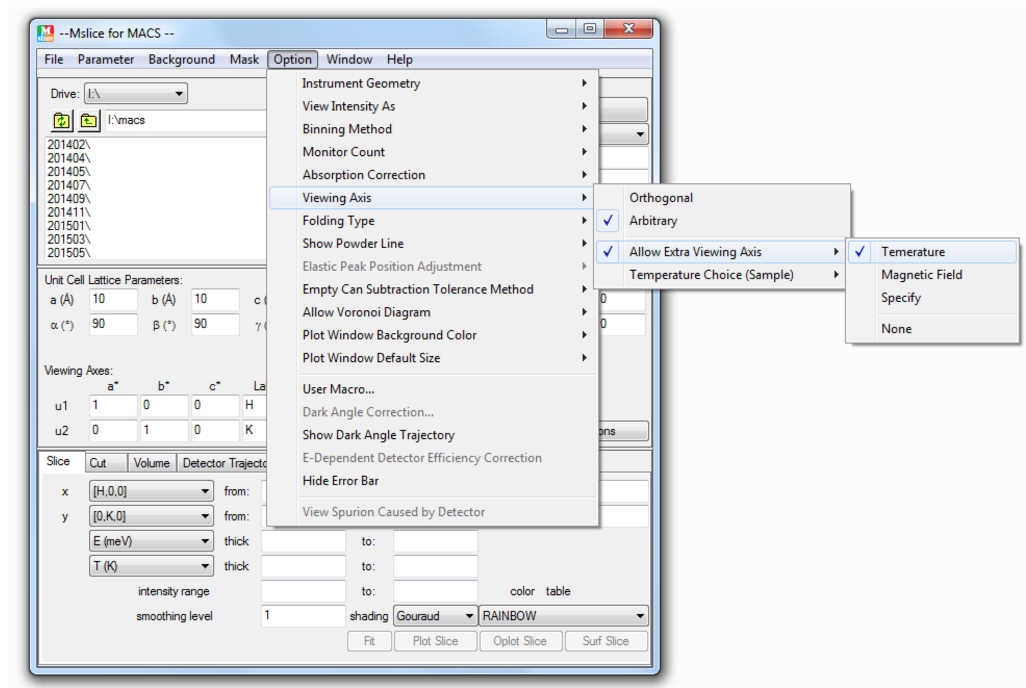
$$\chi''(\tilde{q}=\pi,\omega)=\frac{\pi}{T}Im\left[\rho^2\left(\frac{\hbar\omega}{4\pi k_B T}\right)\right]$$

$$\rho(x)=\frac{\Gamma\left(\frac{1}{4}-ix\right)}{\Gamma\left(\frac{3}{4}-ix\right)}$$

DAVE Mslice

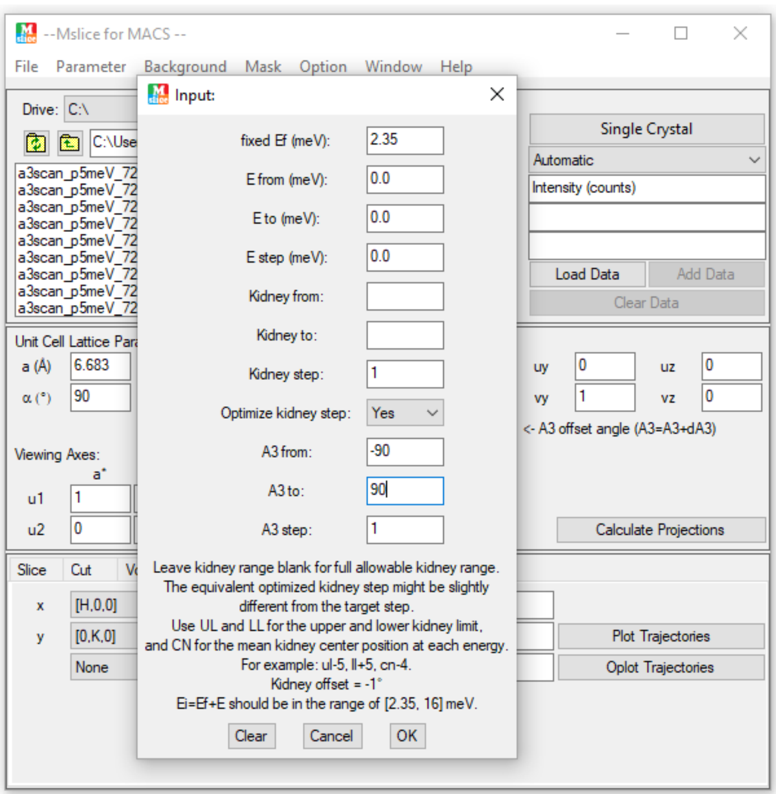
- DAVE->File->Preferences: set data and working directory
- DAVE->Data Reduction->NCNR->MACS Reduction (Mslice)
- Mslice->Option->View Intensity As->S(Q,omega)
- Mslice->Option->Viewing Axis->Allow Extra Viewing Axis->Temperature

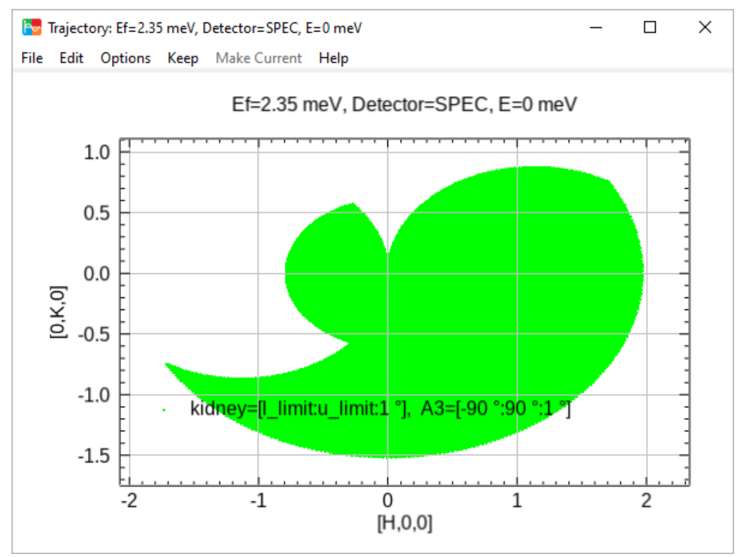




Experiment Planning

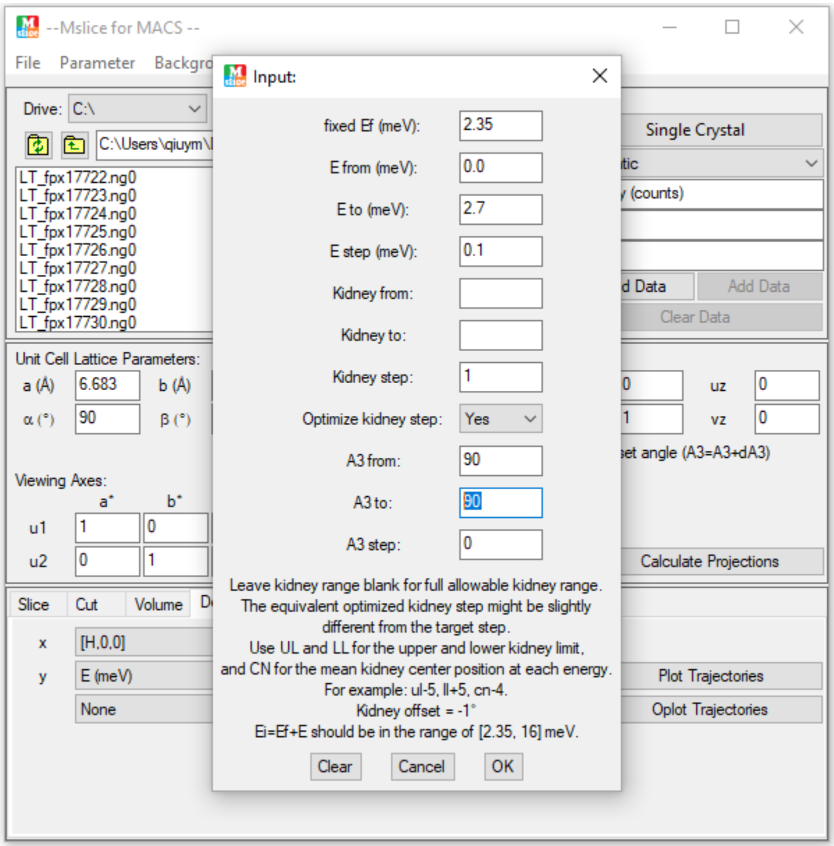
- Enter the lattice parameters and crystal orientation:
  a=6. 683, b=5. 142, c=11. 732, α = β = γ =90,
  u=(1 0 0), v=(0 1 0).
  Or load one data file to preload the lattice parameters, then clear the data.
- Click Calculate Projections button without any data files for experiment planning. Plot detector trajectory H vs K.



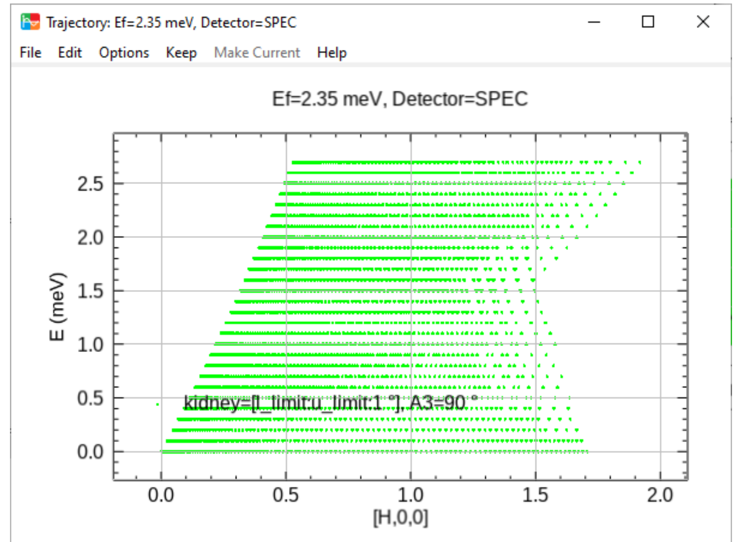


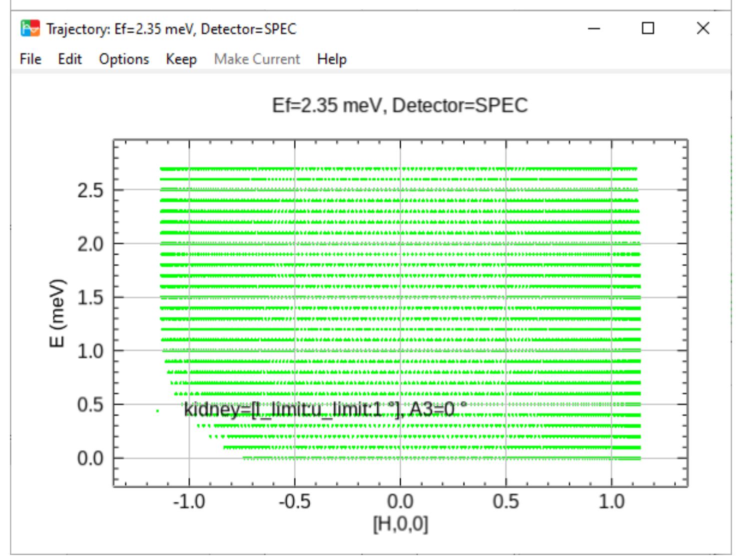
Constant E map.

Experiment Planning



Plot H vs E trajectory.



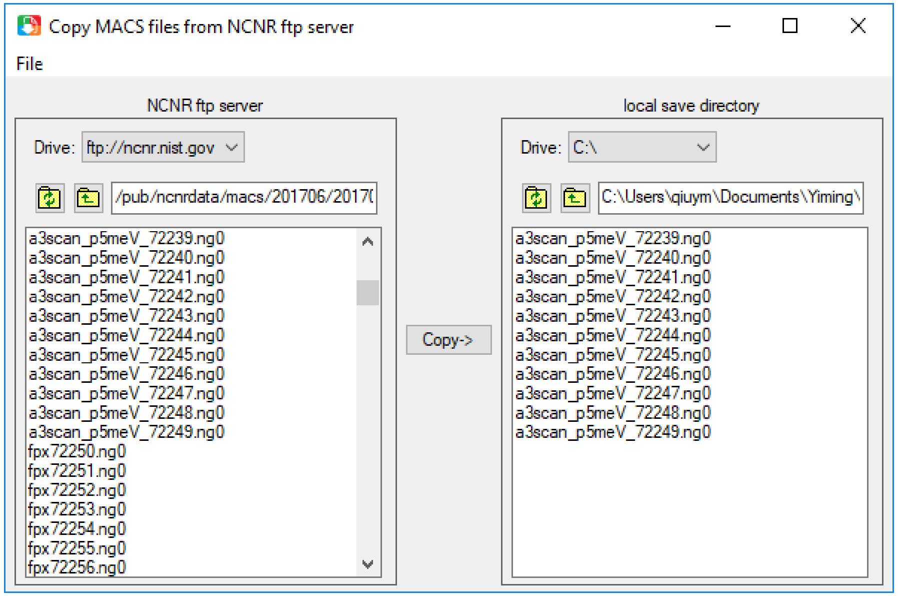


Data Files

- To remotely access NCNR data files, enable the NCNR ftp directory in mslice menu Option->Allow NCNR Ftp Server.
  For windows computer, the ftp directory is ftp://ncnr.nist.gov
  in the drive list. For Mac computers, the ftp directory is in the NCNR_ftp directory in the root directory.
- Or download the files from the ftp site to your computer and view them locally. You can use the tool in the mslice menu File->File Tools->Copy Files from NCNR FTP Server to download the files.
- File list:

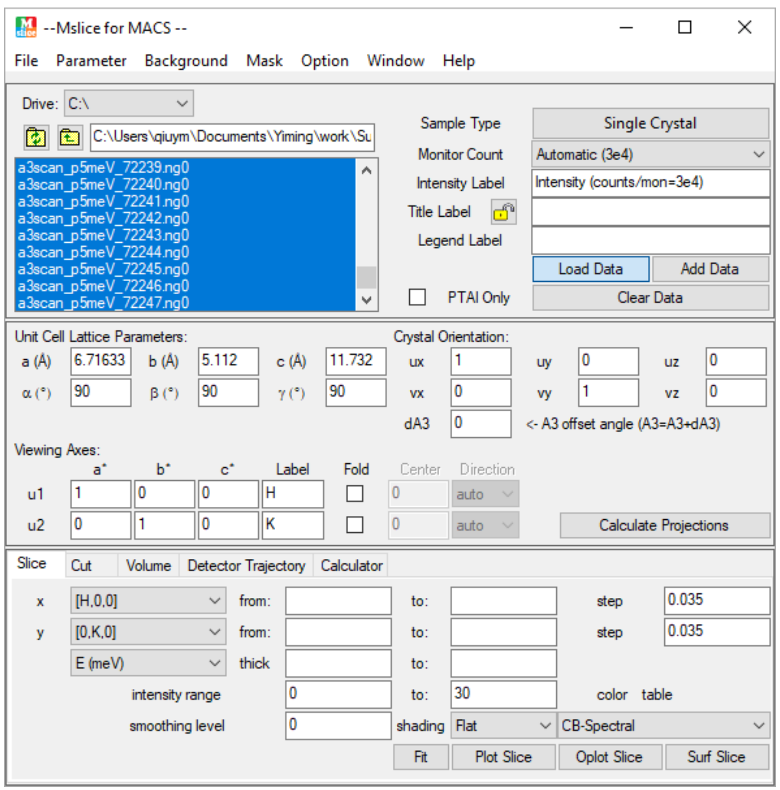
Constant-E A3 scan files:
macs/201706/20170619/data
a3scan_p5meV_72239-72249

Dispersion data files:
macs/201304/20130425/data/
Low-T: (LT_)fpx17722-fpx17879
High-T: (HT_)fpx18314-fpx18397
Empty can: (EC_)fpx18023-fpx18100



Load Data

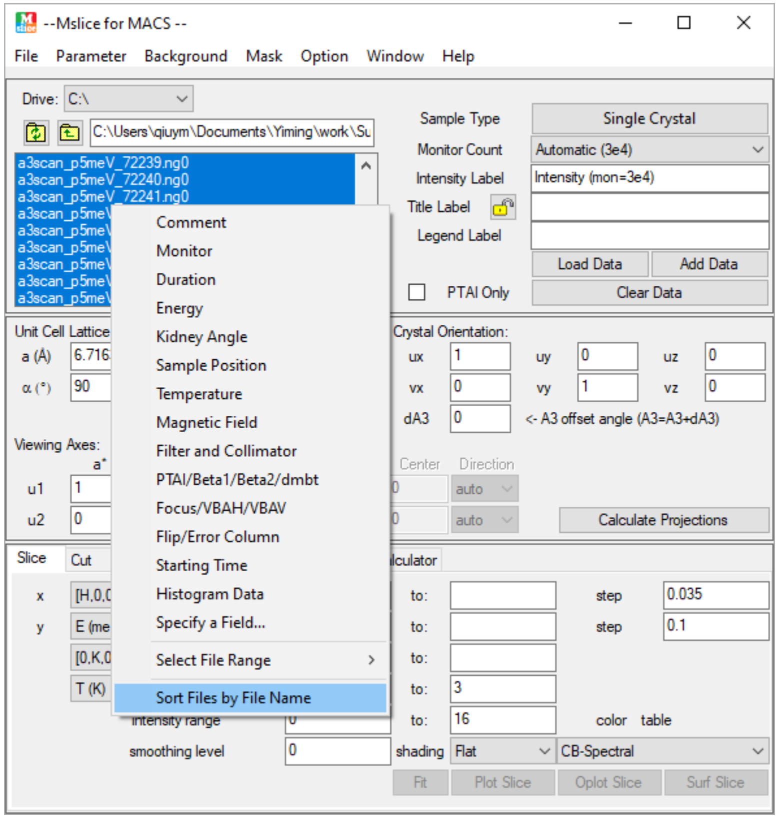
- Choose the data files in the file list panel. Right click to view file info. Press Load Data button to load data. Press Add Data button to append data.
- For background files, choose them in the file list, then in the background menu, click Load Empty Can File(s).



Constant-E A3 scan files:
macs/201706/20170619/data
A3scan_p5meV_72239-72249

Dispersion data files:
macs/201304/20130425/data/
Low-T: LT_fpx17722-17879
High-T: HT_fpx18314-18397
Empty can: EC_fpx18023-18100

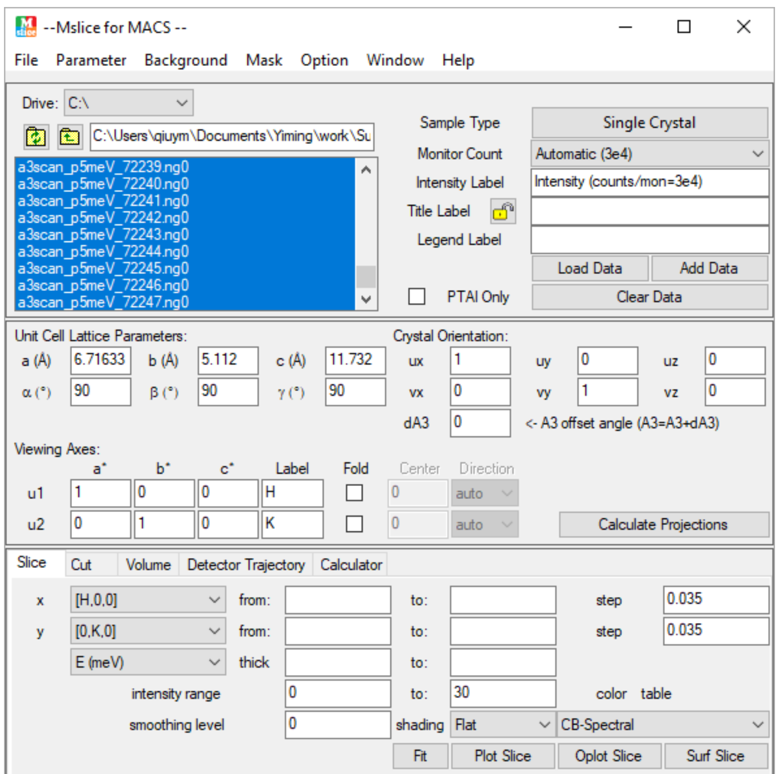
- Right click on the file selector to sort the files by file name.

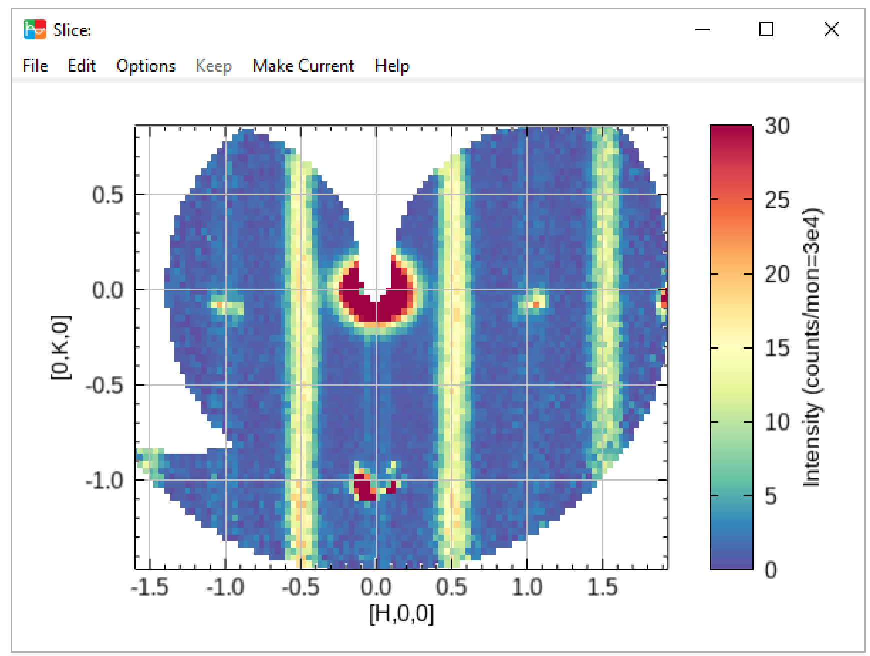


- Disable the monitor lambda/2 correction in the menu Option->Monitor Count->Apply Monitor Lambda/2 Correction.
- Set zero intensity error bar to 1 in the menu Option->Binning Method->Zero Intensity Error->User Specify.

Plot Constant-E Slice

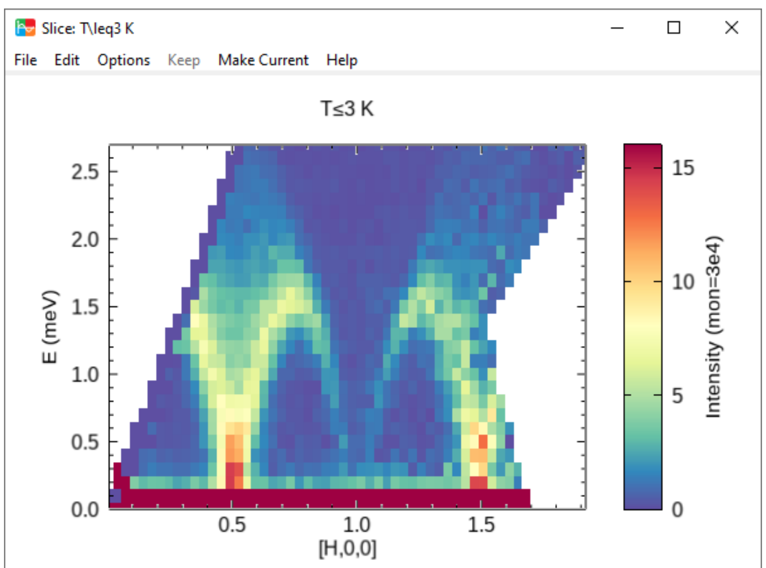
- Load a3 scan files a3scan_p5meV_72239-72249.
- Make sure u1=(1,0,0) and u2=(0,1,0). Press Calculate Projections button.
- In the slice panel, choose [H,0,0] as x axis, step 0.035, and [0,K,0] as y axis, step 0.035. Press Plot Slice button to plot the H vs K contour plot.
- Keep the plot window.

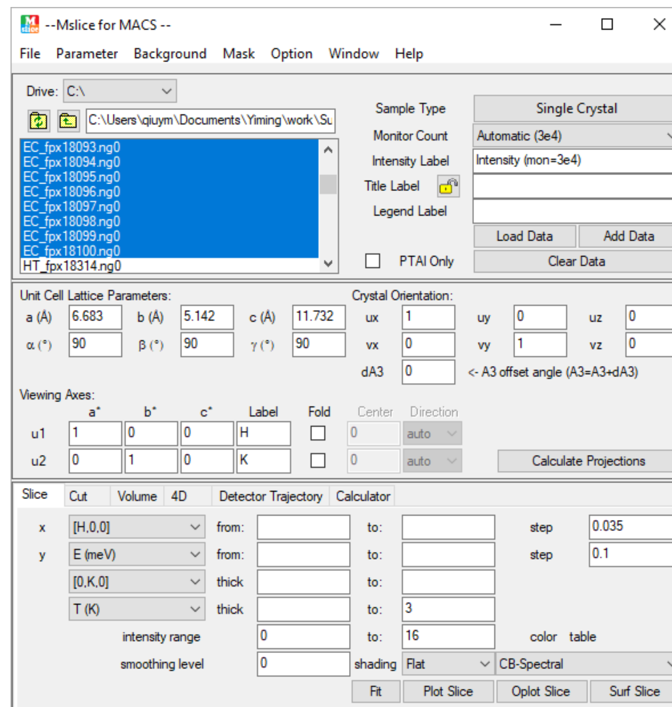




Plot H vs E dispersion Slice

- Load low-T (17722-17879) and high-T (18314-18397) data files. Load empty can files (18023-18100) as background.
- Increase the empty can subtraction tolerance in the menu Parameter-> Change Empty Can Subtraction Tolerance Value to 0.015 for energy, 0.15 for kidney, and 0.1 for A3.
- In the slice panel, choose [H,0,0] as x axis, step 0.035, and E as y axis, step 0.1. Specify the temperature range. Press Plot Slice button to plot the H vs E contour plot.
- Keep the plot window.



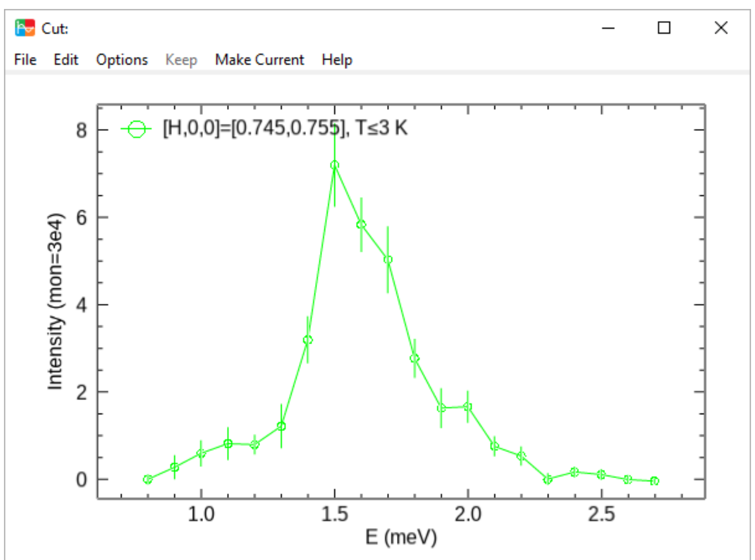


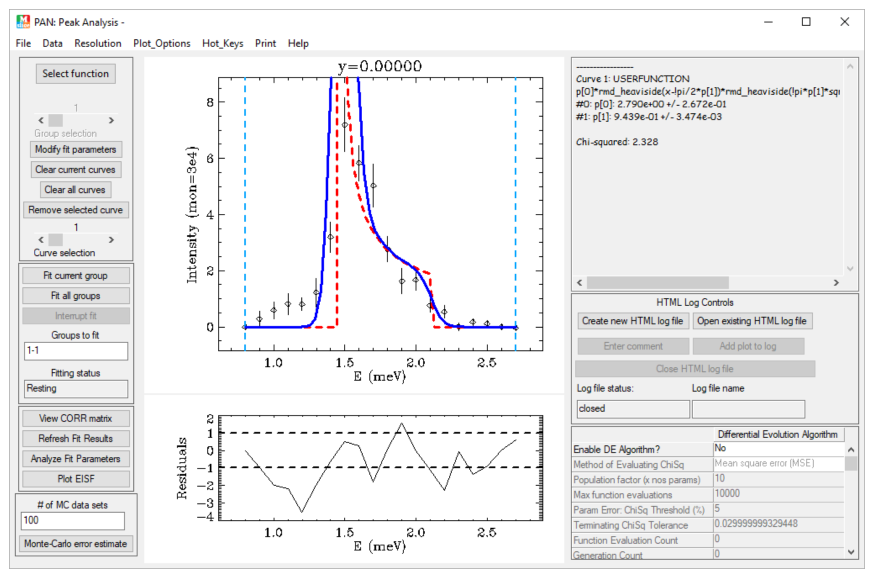
Plot & Fit Cut

- Make a cut along E, with [H,0,0] thickness range of [0.745,0.755] and T<3 K. x range starts from 0.79, step 0.1.
- Keep the plot window.
- Press Fit button in the Cut panel to fit the data. Use Müller Ansatz equ. as the user function (in one line, or use the restore expression to load the equation file equ_MullerAnsatz.eq. initial p[0]=3, p[1]=0.9):

```
p[0]*rmd_heaviside(x-!pi/2*p[1])*rmd_heaviside(!pi*p[1]*sqrt(2)/2-x)
/sqrt(abs(x^2-0.25*(!pi*p[1])^2))
```

- Load pre-generated resolution data (eresl_0p15meV.txt) from Resolution->Load ASCII Res File->Load 3-col ascii resolution function.





PHYSICAL REVIEW B VOLUME 24, NUMBER 3 1 AUGUST 1981

Quantum spin dynamics of the antiferromagnetic linear chain in zero and nonzero magnetic field

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Applying the sum rules (1.38), (1.42), and (1.45) to our analytic expression (1.16) for the dynamic correlation function of the HB AF

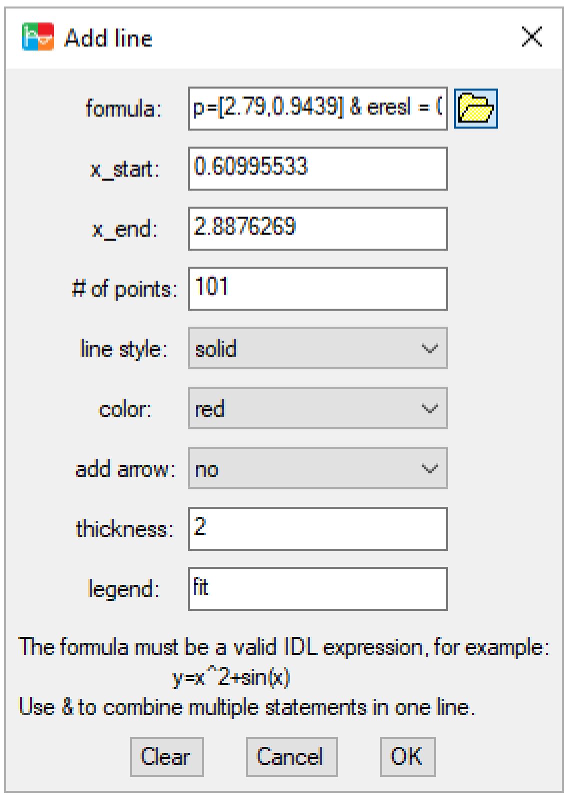
$$S_{zz}(q,\omega)=\frac{A}{(\omega^2-\frac{1}{4}\pi^2J^2\sin^2 q)^{1/2}}\Theta\left[\omega-\frac{\pi}{2}J\sin q\right]\times\Theta\left[\pi J\sin\left(\frac{q}{2}\right)-\omega\right] \tag{1.48}$$

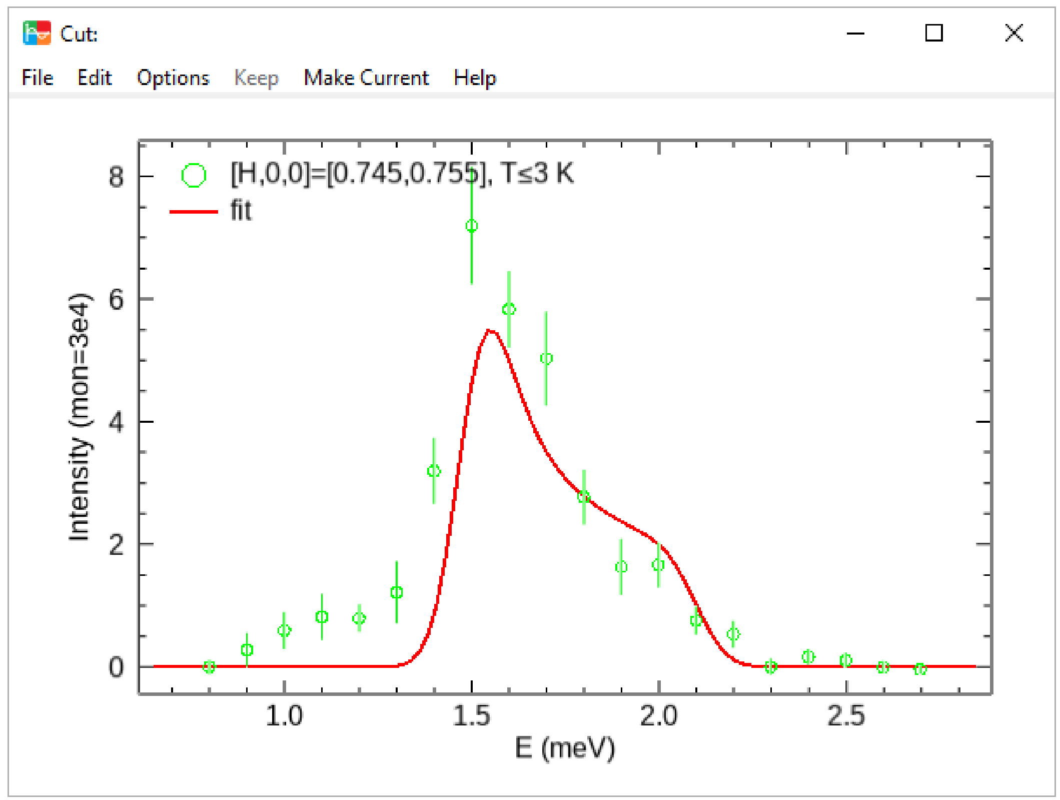
where $\Theta(x)$ is the step function.

- Add a line to the plot from Edit->Add Line :

```
p=[2.79,0.9439] & eresl=0.15 y = gauss_smooth(p[0]*rmd_heaviside(x-!pi/2*p[1])*rmd_heaviside(!pi*p[1]*sqrt(2)/2-x)/sqrt(abs(x^2-0.25*(!pi*p[1])^2)),eresl/(x[1]-x[0])/sqrt(8.*alog(2)))
```

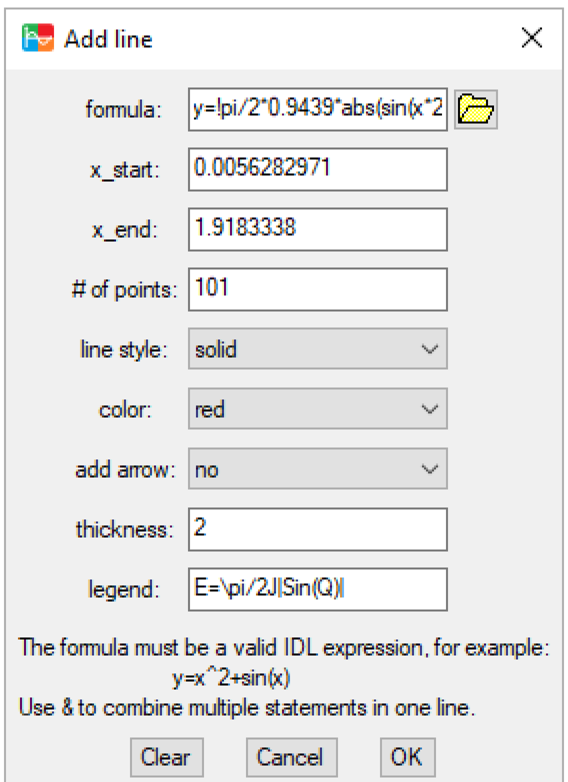
(Or use line equation file line_equation_Ecut.txt.)

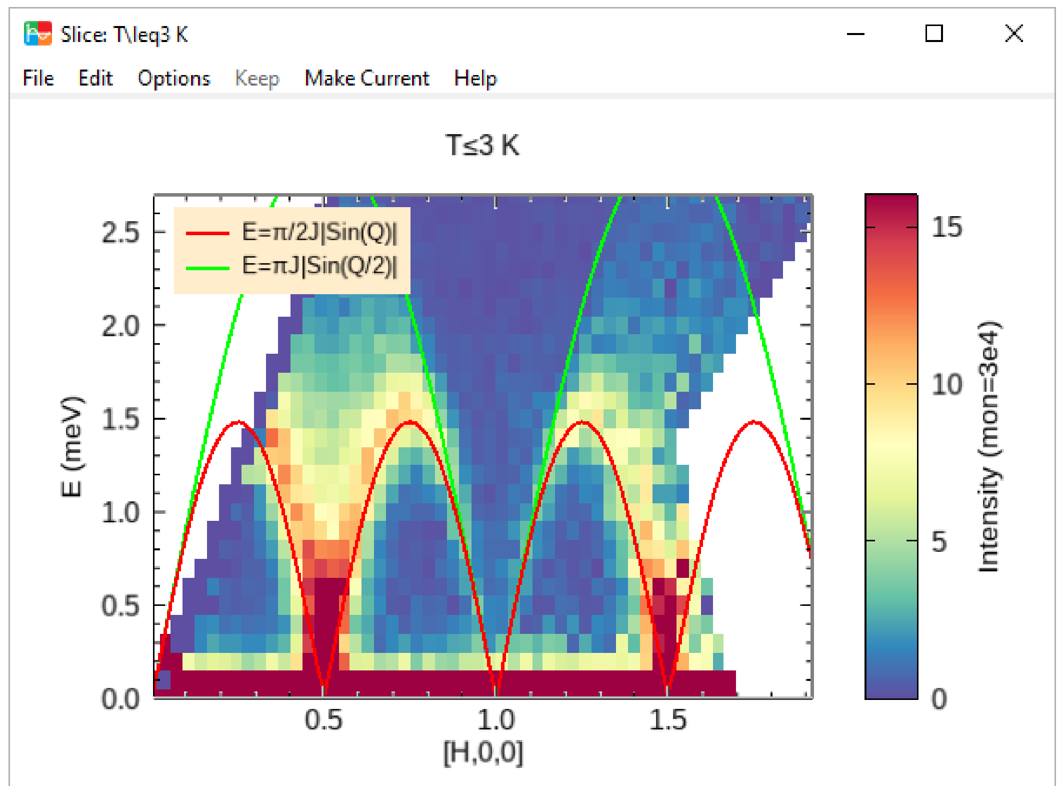




Overplot the Dispersion Curve

- Overplot the lower and upper bound of the continuum in the H vs E window from Edit->Add Line. The formula for the lower bound is `y=!pi/2*0.9439*abs(sin(x*2*!pi))`. Use `E=\pi/2J|Sin(Q)|` as legend. The fomula for the upper bound is `y=!pi*0.9439*abs(sin(x*!pi))`. Use `E=\piJ|Sin(Q/2)|` as legend.



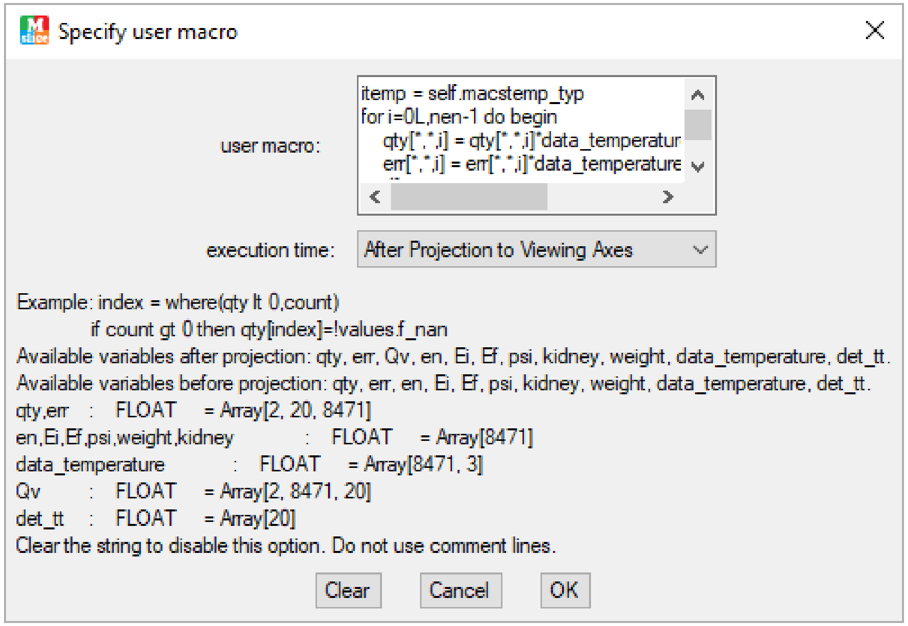


Plot $\chi''T$ vs $\hbar\omega/k_BT$

- In mslice menu Option->User Macro, enter the following script (macro.txt):

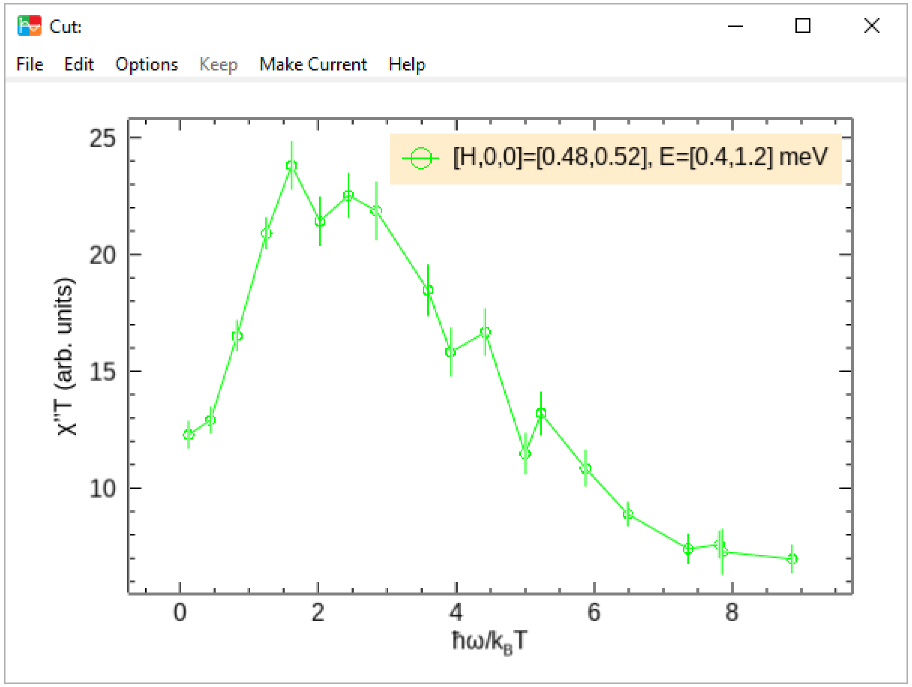
```
itemp = self.macstemp_typ
for i=0L,nen-1 do begin
    qty[*,*,i] = qty[*,*,i]*data_temperature[i,itemp]
    err[*,*,i] = err[*,*,i]*data_temperature[i,itemp]
endfor
data_temperature[*,itemp] = en/(kb*data_temperature[*,itemp])
```

- Choose the execution time to be After Projection to Viewing Axes.



Plot $\chi''T$ vs $\hbar\omega/k_BT$

- Choose Option->View Intensity As-> Chi(Q,omega)
- Recalculate the projection.
- In the cut panel, cut along T, which is E/k_BT now, remove the range, set the step to 0.4. Set H thickness range [0.48,0.52], and E thickness range [0.4,1.2].
- Plot cut. In the plot window, change the x-axis title to \HW/k!dB!nT, and y-axis title to \chi''T (arb. units).



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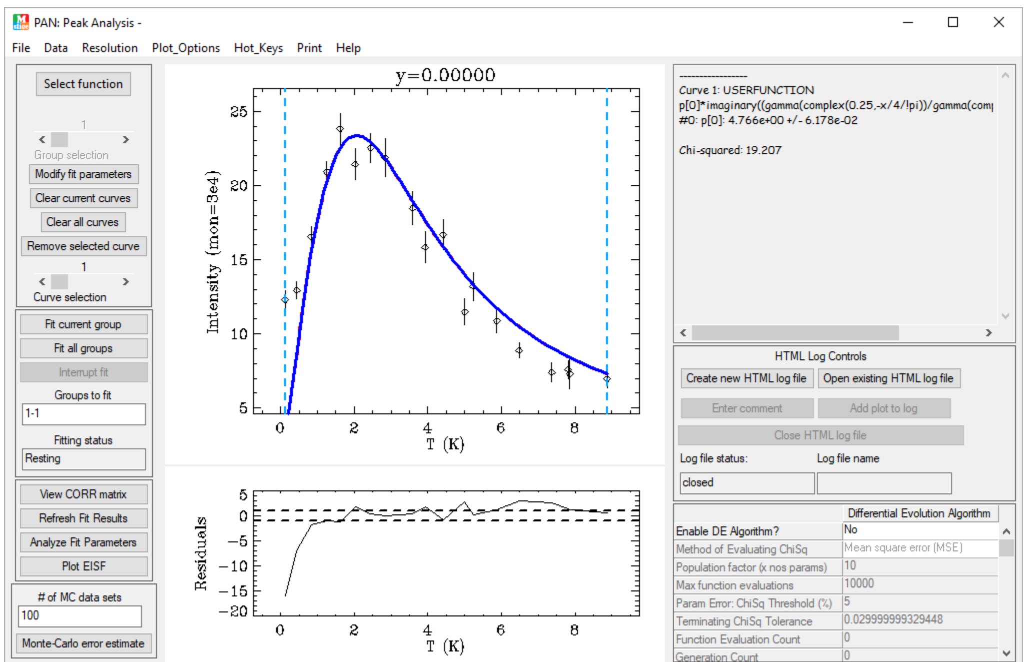
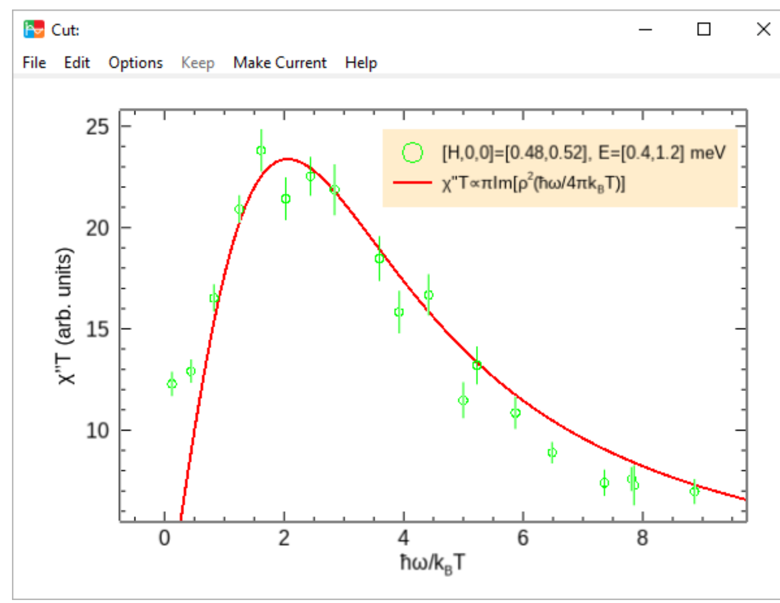
Fit to Scaling Function

- Press Fit button. In PAN, choose user function as the fitting function:
  `p[0]*imaginary((gamma(complex(0.25,-x/4/!pi))/gamma(complex(0.75,-x/4/!pi)))^2)`
  (equ_Scaling.eq)
- Add a line of the scaling function to the previous $\chi''T$ vs $\hbar\omega/k_BT$ plot.
  `y=4.766*imaginary((gamma(complex(0.25,-x/4/!pi))/gamma(complex(0.75,-x/4/!pi)))^2)`
  with `\chi"T\propto\piIm[\rho!u2!n(\HW/4\pik!dB!nT)]` as legend.





Nature Materials **4**, 329 - 334 (2005)
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Subject Categories: Magnetic materials | Computation, modelling and theory

Quantum criticality and universal scaling of a quantum antiferromagnet

Bella Lake[1,2,4], D. Alan Tennant[2,3,5], Chris D. Frost[3] and Stephen E. Nagler[1]

that at the antiferromagnetic zone centre (AFZC) $q_{\mathrm{AFZC}} = \pi/c$, the dynamical structure factor is given by

$$S(\pi,E) = \frac{e^{E/kT}}{e^{E/kT}-1}\,\frac{A}{T}\mathrm{Im}\left[\rho\left(\frac{E}{4\pi T}\right)^{2}\right] \qquad (3)$$

where $\rho(x) = \Gamma(1/4-ix)/\Gamma(3/4-ix)$ and A is a constant[16]. It is clear from this equation that the structure factor multiplied by temperature depends only on the dimensionless ratio of E to T rather than on these quantities separately, and therefore obeys universal scaling. The ideal