Data Analysis

We will use DAVE Mslice to visualize and analyze the data.

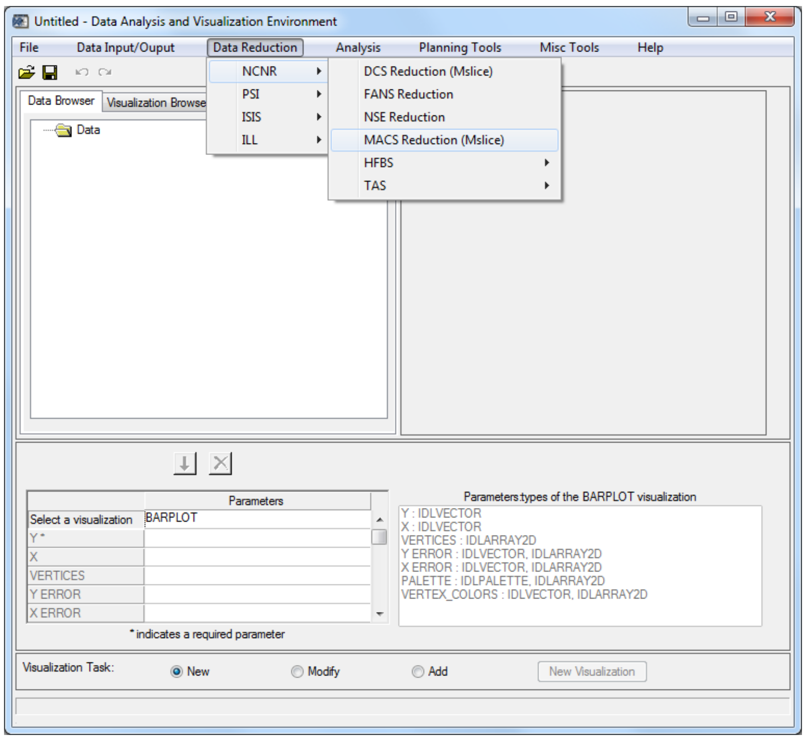
Steps:

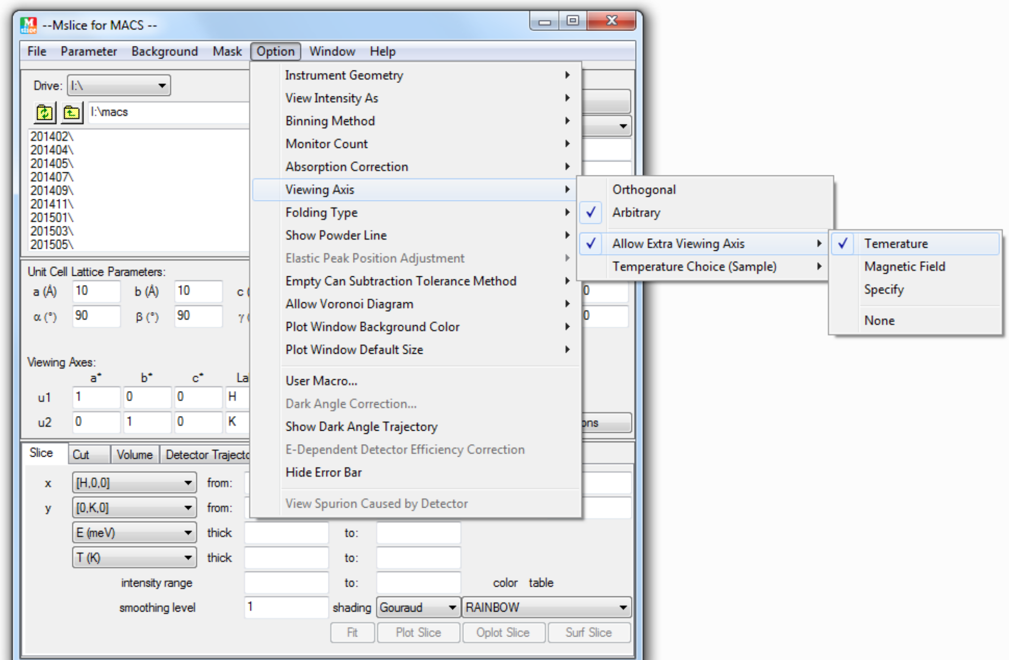
- Start DAVE Mslice.
- Load and plot constant E data.
- Load data and plot H vs E dispersion slice.
- Figure out J and overplot the dispersion curve.
- Plot $\chi''T$ vs $\hbar\omega/k_B T$ at $\tilde{q}=\pi$(H=0.5).
- Fit to the scaling function.

$$\chi''(\tilde{q}=\pi,\omega)=\frac{\pi}{T} Im\left[\rho^2\left(\frac{\hbar\omega}{4\pi k_B T}\right)\right] \qquad \rho(x)=\frac{\Gamma\left(\frac{1}{4}-ix\right)}{\Gamma\left(\frac{3}{4}-ix\right)}$$

DAVE Mslice

- DAVE->Data Reduction->NCNR->MACS Reduction (Mslice)
- Mslice->Option->View Intensity As->S(Q,omega)
- Mslice->Option->Viewing Axis->Allow Extra Viewing Axis->Temperature



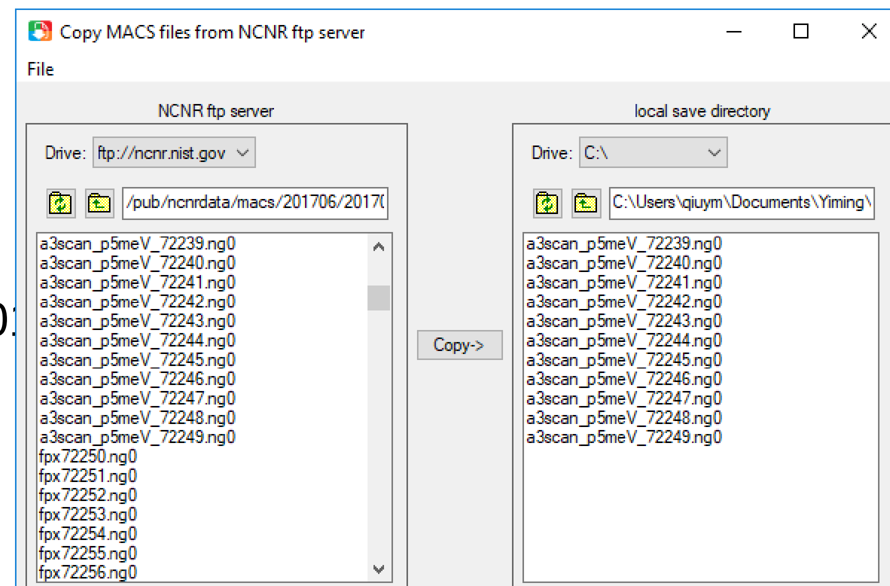


Data Files

- Use the NCNR ftp directory in mslice to remotely load data files. 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 you 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
72239-72249

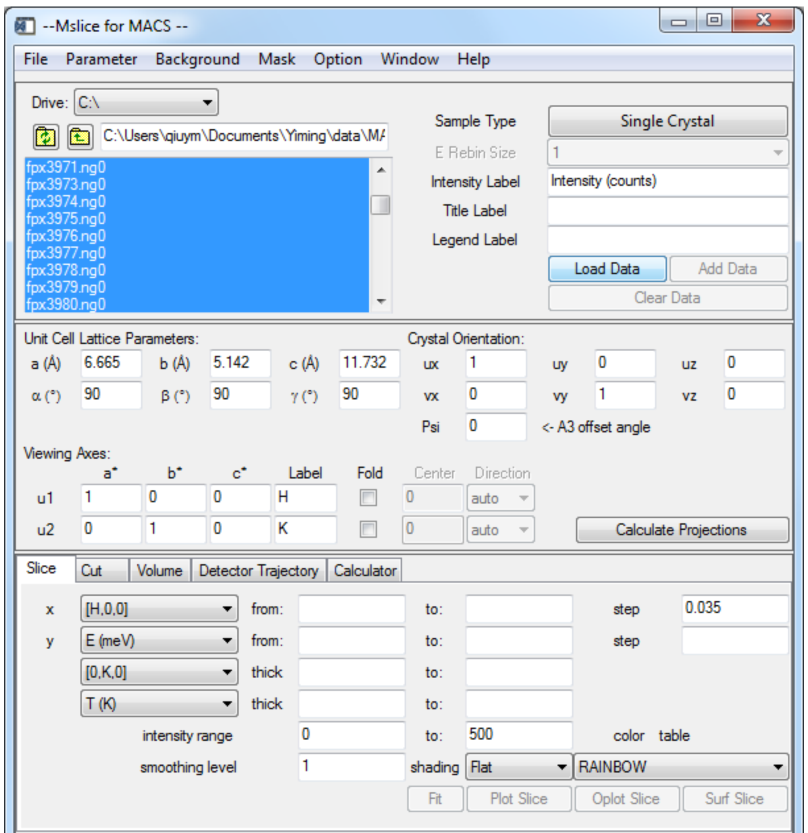
Dispersion data files: macs/201304/20
Low-T: fpx17722-fpx17879
High-T: fpx18314-fpx18397
Empty can: fpx18023-fpx18100



https://tinyurl.com/acns-eresl https://tinyurl.com/acns-macs

Load Data

- Choose the data files in the file list panel. Right click to view file info. Press Load Data button. 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).

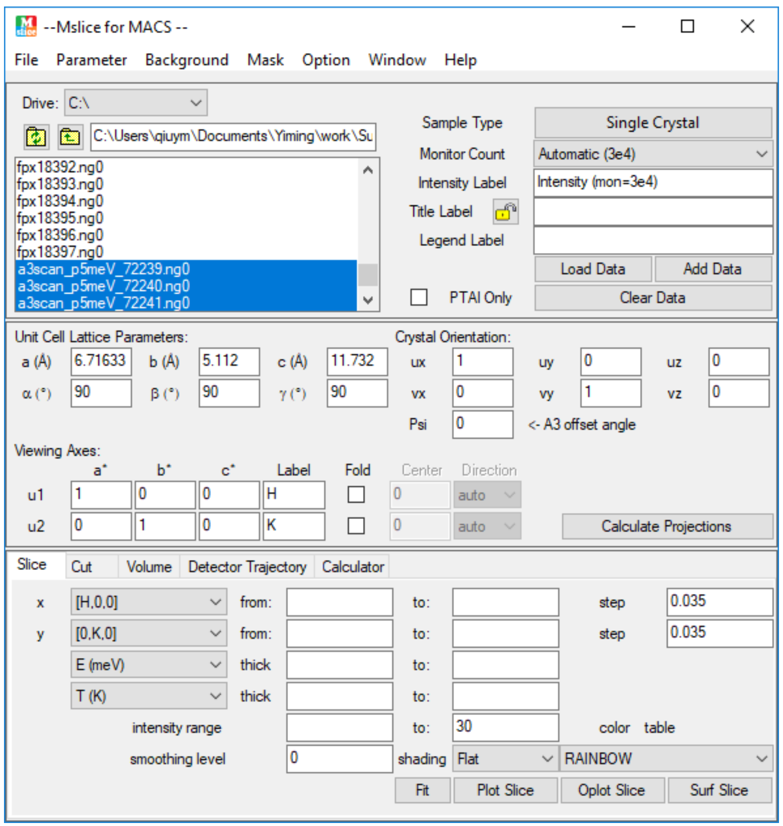


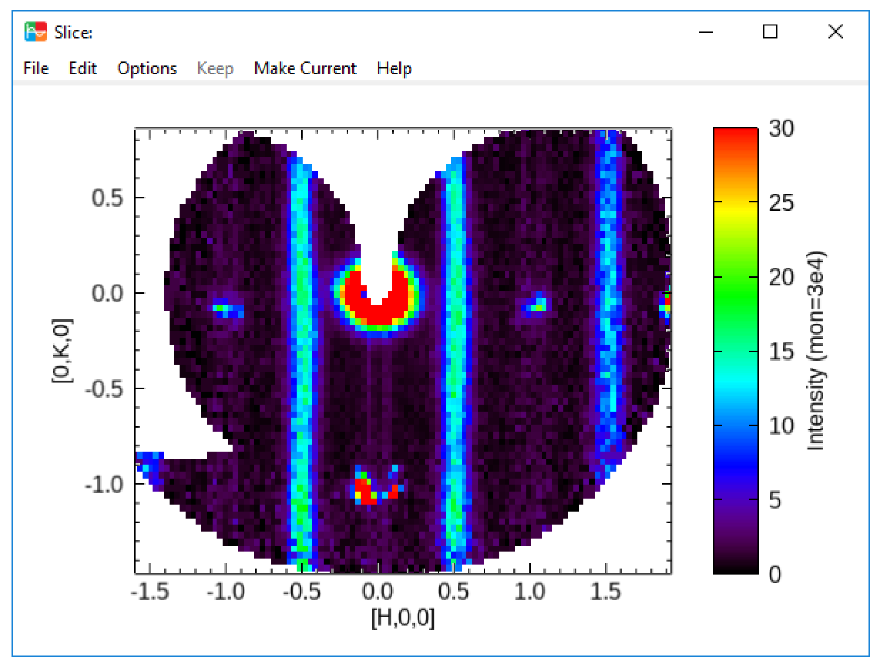
Constant-E A3 scan files:
macs/201706/20170619/data
72239-72249

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

Plot Constant-E Slice

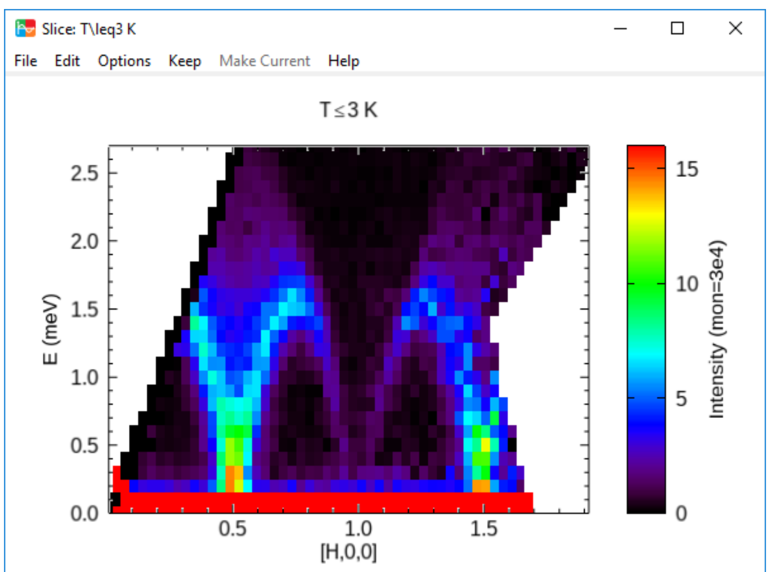
- Load a3 scan files 72239-72249
- Make sure u1=(1,0,0) and u2=(0,1,0). Press Calculate Projections button.
- In the slice panel, choose [H,0,0] as x axis, step 0.035, and [0,K,0] as
- y axis, step 0.035. Press Plot Slice button to plot the H vs K contour plot.
- Keep the plot window.

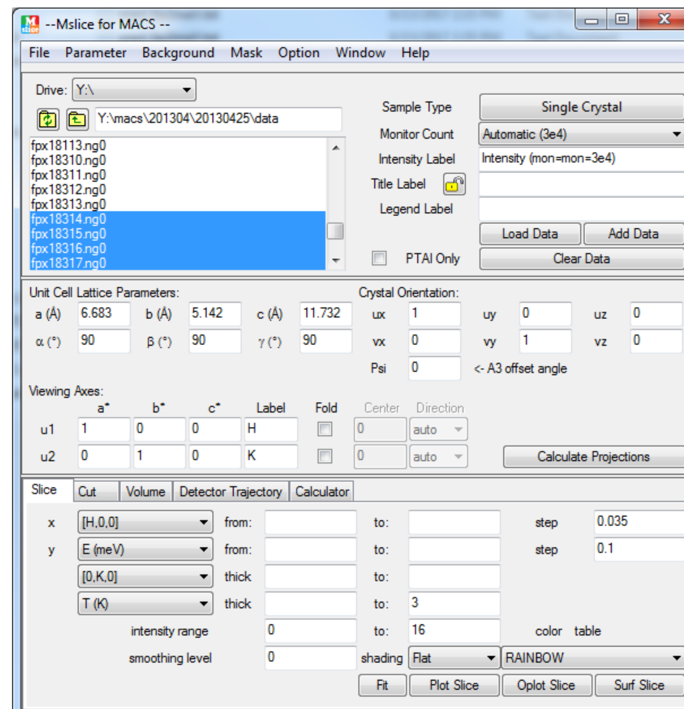




Plot H vs E dispersion Slice

- Load low-T (17722-17879) and high-T (18314-18397) data files. Load empty can files (18023-18100) as background.
- Disable the monitor lambda/2 correction in the Option menu. Calculate projection. Increase the empty can subtraction tolerance in the Parameter menu to 0.015 for energy and 0.15 for kidney.
- 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.



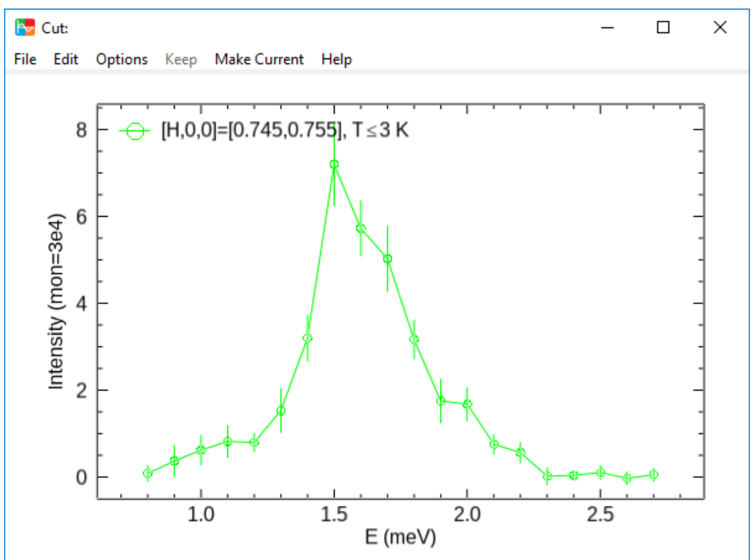


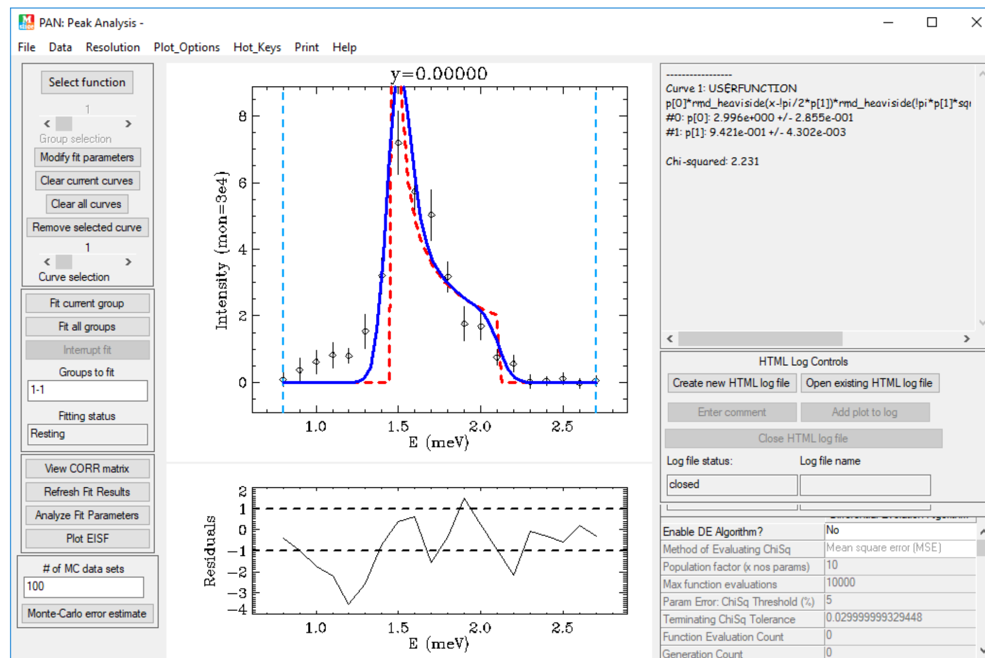
Plot & Fit Cut

- 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, 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 from Resolution->Load ASCII Res File.





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

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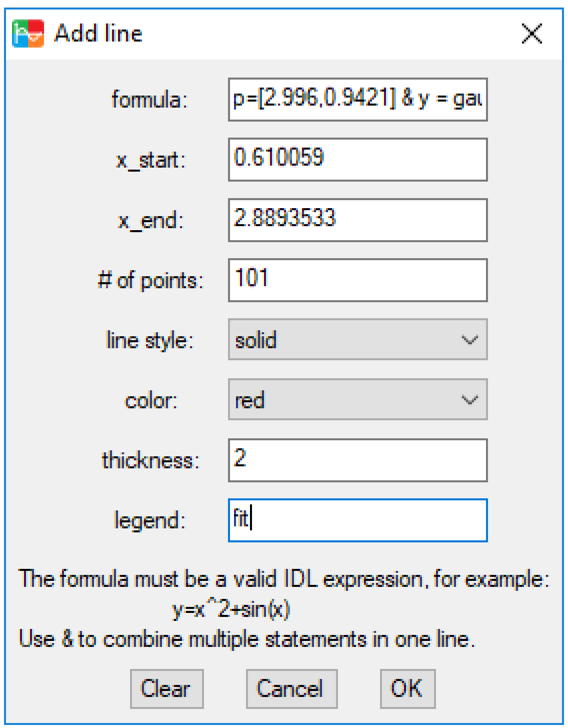
Applying the sum rules (1.38), (1.42), and (1.45) to our analytic expression (1.16) for the dynamic correlation function of the HB AF

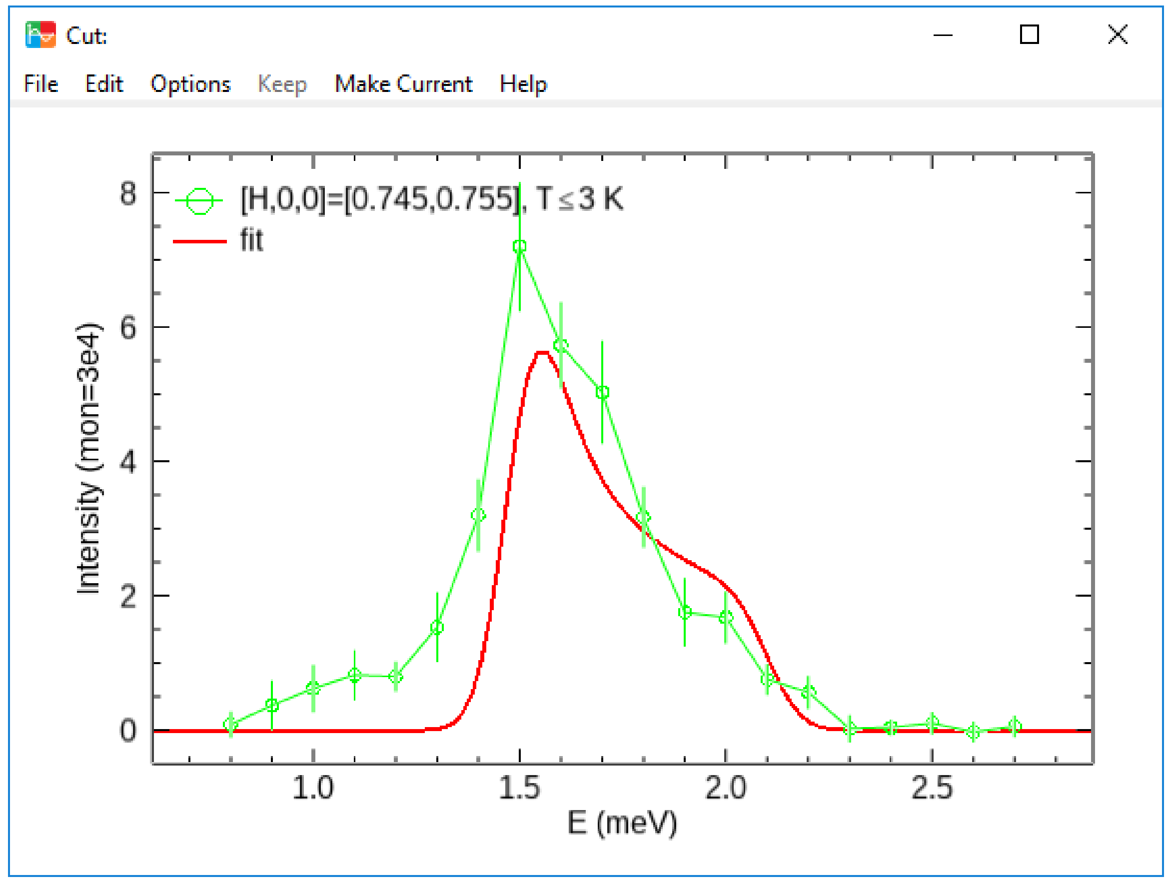
$$S_{zz}(q,\omega)=\frac{A}{\left(\omega^2-\frac{1}{4}\pi^2J^2\sin^2 q\right)^{1/2}}\Theta\left[\omega-\frac{\pi}{2}J\sin q\right]\times\Theta\left[\pi J\sin\left|\frac{q}{2}\right|-\omega\right] \qquad (1.48)$$

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

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

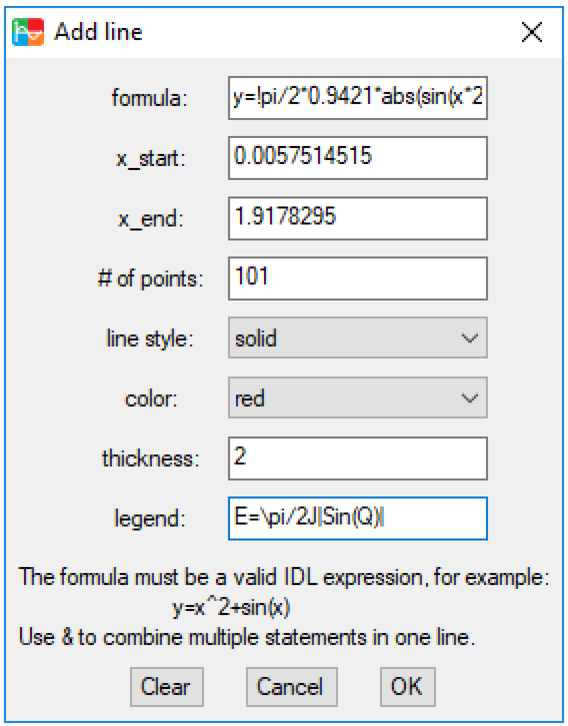
```
p=[2.996,0.9421] & y = gauss_smooth(p[0]*rmd_heaviside(x-!pi/2*p[1])*
rmd_heaviside(!pi*p[1]*sqrt(2)/2-x)/sqrt(abs(x^2-0.25*(!pi*p[1])^2)),
0.15/(x[1]-x[0])/sqrt(8.*alog(2)))
```

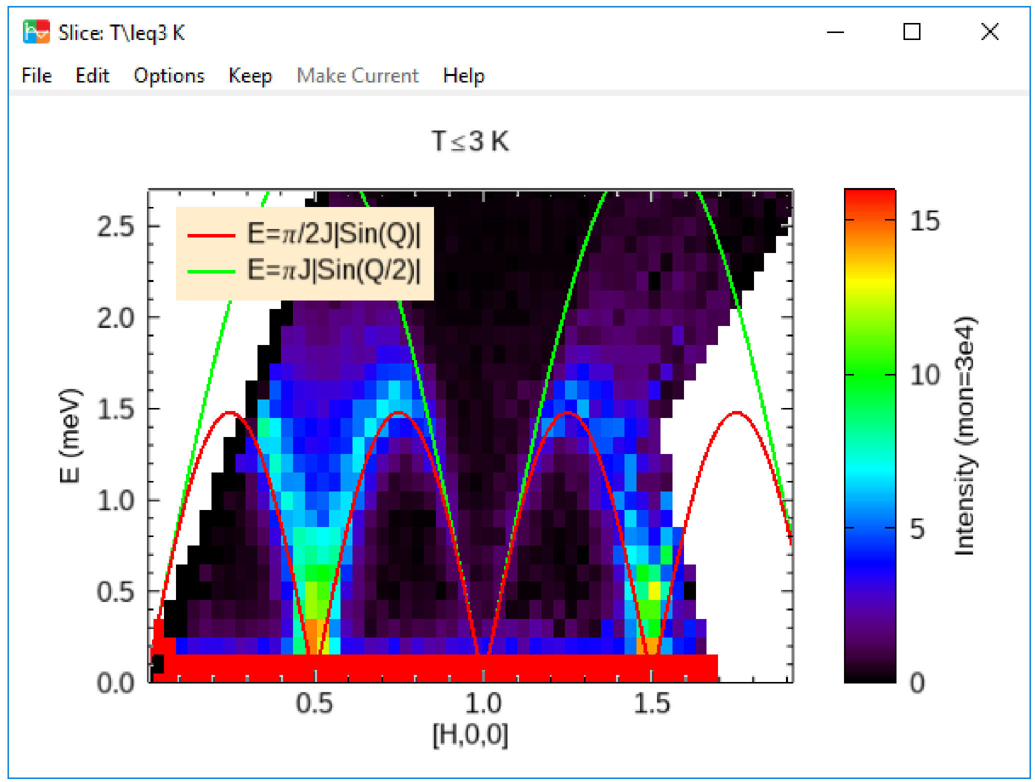




Overplot the Dispersion Curve

- 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*0.9421*abs(sin(x*2*!pi))`. Use `E=\pi/2J|Sin(Q)|` as legend. The fomula for the upper bound is `y=!pi*0.9421*abs(sin(x*!pi))`. Use `E=\piJ|Sin(Q/2)|` as legend.



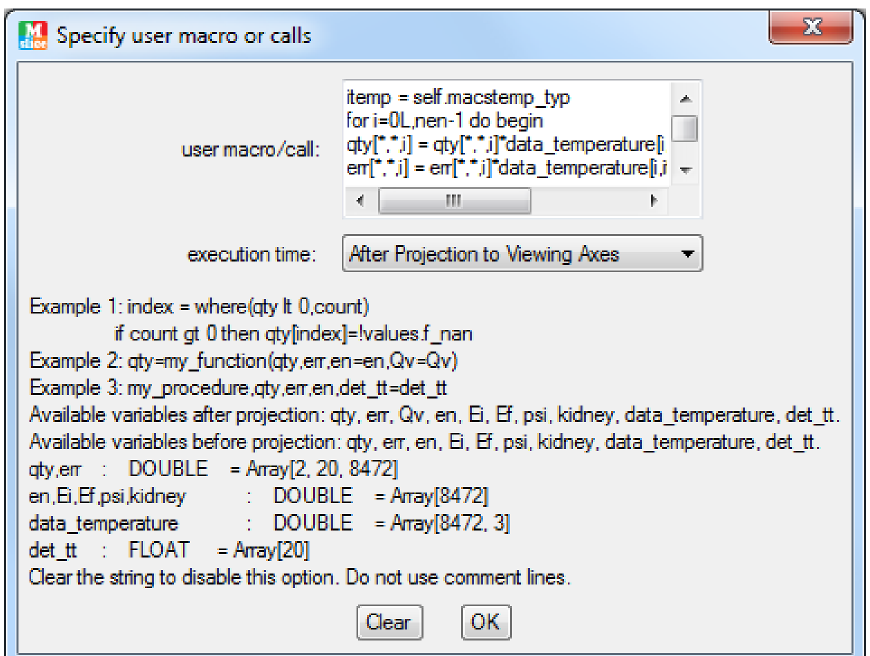


Plot $\chi'' T$ vs $\hbar\omega/k_B T$

- In mslice menu Option->User Macro, enter the following script:

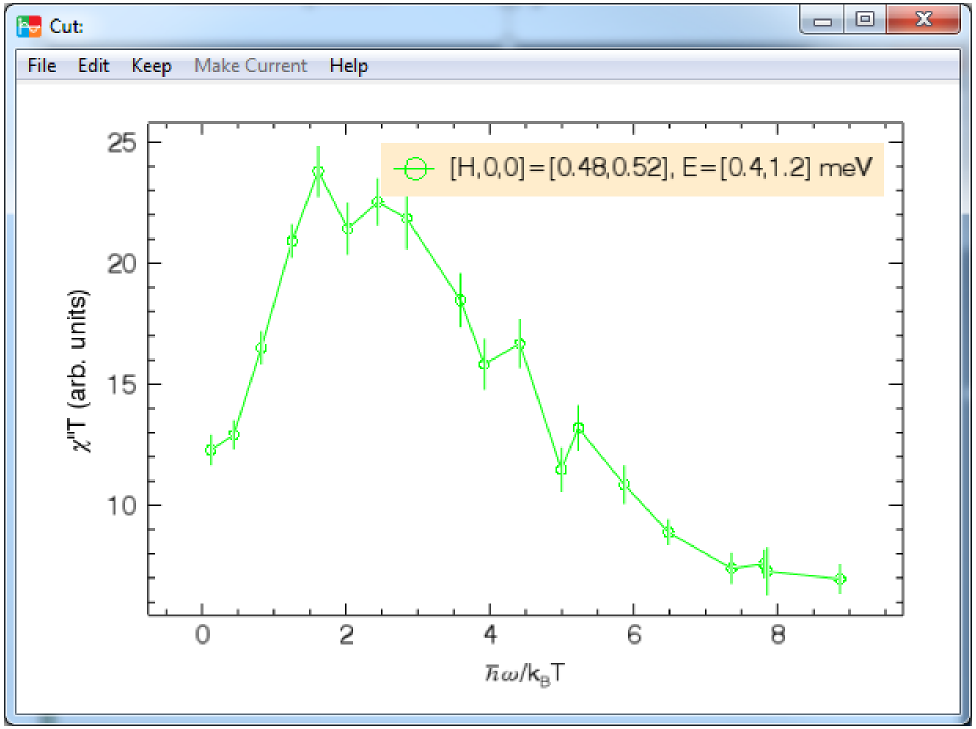
```
itemp = self.macstemp_typ
for i=0L,nen-1 do begin
    qty[*,*,i] = qty[*,*,i]*data_temperature[i,itemp]
    err[*,*,i] = err[*,*,i]*data_temperature[i,itemp]
endfor
data_temperature[*,itemp] = en/(kb*data_temperature[*,itemp])
```

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



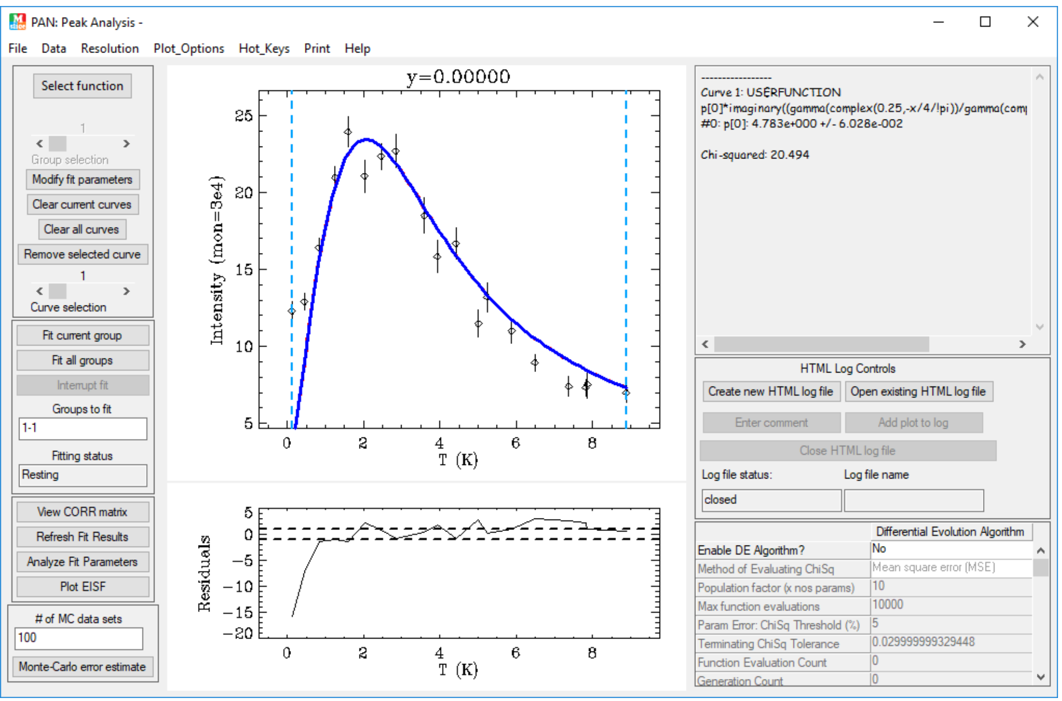
Plot $\chi''T$ vs $\hbar\omega/k_BT$

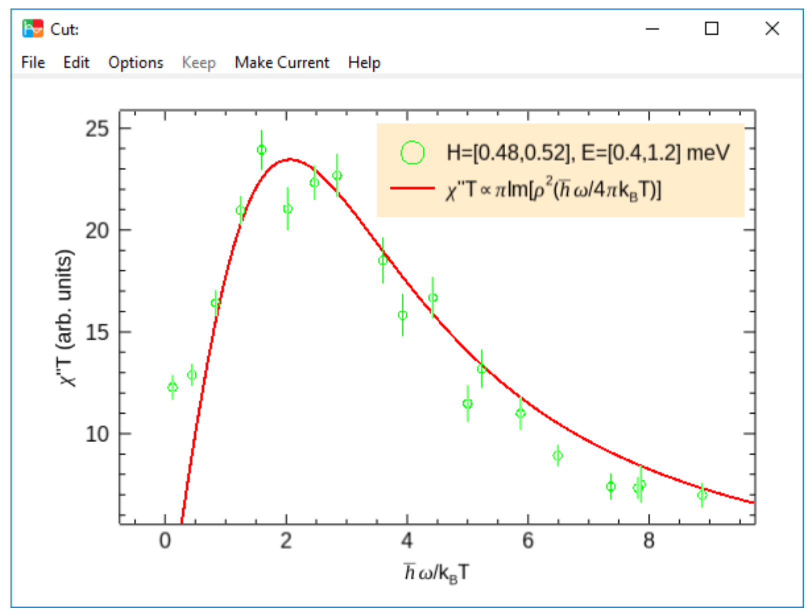
- Choose Option->View Intensity As-> Chi(Q,omega)
- Recalculate the projection.
- In the cut panel, cut along T, which is E/k_BT now, step 0.4.
  Set H thickness range [0.48,0.52], and E thickness range [0.4,1.2].
- Plot cut. In the plot window, change the x-axis title to \HW/k!dB!nT, and y-axis title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



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)
- Add a line of the scaling function to the previous $\chi''T$ vs $\hbar\omega/k_BT$ plot.
  y=4.783*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.





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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) $q_{AFZC} = \pi/c$, 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