

# Data Analysis

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

Steps:

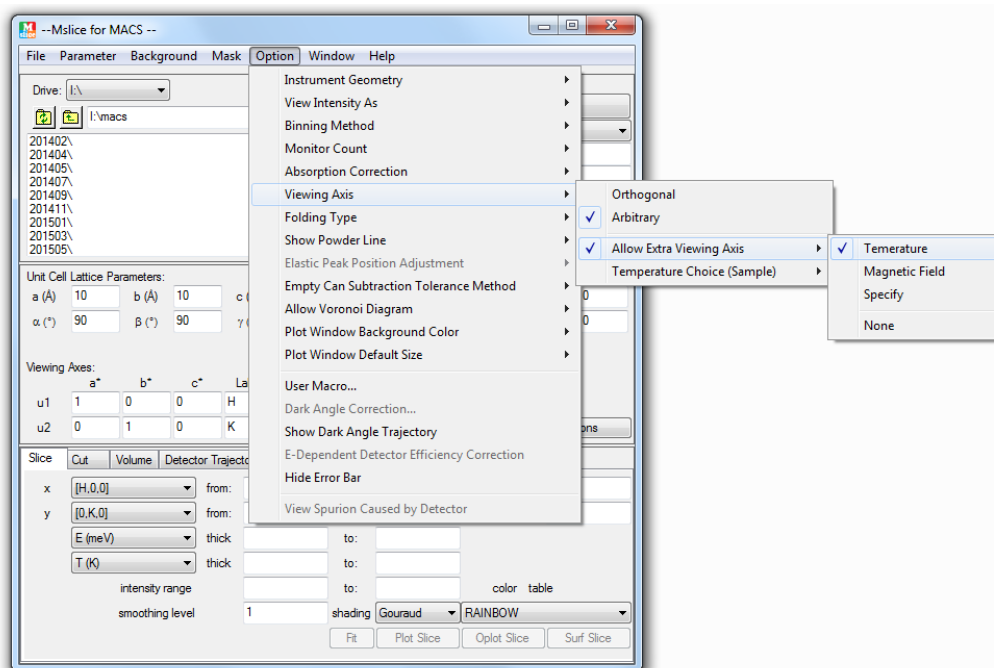
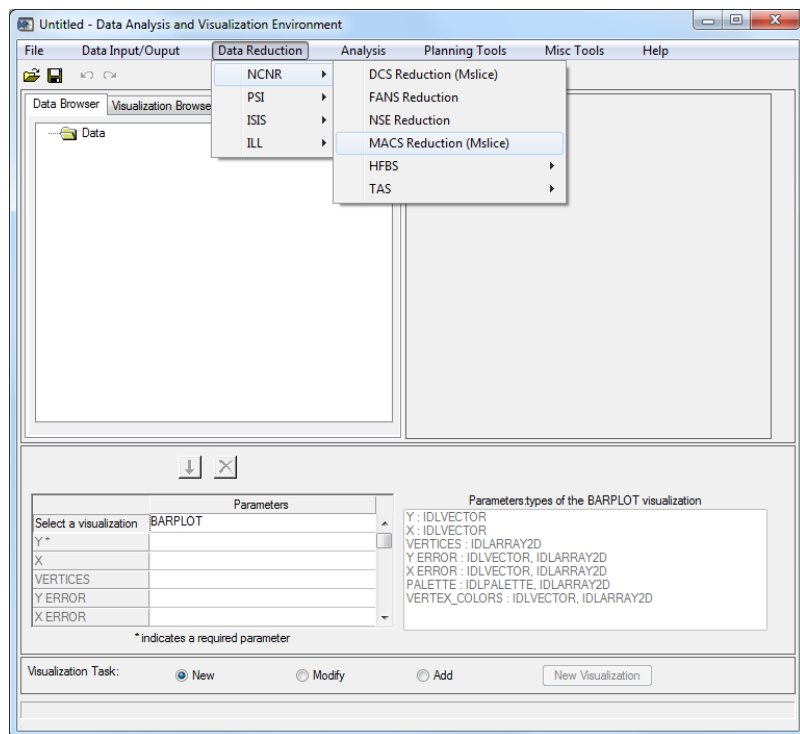
- Start DAVE. Use Mslice for experiment planning.
- Load and plot constant E data.
- Load data and plot H vs E dispersion slice.
- Figure out J and overplot the dispersion curve.
- Plot  $\chi''T$  vs  $\hbar\omega/k_B T$  at  $\tilde{q}=\pi(H=0.5)$ .
- Fit to the scaling function.

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

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

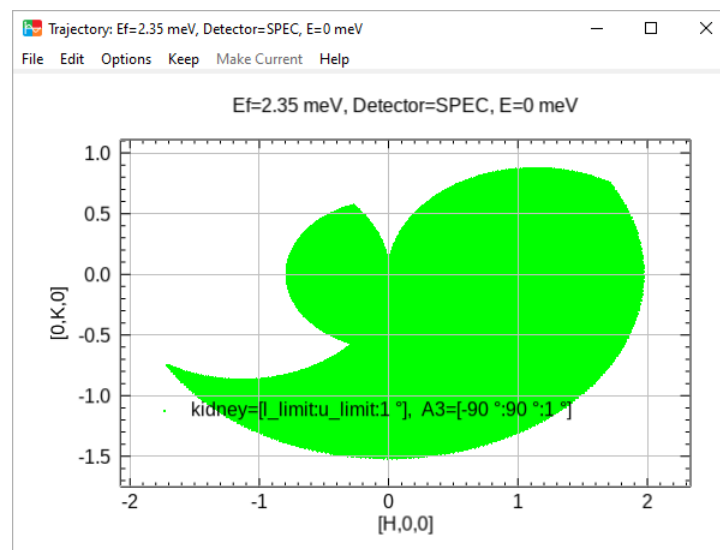
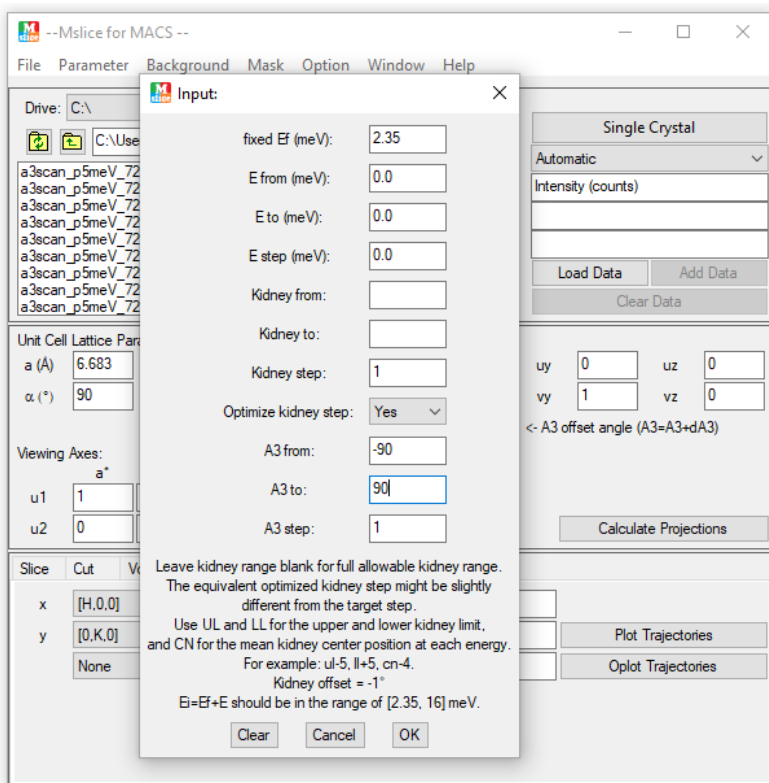
# DAVE Mslice

- Download DAVE (latest development version) from <https://www.ncnr.nist.gov/dave/download.html>.
- 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:  
 $a=6.683$ ,  $b=5.142$ ,  $c=11.732$ ,  $\alpha = \beta = \gamma = 90$ ,  
 $u=(1 \ 0 \ 0)$ ,  $v=(0 \ 1 \ 0)$ .  
 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.

--Mslice for MACS --

File Parameter Background

Drive: C:\

C:\Users\qium\...

LT\_fpx17722.ng0  
LT\_fpx17723.ng0  
LT\_fpx17724.ng0  
LT\_fpx17725.ng0  
LT\_fpx17726.ng0  
LT\_fpx17727.ng0  
LT\_fpx17728.ng0  
LT\_fpx17729.ng0  
LT\_fpx17730.ng0

Unit Cell Lattice Parameters:

a (Å) 6.683 b (Å)  
α (°) 90 β (°)

Viewing Axes:

a\* b\*  
u1 1 0  
u2 0 1

Slice Cut Volume D

x [H,0,0]  
y E (meV)  
None

Input:

fixed Ef (meV): 2.35  
E from (meV): 0.0  
E to (meV): 2.7  
E step (meV): 0.1  
Kidney from:  
Kidney to:  
Kidney step: 1  
Optimize kidney step: Yes  
A3 from: 90  
A3 to: 90  
A3 step: 0

Single Crystal

tic

y (counts)

d Data Add Data  
Clear Data

0 uz 0  
1 vz 0

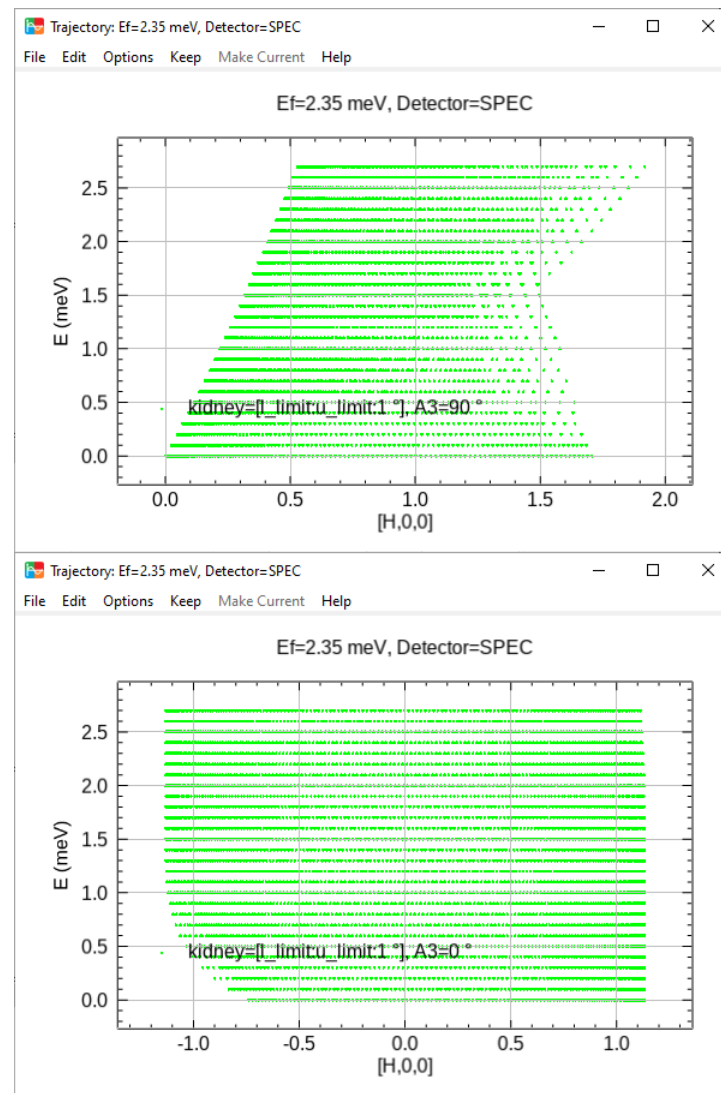
net angle (A3=A3+dA3)

Calculate Projections

Plot Trajectories  
Oplot Trajectories

Leave kidney range blank for full allowable kidney range.  
The equivalent optimized kidney step might be slightly different from the target step.  
Use UL and LL for the upper and lower kidney limit, and CN for the mean kidney center position at each energy.  
For example: ul-5, ll+5, cn-4.  
Kidney offset = -1°  
Ei=Ef+E should be in the range of [2.35, 16] meV.

Clear Cancel OK



# Data Files

- To remotely access NCNR data files, enable the NCNR ftp directory in mslice menu **Option->Allow NCNR Data Repository**.  
For windows computer, the ftp directory is <https://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 Data Repository** to download the files.
- File list:

Constant-E A3 scan files:

macs/201706/20170619/data  
a3scan\_p5meV\_72239-72249

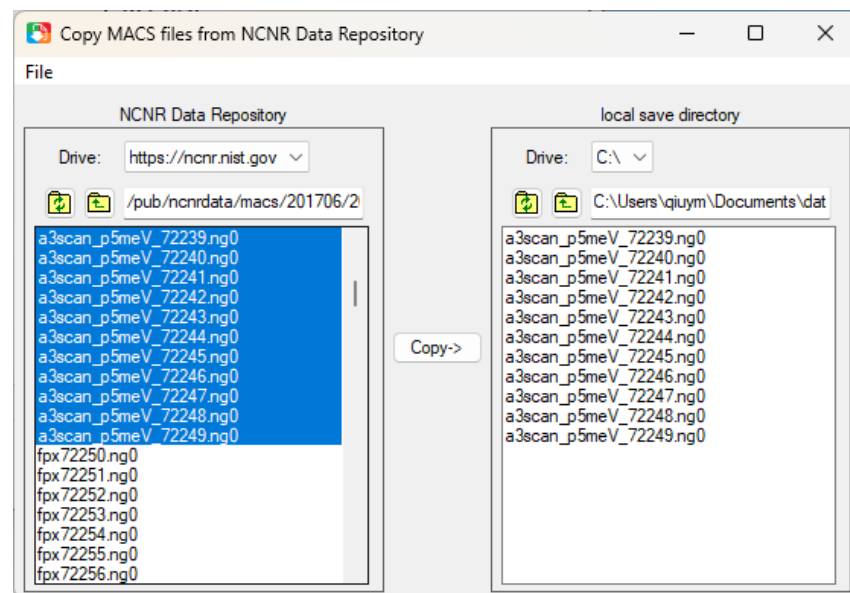
Dispersion data files:

macs/201304/20130425/data/

Low-T: (LT\_)fpx17722-fpx17879

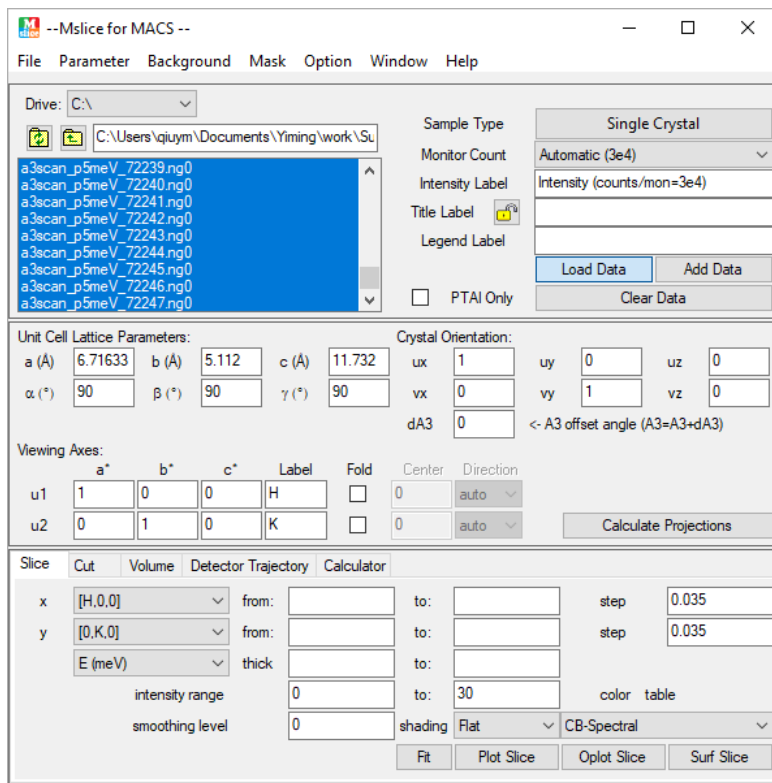
High-T: (HT\_)fpx18314-fpx18397

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)**.

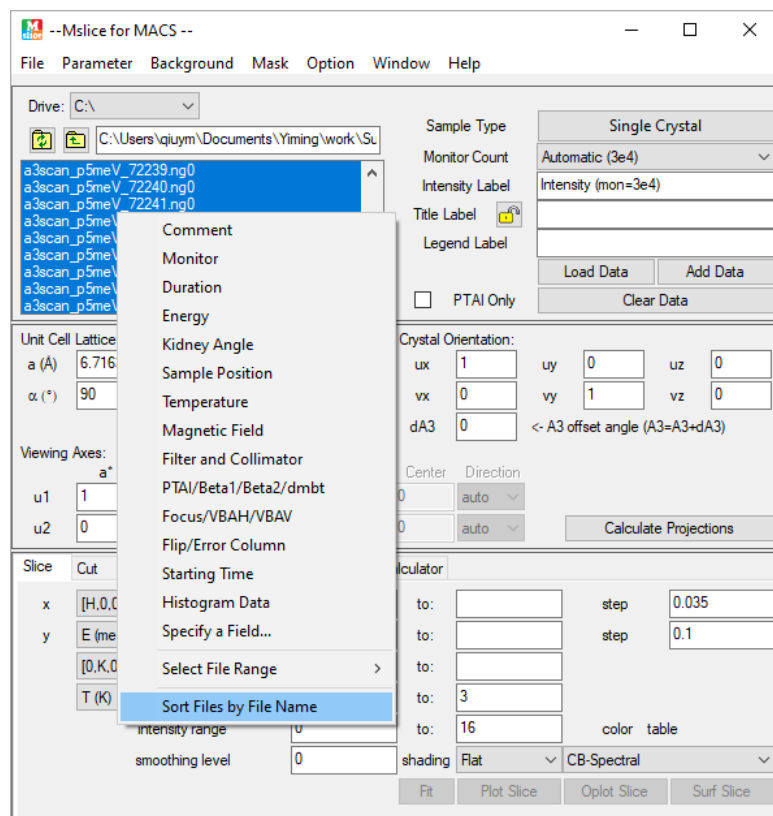


The screenshot shows the --Mslice for MACS -- software interface. The main window has a menu bar (File, Parameter, Background, Mask, Option, Window, Help) and a toolbar. The Drive is set to C:\. The file list shows several A3 scan files (a3scan\_p5meV\_72239.ng0 to a3scan\_p5meV\_72247.ng0). The Sample Type is Single Crystal, Monitor Count is Automatic (3e4), and Intensity Label is Intensity (counts/mon=3e4). The Title and Legend labels are empty. The Load Data and Add Data buttons are visible. The Unit Cell Lattice Parameters are: a (Å) 6.71633, b (Å) 5.112, c (Å) 11.732, α (°) 90, β (°) 90, γ (°) 90. The Crystal Orientation is: ux 1, uy 0, uz 0, vx 0, vy 1, vz 0, dA3 0. The Viewing Axes are: u1 1, u2 0, a\* 0, b\* 0, c\* 0, Label H, K, Center 0, Direction auto. The Slice panel shows Cut, Volume, Detector Trajectory, and Calculator tabs. The Calculator tab is active, showing x [H,0,0], y [0,K,0], E (meV), intensity range 0 to 30, smoothing level 0, shading Flat, and CB-Spectral. The Fit, Plot Slice, Oplot Slice, and Surf Slice buttons are at the bottom.

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

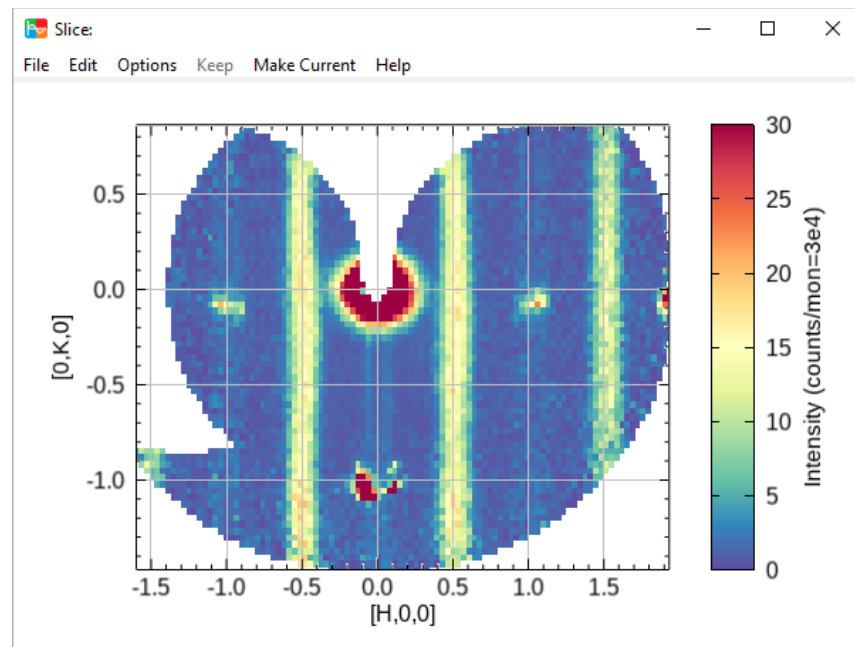
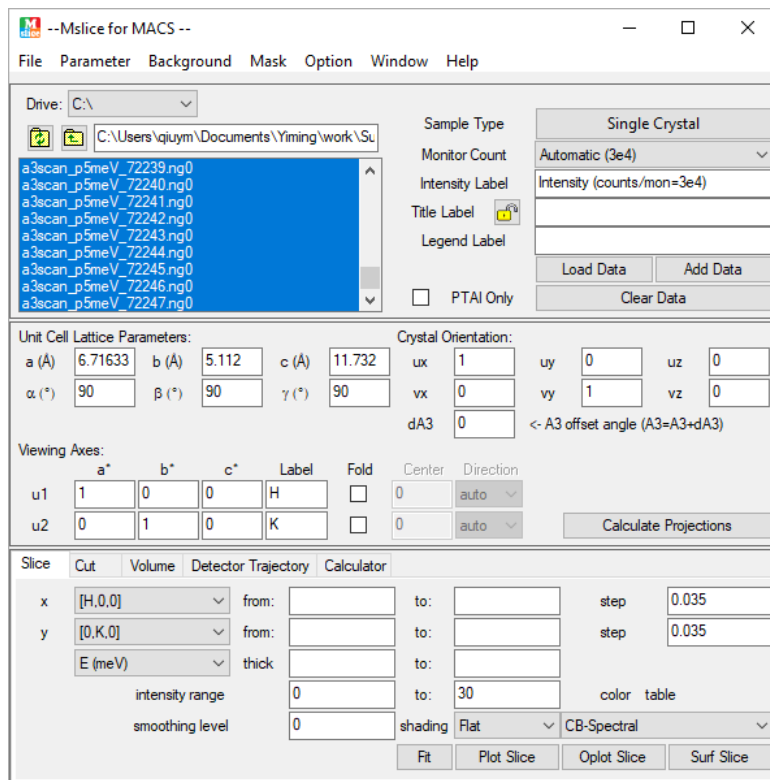
- Right click on the file selector to sort the files by file name.



- 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

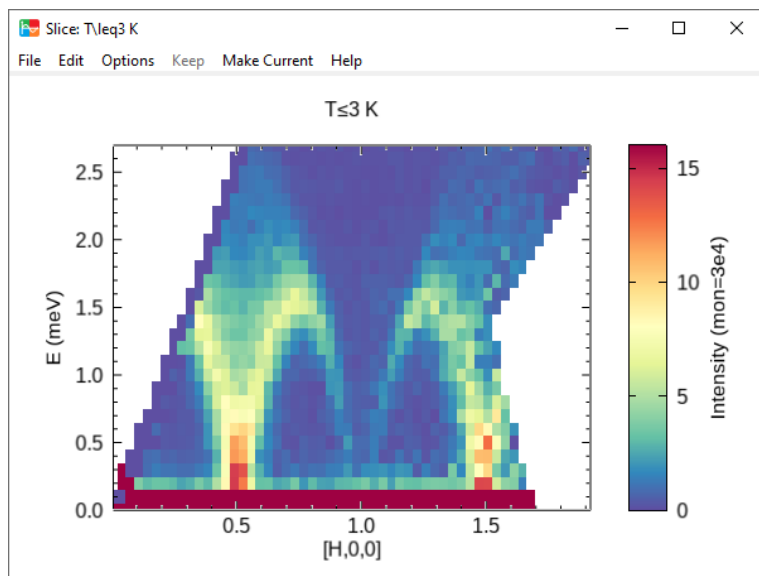
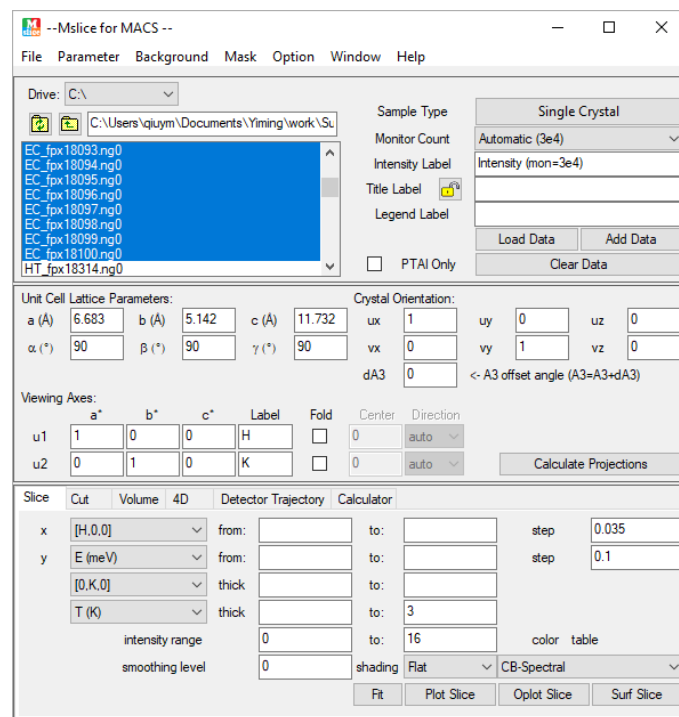
- Load a3 scan files a3scan\_p5meV\_72239-72249.
- Make sure  $u1=(1,0,0)$  and  $u2=(0,1,0)$ . Press [Calculate Projections](#) button.
- In the slice panel, choose  $[H,0,0]$  as x axis, step 0.035, and  $[0,K,0]$  as y axis, step 0.035. Press Plot Slice button to plot the H vs K contour plot.
- Keep 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.

The image shows the "Mslice for MACS" software interface. The "Drive" is set to "C:\". The "Sample Type" is "Single Crystal". The "Monitor Count" is "Automatic (3e4)". The "Intensity Label" is "Intensity (mon=3e4)". The "Title Label" and "Legend Label" are empty. The "Load Data" and "Add Data" buttons are visible. The "Clear Data" button is also present.

The "Unit Cell Lattice Parameters" section shows:

a (Å)	6.683	b (Å)	5.142	c (Å)	11.732
α (°)	90	β (°)	90	γ (°)	90

The "Crystal Orientation" section shows:

ux	1	uy	0	uz	0
vx	0	vy	1	vz	0
dA3	0	<- A3 offset angle (A3=A3+dA3)			

The "Viewing Axes" section shows:

	a*	b*	c*	Label	Fold	Center	Direction
u1	1	0	0	H		0	auto
u2	0	1	0	K		0	auto

The "Slice" section shows:

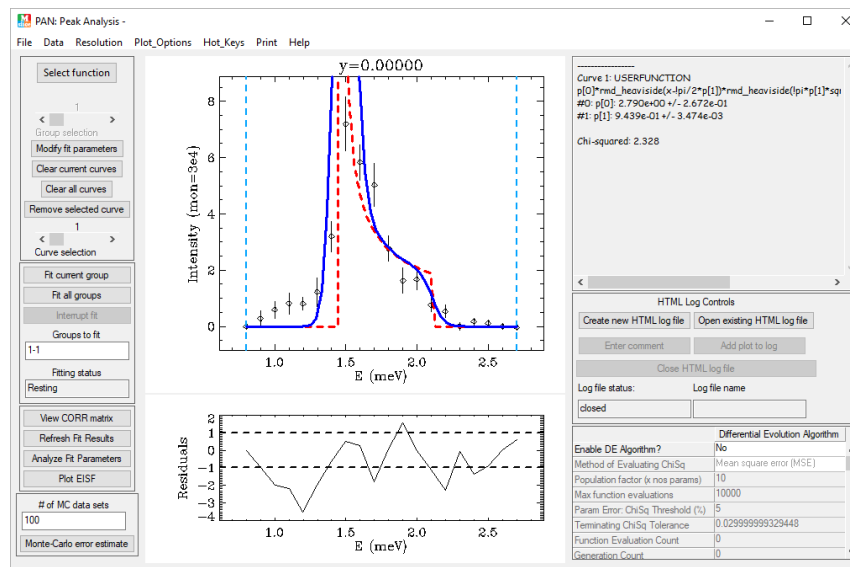
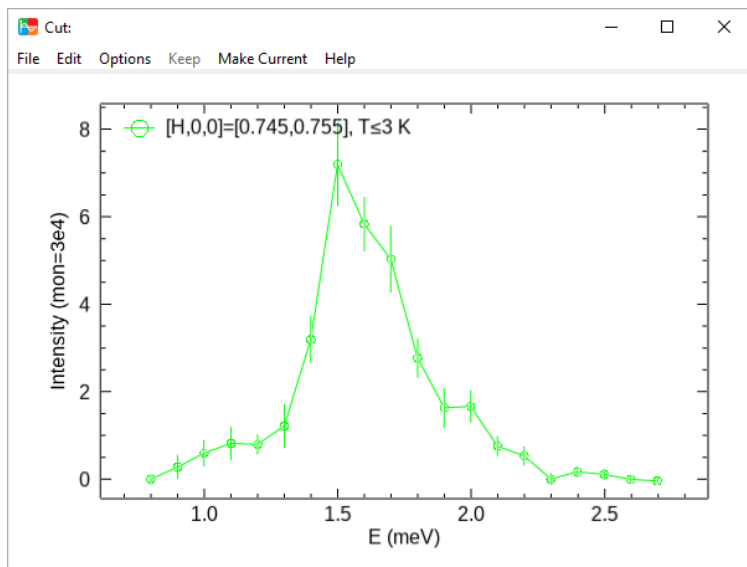
	Cut	Volume	4D	Detector Trajectory	Calculator
x	[H,0,0]			from: to: step: 0.035	
y	E (meV)			from: to: step: 0.1	
	[0,K,0]			thick: to: 3	
	T (K)			thick: to: 16	

The "intensity range" is 0 to 16. The "smoothing level" is 0. The "shading" is "Flat". The "color table" is "CB-Spectral". The "Fit", "Plot Slice", "Oplot Slice", and "Surf Slice" buttons are visible.

# 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  $p[0]=3$ ,  $p[1]=0.9$ ):  

$$p[0] * \text{rmd\_heaviside}(x - !\pi/2 * p[1]) * \text{rmd\_heaviside}(!\pi * p[1] * \text{sqrt}(2) / 2 - x) / \text{sqrt}(\text{abs}(x^2 - 0.25 * (!\pi * p[1])^2))$$
- Load pre-generated resolution data (eresl\_0p15meV.txt) from  
**Resolution->Load ASCII Res File->Load 3-col ascii resolution function.**



# 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

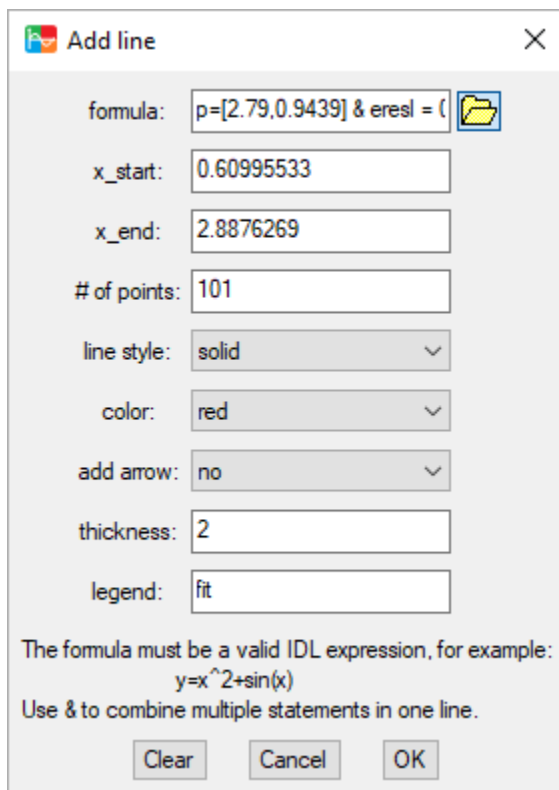
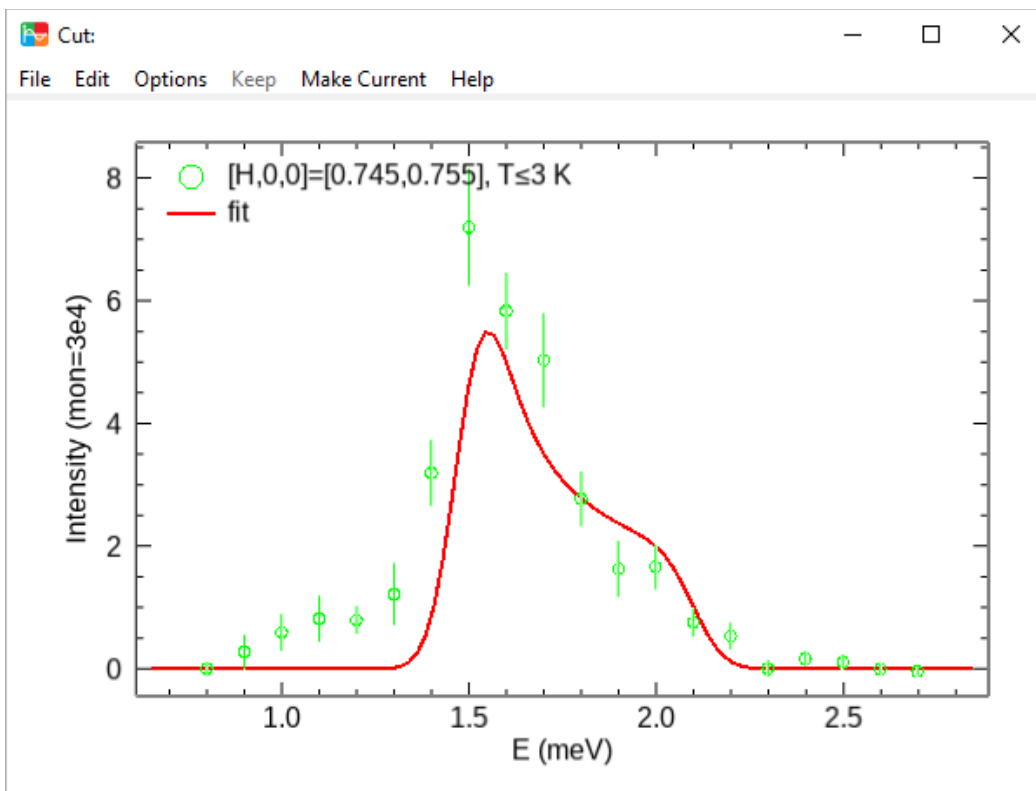
$$S_{\pm\pm}(q, \omega) = \frac{A}{(\omega^2 - \frac{1}{4}\pi^2 J^2 \sin^2 q)^{1/2}} \Theta\left(\omega - \frac{\pi}{2} J \sin q\right) \\ \times \Theta\left[\pi J \sin\left(\frac{q}{2}\right) - \omega\right] \quad (1.48)$$

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

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

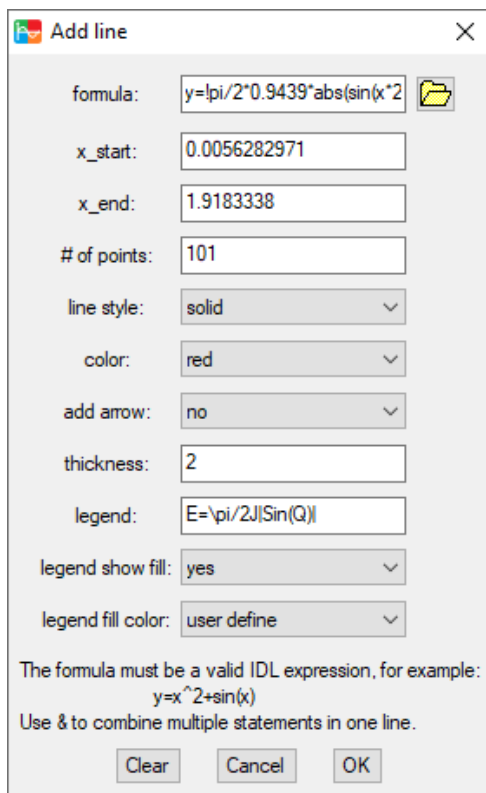
```
p=[2.79, 0.9439] & eresl=0.15 y = gauss_smooth(p[0]*rmd_heaviside(x-
!pi/2*p[1])*rmd_heaviside(!pi*p[1]*sqrt(2)/2-x)/sqrt(abs(x^2-
0.25*(!pi*p[1])^2)), eresl/(x[1]-x[0])/sqrt(8.*alog(2)))
```

(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  $y = \pi/2 * 0.9439 * \text{abs}(\sin(x * 2 * \pi))$ . Use  $E = \pi/2 J |\sin(Q)|$  as legend. The formula for the upper bound is  $y = \pi * 0.9439 * \text{abs}(\sin(x * \pi))$ . Use  $E = \pi J |\sin(Q/2)|$  as legend.



**Add line**

formula:

x\_start:

x\_end:

# of points:

line style:

color:

add arrow:

thickness:

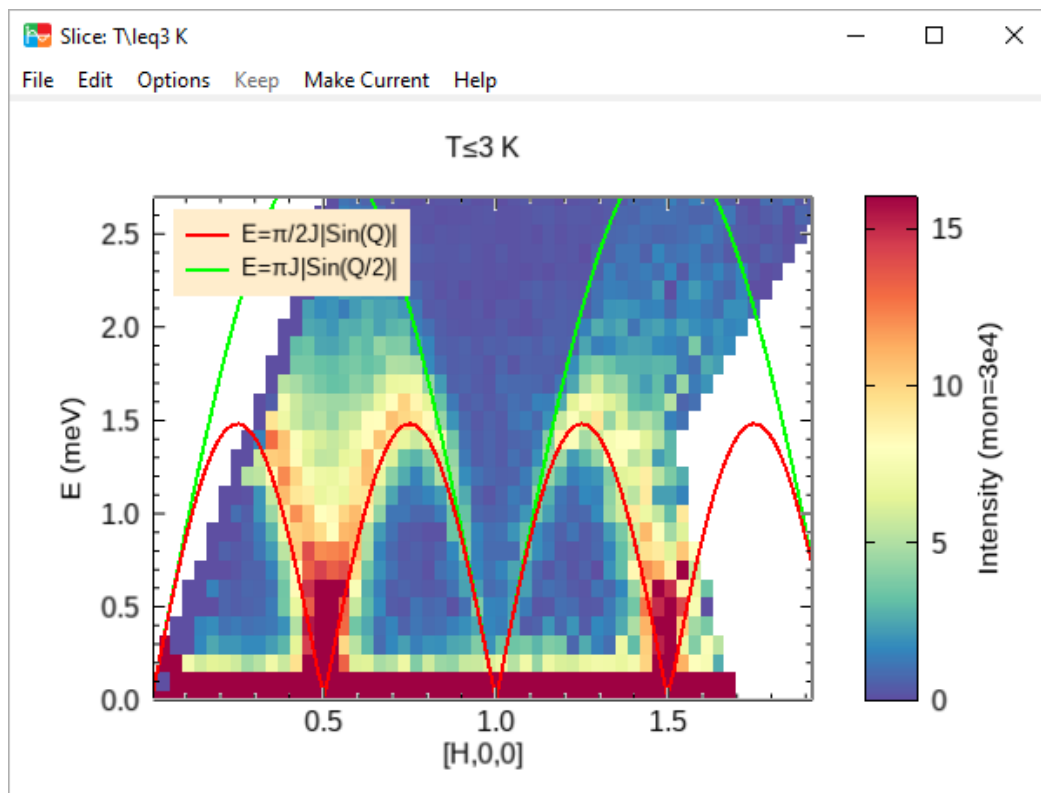
legend:

legend show fill:

legend fill color:

The formula must be a valid IDL expression, for example:  
 $y = x^2 + \sin(x)$   
 Use & to combine multiple statements in one line.

Clear Cancel OK



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

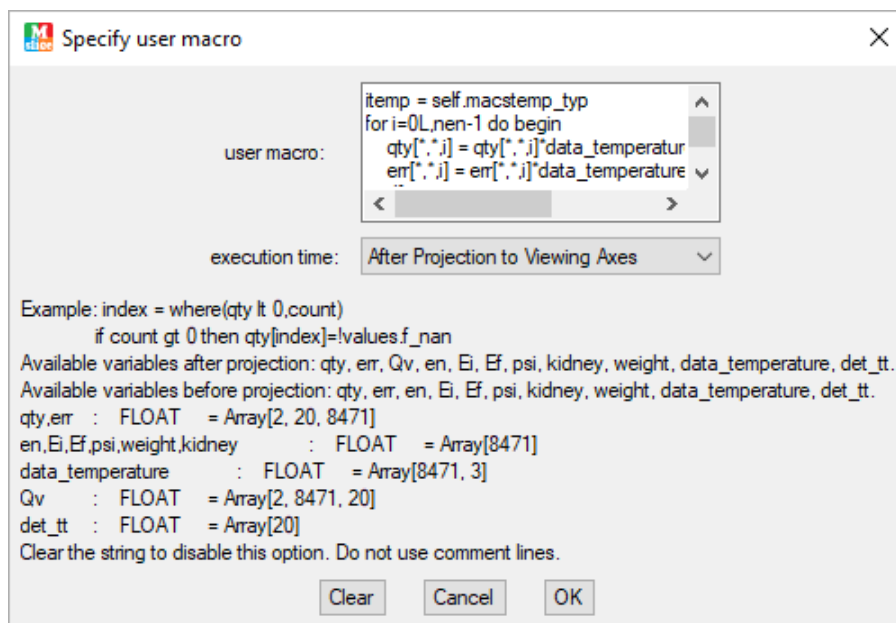
- In mslice menu **Option->User Macro**, enter the following script (macro.txt):

```

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])

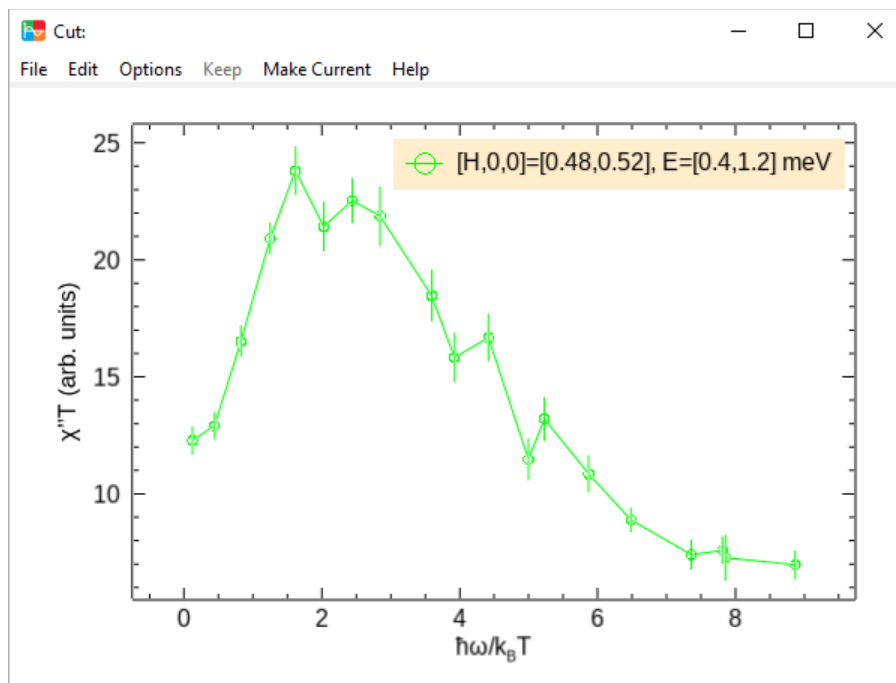
```

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



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

- Choose **Option->View Intensity As-> Chi(Q,omega)**
- Recalculate the projection.
- In the cut panel, cut along T, which is  $E/k_B T$  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  $\hbar\omega/k_B T$ , and y-axis title to  $\chi''T$  (arb. units).

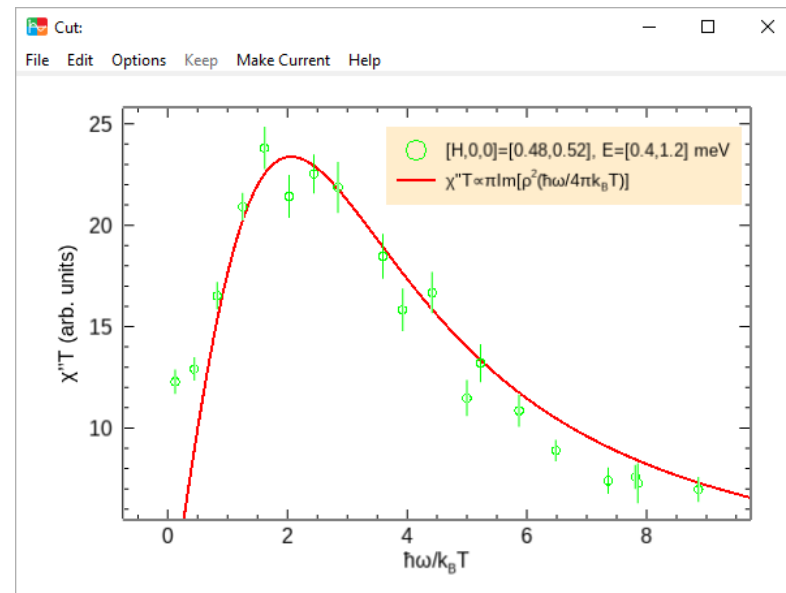
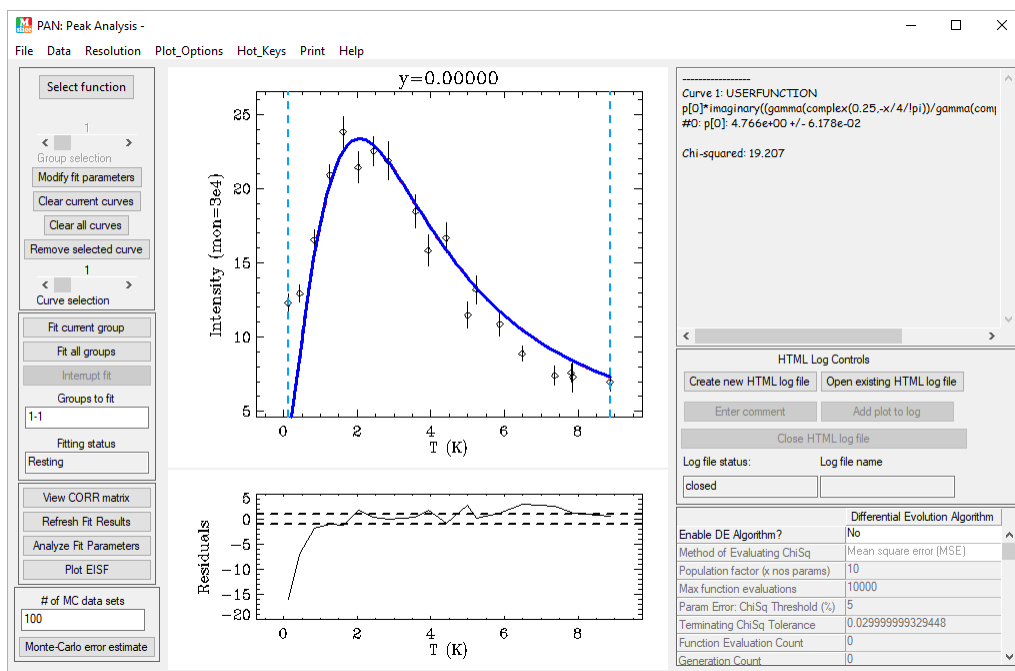


# Fit to Scaling Function

- Press Fit button. In PAN, choose user function as the fitting function:  

$$p[0] * \text{imaginary} \left( \frac{\gamma(\text{complex}(0.25, -x/4/\pi))}{\gamma(\text{complex}(0.75, -x/4/\pi))} \right)^2$$
(equ\_Scaling.eq)
- Add a line of the scaling function to the previous  $\chi''T$  vs  $\hbar\omega/k_B T$  plot.  

$$y = 4.766 * \text{imaginary} \left( \frac{\gamma(\text{complex}(0.25, -x/4/\pi))}{\gamma(\text{complex}(0.75, -x/4/\pi))} \right)^2$$
with  $\backslash \chi''T \backslash \text{propto} \backslash \pi \text{Im}[\backslash \rho^2 \backslash n(\backslash HW/4 \backslash \pi k \backslash dB \backslash nT)]$  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<sup>1,2,4</sup>, D. Alan Tennant<sup>2,3,5</sup>, Chris D. Frost<sup>3</sup> and Stephen E. Nagler<sup>1</sup>

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

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

where  $\rho(x) = \Gamma(1/4 - ix)/\Gamma(3/4 - ix)$  and  $A$  is a constant<sup>16</sup>. 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