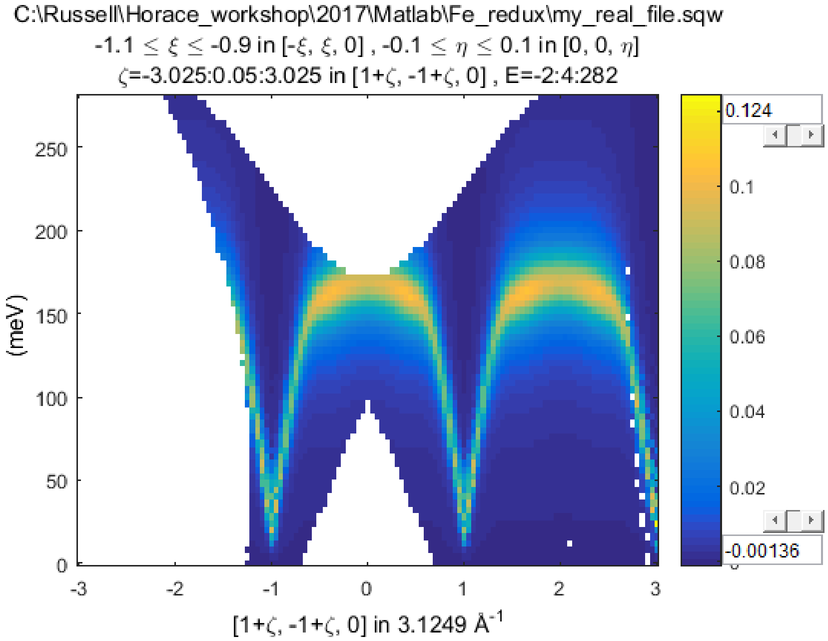
Contents

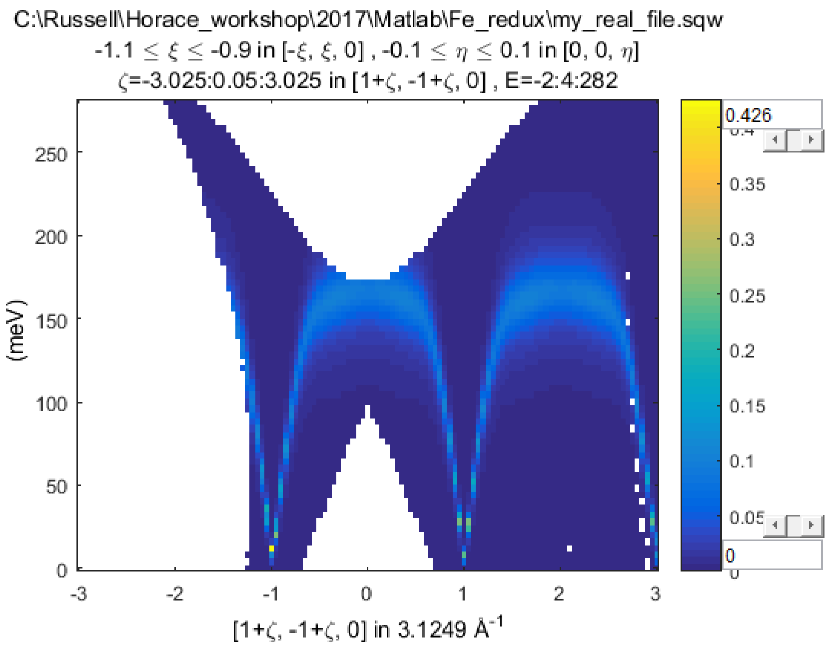
Simulation and Fitting

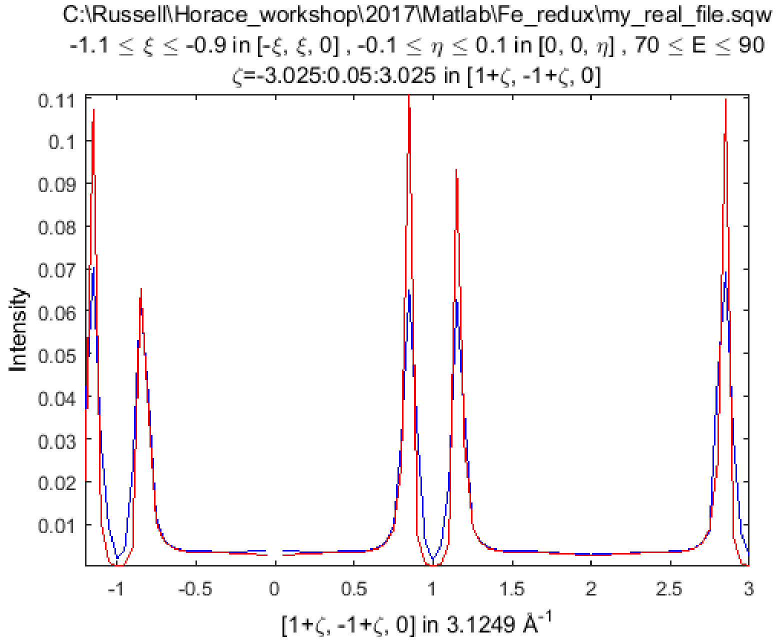
```
%Perform quantitative analysis of your data. If you have a function, or a
%program, that calculates S(Q,w) then you can access it directly from
%Horace and calculate / fit your data directly.
```

Simulating a pre-prepared S(Q,w) function (not related to Fe)

```
%2d slice
my_slice=cut_sqw(sqw_file,proj,[-3,0.05,3],[-1.1,-0.9],[-0.1,0.1],[0,4,280]);

%array of 1d cuts
energy_range=[80:20:160];
for i=1:numel(energy_range)
    my_cut(i)=cut_sqw(sqw_file,proj,[-3,0.05,3],[-1.1,-0.9],[-0.1,0.1],[energy_range(i)-10,energy_range(i)+10]);
end

%simulate on sqw objects
sim_slice=sqw_eval(my_slice,@sr122_xsec,[1,0,0,35,-5,15,10,0.1]);
sim_cut=sqw_eval(my_cut,@sr122_xsec,[1,0,0,35,-5,15,10,0.1]);

%note that the sr122_xsec function is an analytical function for S(q,w)
%that was written specially for this example, and is not generally
%available. You can write your own routine and call it in the same way,
%however!

%repeat on dnd objects
sim_slice_dnd=sqw_eval(d2d(my_slice),@sr122_xsec,[1,0,0,35,-5,15,10,0.1]);
sim_cut_dnd=sqw_eval(d1d(my_cut),@sr122_xsec,[1,0,0,35,-5,15,10,0.1]);

plot(sim_slice); keep_figure;
plot(sim_slice_dnd); keep_figure;

acolor blue
dl(sim_cut(1));
acolor red
pl(sim_cut_dnd(1));
keep_figure;

%note the differences between simulations of notionally the same data. This
%is because dnd just takes the centre point of the integration range,
%whereas sqw takes all of the contributing detector pixels. This is
%imperative if the dispersion varies significantly in a direction
%perpendicular to your cut/slice, as it introduces broadening that the dnd
%simulation fails to capture.
```

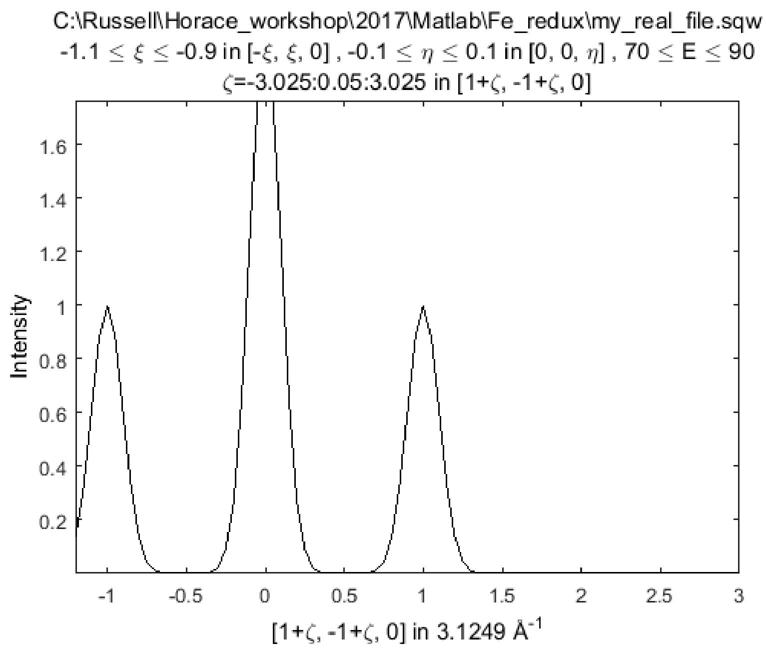

C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η]
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0] , E=-2:4:282
(meV)
[1+ζ, -1+ζ, 0] in 3.1249 Å^-1
0.124
-0.00136


C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η]
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0] , E=-2:4:282
(meV)
[1+ζ, -1+ζ, 0] in 3.1249 Å^-1
0.426
0



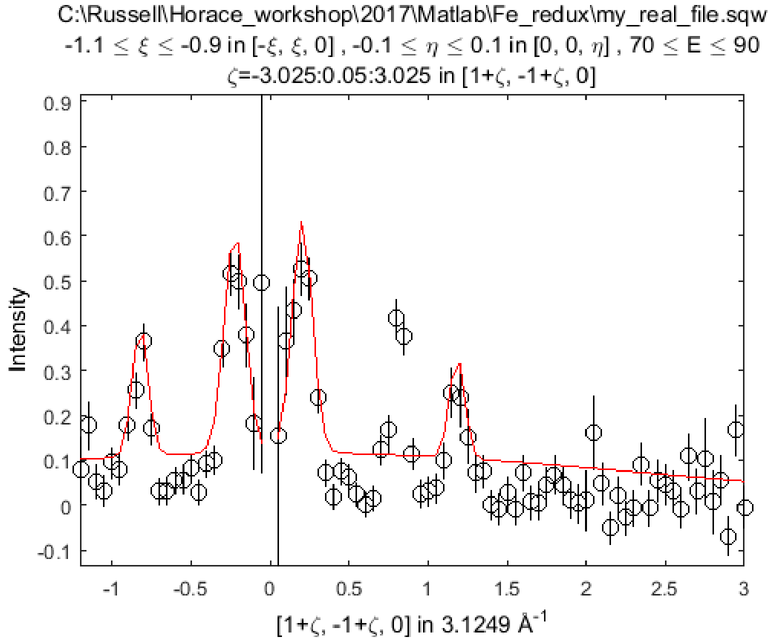
Simulate a peak function with a cut

```
peak_cut=func_eval(my_cut(1),@mgauss,[1,-1,0.1,2,0,0.1,1,1,0.1]);
acolor black
dl(peak_cut);
%note the mgauss function is built-in to Horace, so you can use it
```



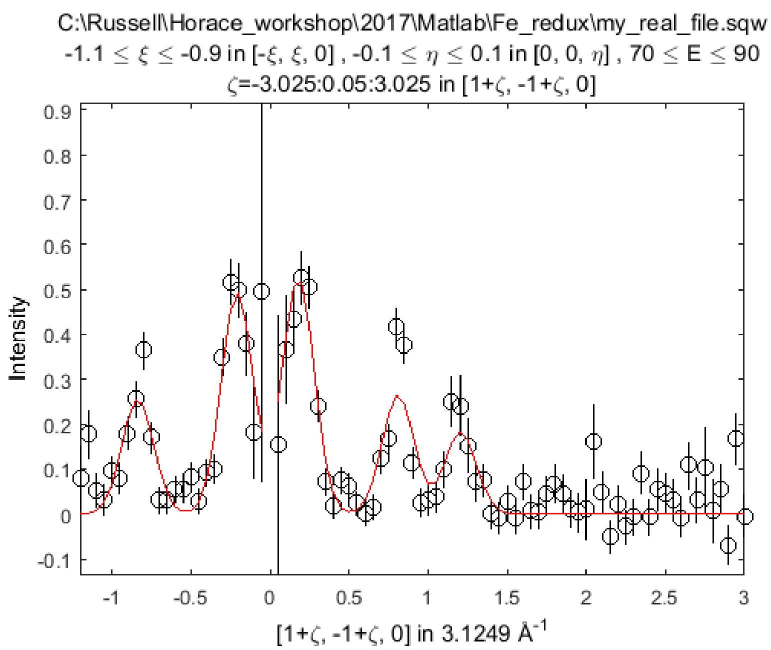
Fit a single cut with a peak function

```
%Allow all parameters to be free
pars_in=[0.4,-0.7,0.1,0.5,-0.2,0.1,0.5,0.2,0.1,0.4,0.6,0.1,0.4,1.3,0.1];
[wfit,fitdata]=fit_func(my_cut(1)-0.3,@mgauss,pars_in);

acolor black
plot(my_cut(1)-0.35);
acolor red
pl(wfit);
```



Fit gaussians, keeping the widths of all the peaks fixed, but allow heights and centres to vary;

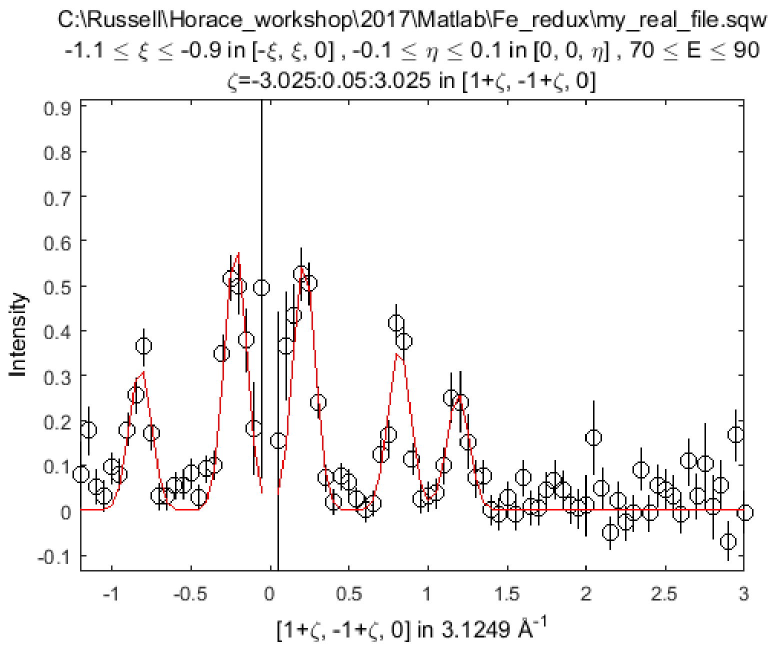
```
pars_in=[0.4,-0.8,0.1,0.5,-0.22,0.1,0.5,0.22,0.1,0.4,0.8,0.1,0.4,1.2,0.1];
pars_free=[1,1,0,1,1,0,1,1,0,1,1,0,1,1,0];
[wfit,fitdata]=fit_func(my_cut(1)-0.35,@mgauss,pars_in,...
    pars_free);
acolor black
plot(my_cut(1)-0.35);
acolor red
pl(wfit);
```



Fix with more realistic values and bind some of the positions to follow symmetry (i.e. position of peaks for Q<0 are reflection of those at Q>0)

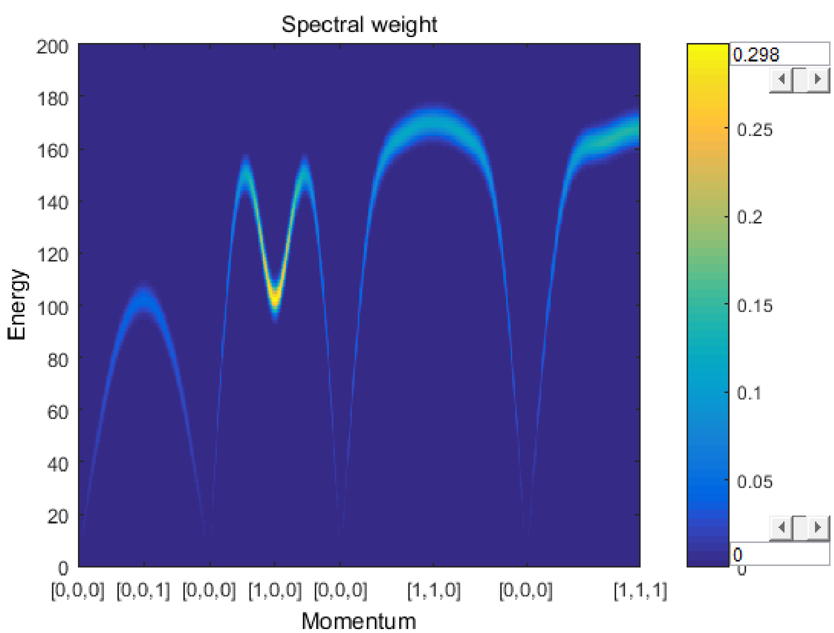
```
pars_in=[0.4,-0.8,0.07,0.5,-0.22,0.07,0.5,0.22,0.07,0.4,0.8,0.07,0.4,1.2,0.07];
pars_free=[1,1,0,1,1,0,1,1,0,1,1,0,1,1,0];
pars_bind={{2,11,0,-1},{5,8,0,-1}};%ensures symmetry about x=0
[wfit,fitdata]=fit_func(my_cut(1)-0.35,@mgauss,pars_in,...
    pars_free,pars_bind);
acolor black
plot(my_cut(1)-0.35);
```

```
acolor red
pl(wfit);
```



Make dispersion plots

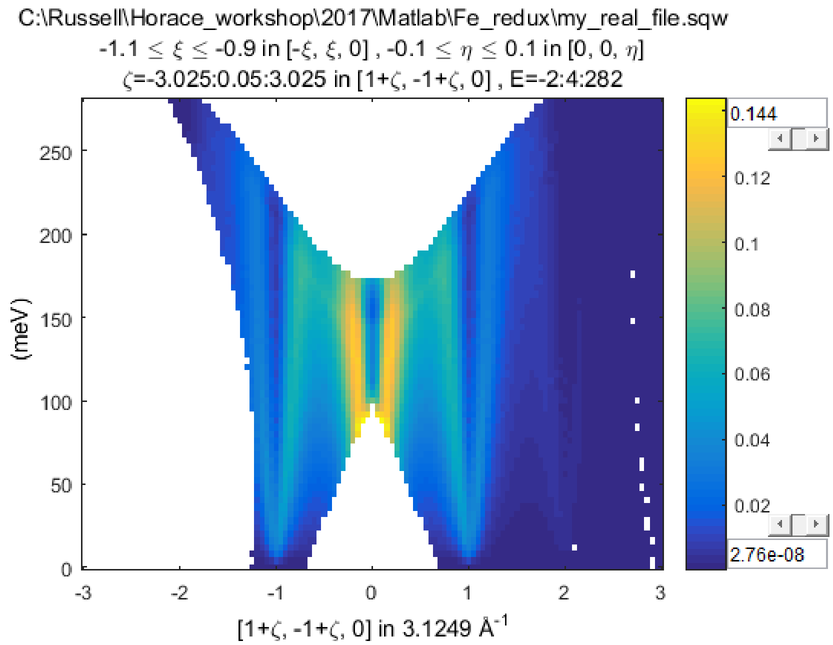
```
alatt=[2.87,2.87,2.87];
angdeg=[90,90,90];
lattice=[alatt,angdeg];
rlp=[0,0,0; 0,0,1; 0,0,0; 1,0,0; 0,0,0; 1,1,0; 0,0,0; 1,1,1];
pars=[1,0.05,0.05,35,-5,15,10,0.1];
ecent=[0,1,200];
fwhh=8;
disp2sqw_plot(lattice,rlp,@sr122_disp,pars,ecent,fwhh);
```

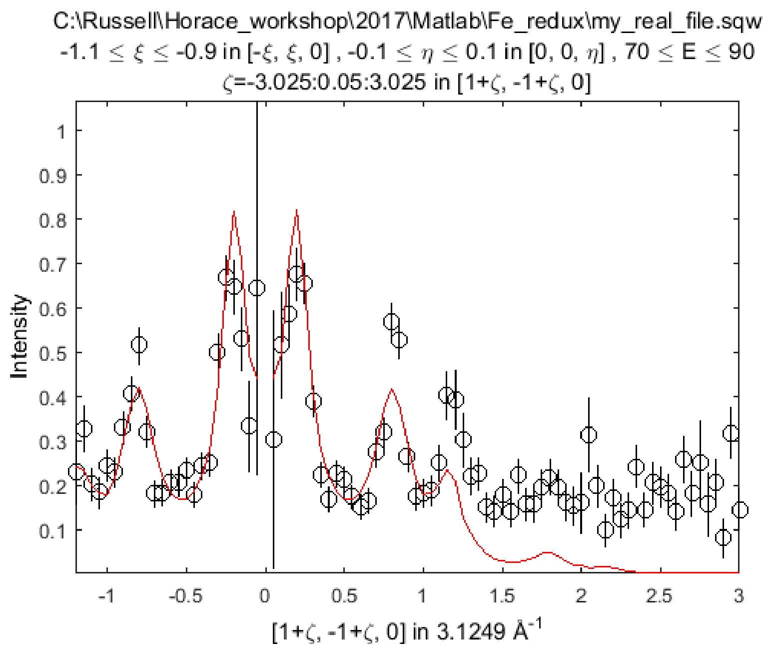


Fit a single cut with an S(Q,w) model

```
%Fit only a small section...
my_new_cut=cut_sqw(sqw_file,proj,[0.5,0.05,1.5],[-1.1,-0.9],[-0.1,0.1],[100,120]);

% Write your own FM spin-waves function
test_slice=sqw_eval(my_slice,@Fe_FM_spinwaves_FF,[250 0 2.4 5 1]);
plot(test_slice);
```

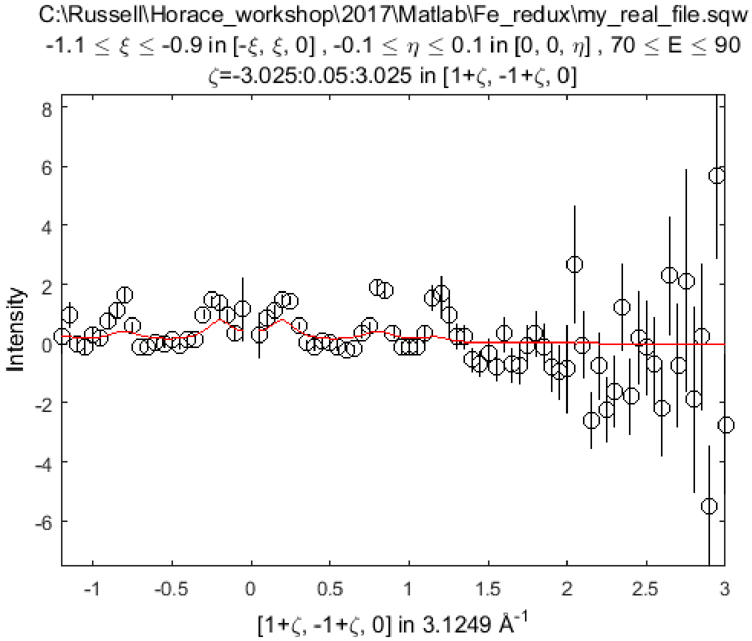
```
keep_figure

pars=[350,0,2.4,5,1];
pfree=[1,1,1,1,1];
[wfit,fitdata]=fit_sqw(my_cut(1)-0.2,@Fe_FM_spinwaves_FF,pars,pfree,'list',1);
acolor black
plot(my_cut(1)-0.2)
acolor red
pl(wfit)
```





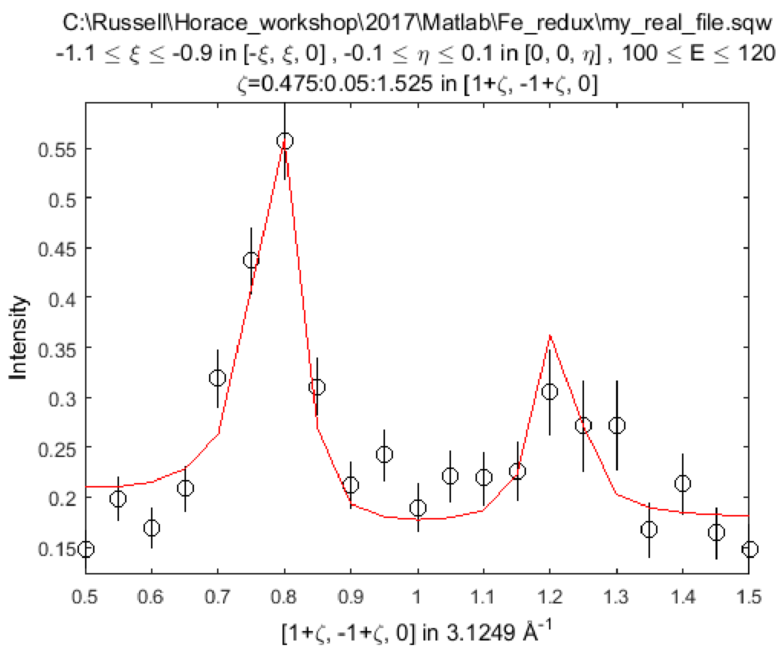
Fit with background subtracted, and magnetic form factor correction

```
mi= MagneticIons('Fe0');
my_cut_corrected = mi.fix_magnetic_ff(my_cut(1)-0.4);

acolor black
amark o
plot(my_cut_corrected(1));
acolor red
pl(wfit)
ly
```



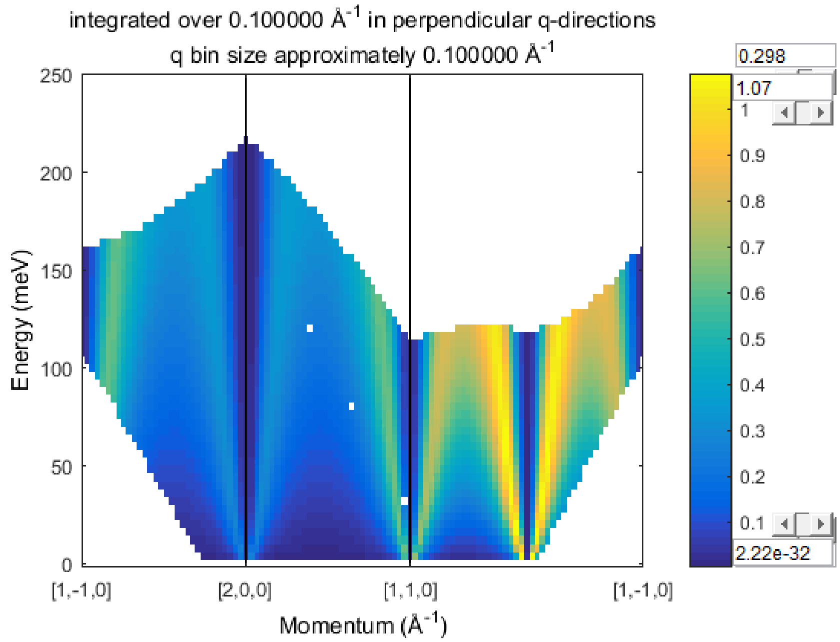
Add a linear background a linear background to your function (in case background subtraction difficult)

```
pars=[250,0,2.4,10,5];
pfree=[1,0,1,0,1];
bgpars=[0.08,0.001];
bgfree=[1,0];
[wfit,fitdata]=fit_sqw(my_new_cut,@Fe_FM_spinwaves_FF,pars,pfree,...
    @linear_bg,bgpars,bgfree,'list',1);

acolor black
plot(my_new_cut)
acolor red
pl(wfit)
```



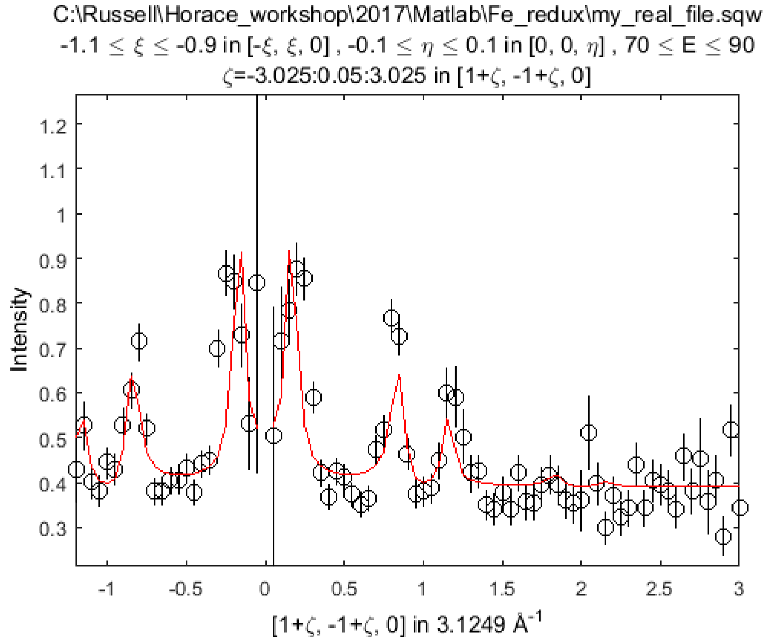
Simulate spaghetti plot

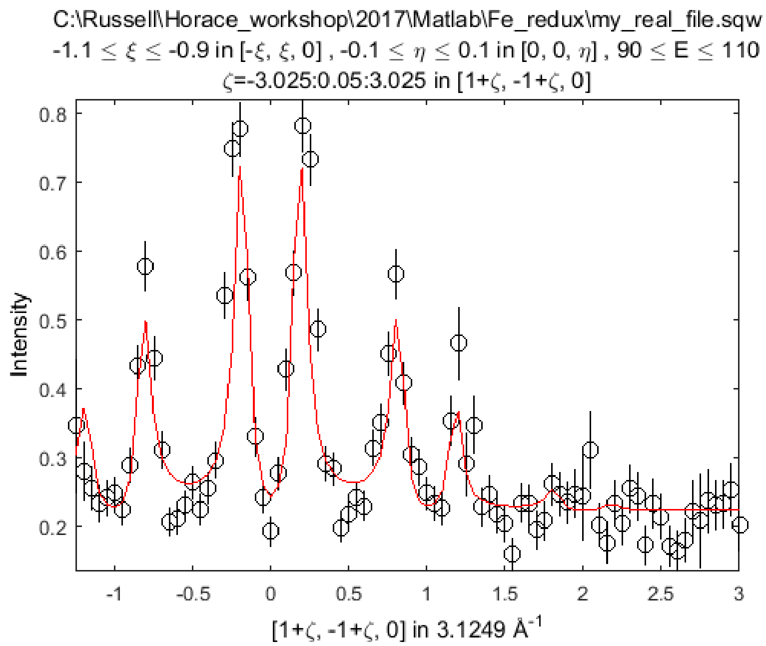
```
rlp=[1,-1,0; 2,0,0; 1,1,0; 1,-1,0];
wdisp=spaghetti_plot(rlp,sqw_file,'qbin',0.1,'ebin',[0,4,250]);

pars=[250,0,2.4,10,5];
wdisp_sim=sqw_eval(wdisp,@Fe_FM_spinwaves_FF,pars);

spaghetti_plot(wdisp_sim)
```

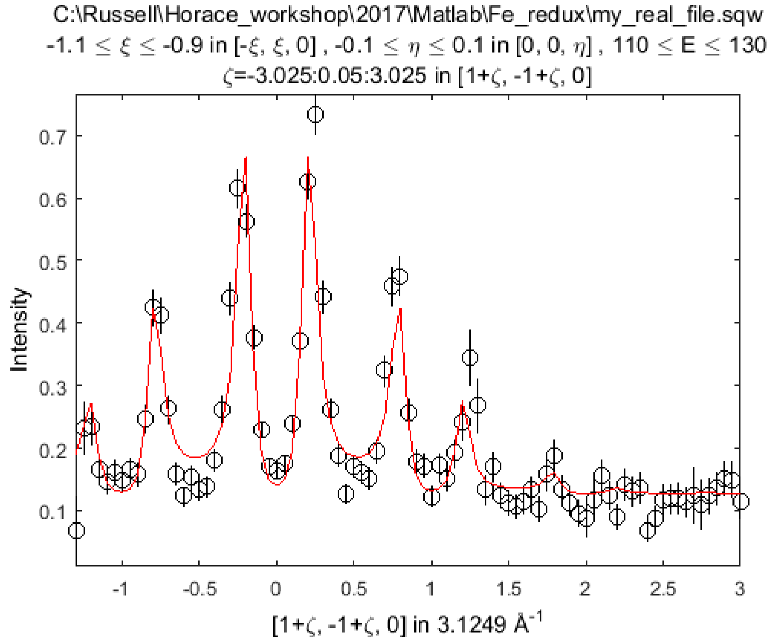


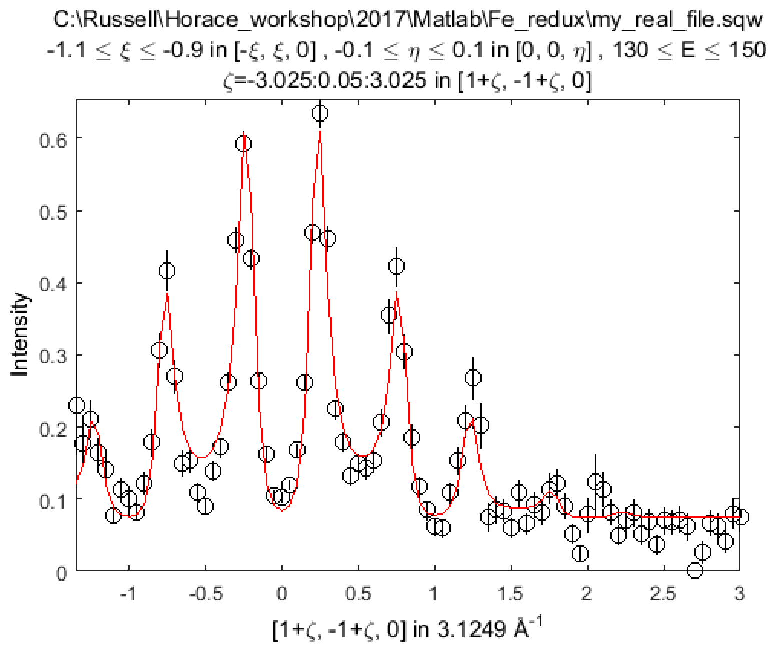
Fit multiple cuts simultaneously with a single S(Q,w) model

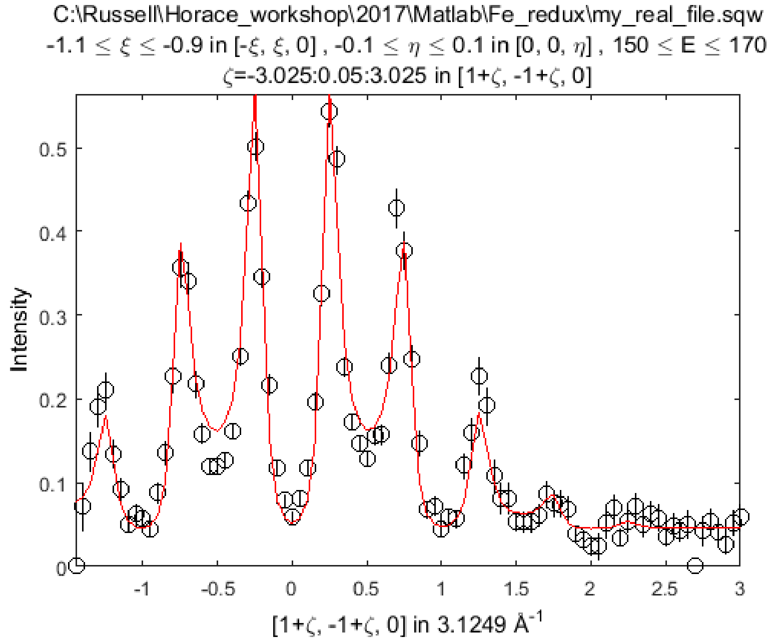
```
%We will use the array of 1d cuts we made earlier

%To begin just use the same input as above, i.e. single parameter set and a
%single set of parameters for the background functions
pars=[250,0,2.4,10,5];
pfree=[1,0,1,0,1];
bgpars=[0.08,0.001];
bgfree=[1,0];
[wfit,fitdata]=multifit_sqw(my_cut,@Fe_FM_spinwaves_FF,pars,pfree,...
    @linear_bg,bgpars,bgfree,'list',1);

for i=1:numel(my_cut)
    acolor black
    plot(my_cut(i));
    acolor red
    pl(wfit(i));
    %lx -2 2
    keep_figure;
end

%%Do something a bit more sophisticated with the backgrounds

%Use different background functions for each cut, and different parameters

bgfunc={@linear_bg,@linear_bg,@linear_bg,@quadratic_bg,@quadratic_bg};
bgpars={[0.37,0],[0.2,0],[0.14,0],[0.08,0,0],[0.03,0,0]};%use different initial guesses and different free/fixed parameters for the background
bgfree={[1,1],[1,1],[1,1],[1,1,1],[1,1,1]};

[wfit,fitdata]=multifit_sqw(my_cut,@Fe_FM_spinwaves_FF,pars,pfree,...
    bgfunc,bgpars,bgfree,'list',1);

for i=1:numel(my_cut)
    acolor black
    plot(my_cut(i));
    acolor red
    pl(wfit(i));
    %lx -2 2
    keep_figure;
end
```

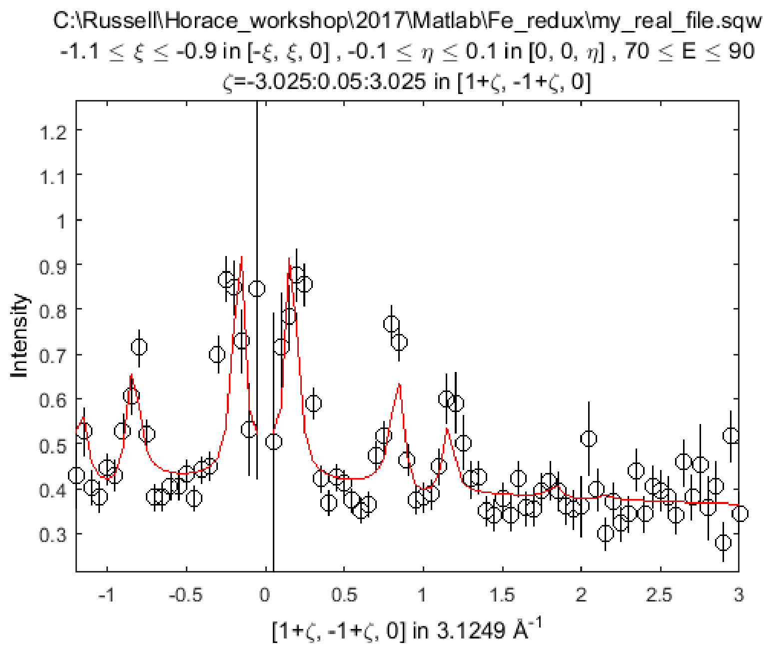

C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 70 ≤ E ≤ 90
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
[1+ζ, -1+ζ, 0] in 3.1249 Å-1

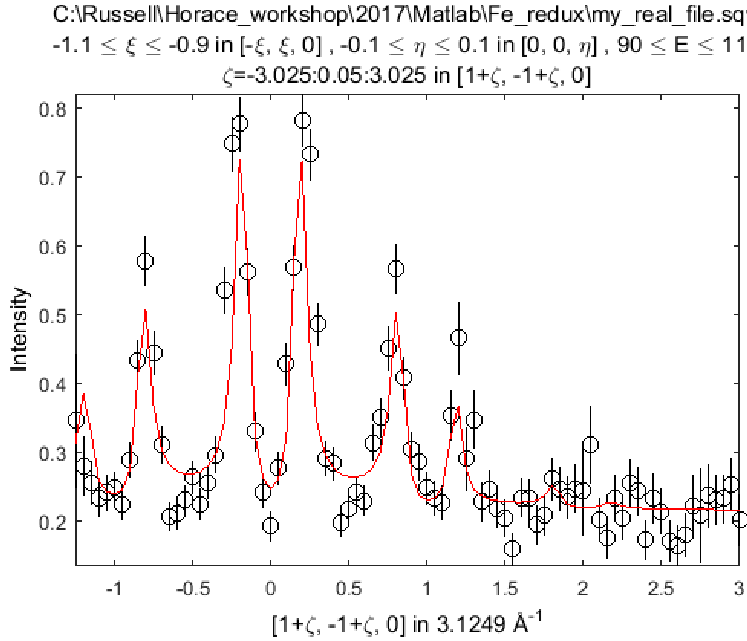

C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 90 ≤ E ≤ 110
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
[1+ζ, -1+ζ, 0] in 3.1249 Å-1

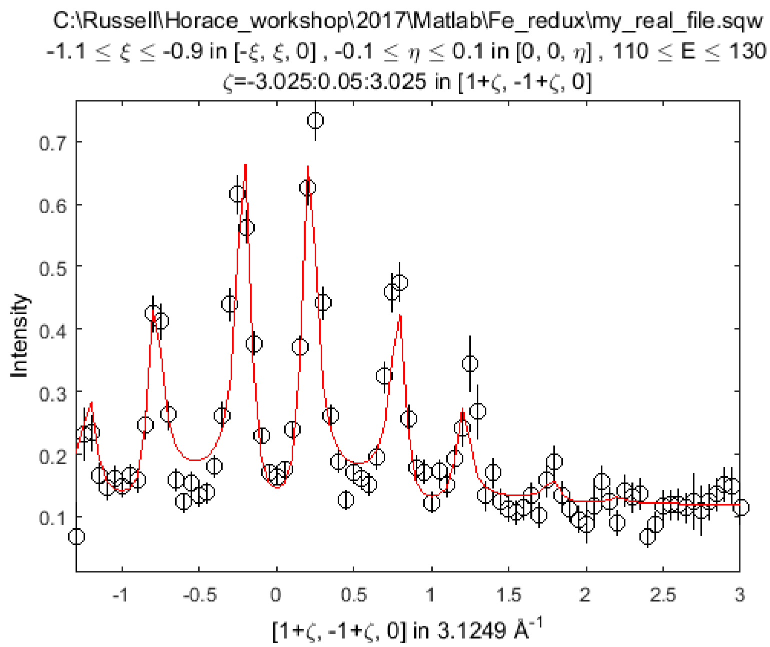

C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 110 ≤ E ≤ 130
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
0.7
0.6
0.5
0.4
0.3
0.2
0.1
-1
-0.5
0
0.5
1
1.5
2
2.5
3
[1+ζ, -1+ζ, 0] in 3.1249 Å-1


C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 130 ≤ E ≤ 150
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
0.6
0.5
0.4
0.3
0.2
0.1
0
-1
-0.5
0
0.5
1
1.5
2
2.5
3
[1+ζ, -1+ζ, 0] in 3.1249 Å-1

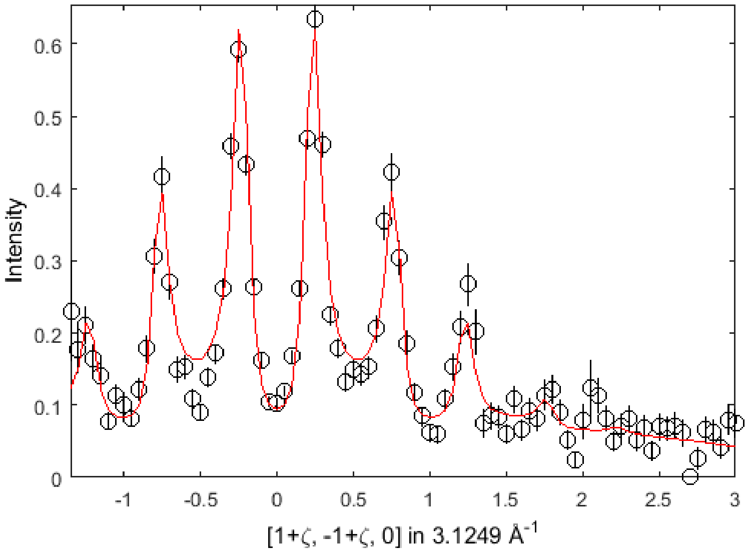

C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 150 ≤ E ≤ 170
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
[1+ζ, -1+ζ, 0] in 3.1249 Å^{-1}


C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 70 ≤ E ≤ 90
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
[1+ζ, -1+ζ, 0] in 3.1249 Å^{-1}

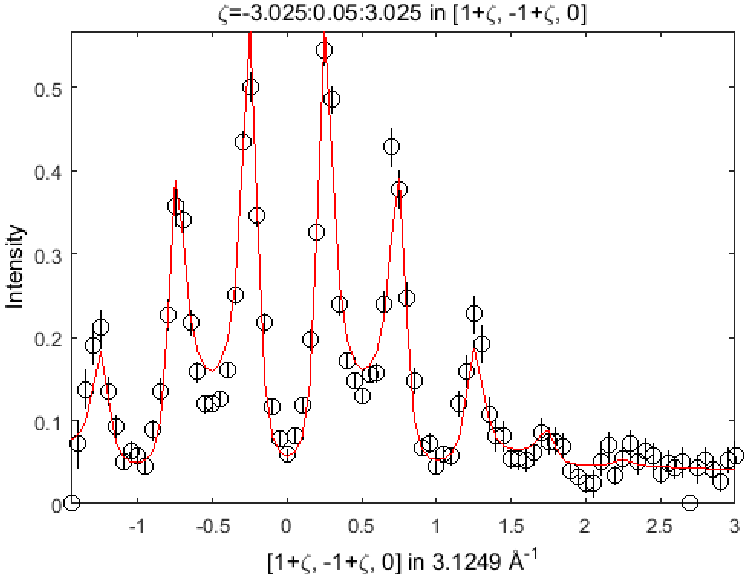

C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 90 ≤ E ≤ 110
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
[1+ζ, -1+ζ, 0] in 3.1249 Å^-1


C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 ≤ ξ ≤ -0.9 in [-ξ, ξ, 0] , -0.1 ≤ η ≤ 0.1 in [0, 0, η] , 110 ≤ E ≤ 130
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]
Intensity
[1+ζ, -1+ζ, 0] in 3.1249 Å^-1

C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 $\leq \xi \leq$ -0.9 in [-ξ, ξ, 0] , -0.1 $\leq \eta \leq$ 0.1 in [0, 0, η] , 130 $\leq$ E $\leq$ 150
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]



C:\Russell\Horace_workshop\2017\Matlab\Fe_redux\my_real_file.sqw
-1.1 $\leq \xi \leq$ -0.9 in [-ξ, ξ, 0] , -0.1 $\leq \eta \leq$ 0.1 in [0, 0, η] , 150 $\leq$ E $\leq$ 170
ζ=-3.025:0.05:3.025 in [1+ζ, -1+ζ, 0]



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