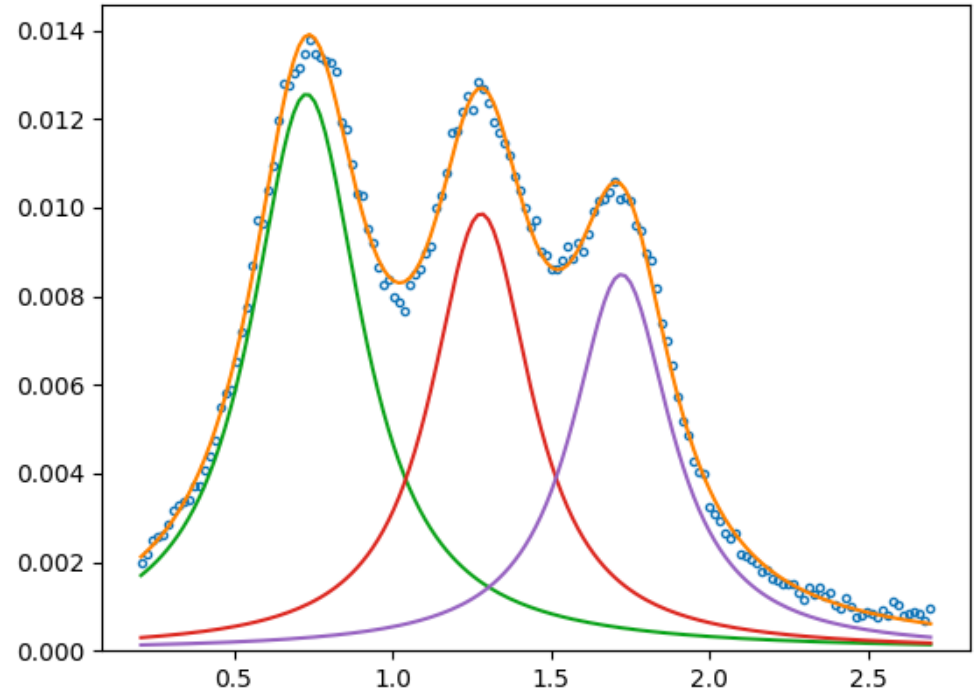
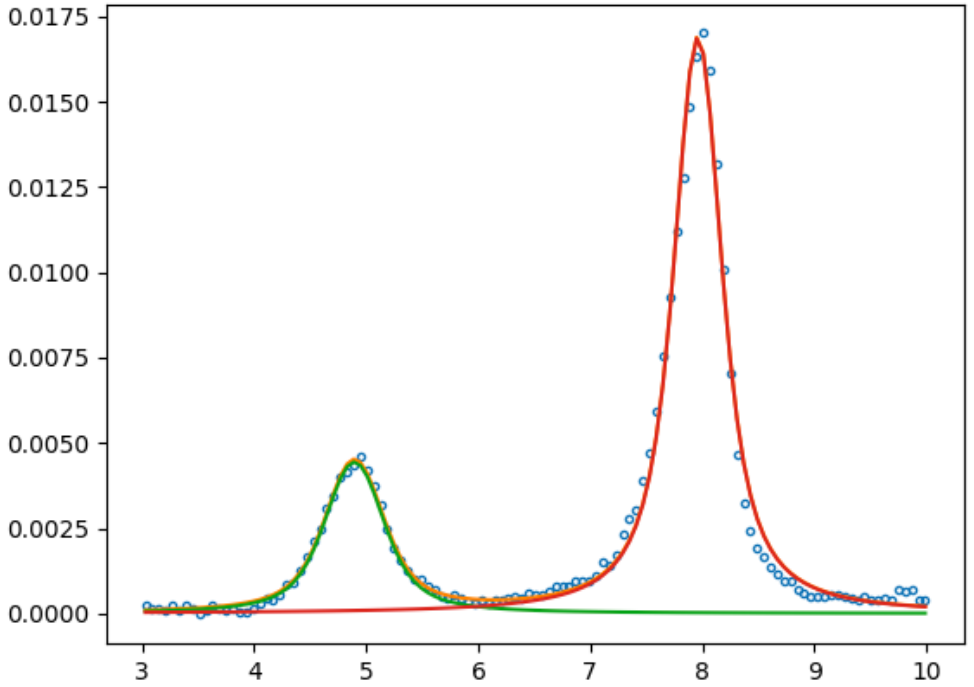
To get a good simulation on peak shape: (Take 60K as an example)





The intensity is calculated using the voigt function (convolution of Gaussian and Lorentzian)
The Gaussian FWHM is the instrument resolution, and the Lorentzian FWHM is from fitting to the data peak.

```
v1_amplitude: value=0.008203 +/- 0.000341
v1_mean: value=0.729580 +/- 0.002128
v1_fwhm: value=0.087749 +/- 0.000000
v1_gamma: value=0.402641 +/- 0.011675
v2_amplitude: value=0.005881 +/- 0.000172
v2_mean: value=1.280150 +/- 0.002239
v2_fwhm: value=0.067779 +/- 0.000000
v2_gamma: value=0.371048 +/- 0.010340
v3_amplitude: value=0.005034 +/- 0.000157
v3_mean: value=1.722628 +/- 0.002602
v3_fwhm: value=0.056329 +/- 0.000000
v3_gamma: value=0.371406 +/- 0.010060
```

Intrinsic width for 60K at 3.32meV: (0.3714+0.3710+0.4026)/3 =0.3817

v1_amplitude: value=0.003844 +/- 0.000281
v1_mean: value=4.894831 +/- 0.012914
v1_fwhm: value=0.389938 +/- 0.000000
v1_gamma: value=0.387940 +/- 0.050528
v2_amplitude: value=0.012727 +/- 0.000239
v2_mean: value=7.961387 +/- 0.003138
v2_fwhm: value=0.239656 +/- 0.000000
v2_gamma: value=0.403278 +/- 0.011223

Instrument resolution

Intrinsic width for 60K at 12meV: (0.4033+0.3879)/2 =0.3956

χ^2 as a function of scaling ratio between neutron spectrum with two E_i and B66

χ^2 is get by fitting all temperature and entire energy range (0.2meV to 12 meV)

B20, B40, and B60 are fitted and calculate the χ^2 .
Start guess B20 = -0.1, B40 = -6e-4, B60 = 2e-6

Using the voigt function as the peak shape to calculate the neutron spectrum at different excitation energies.

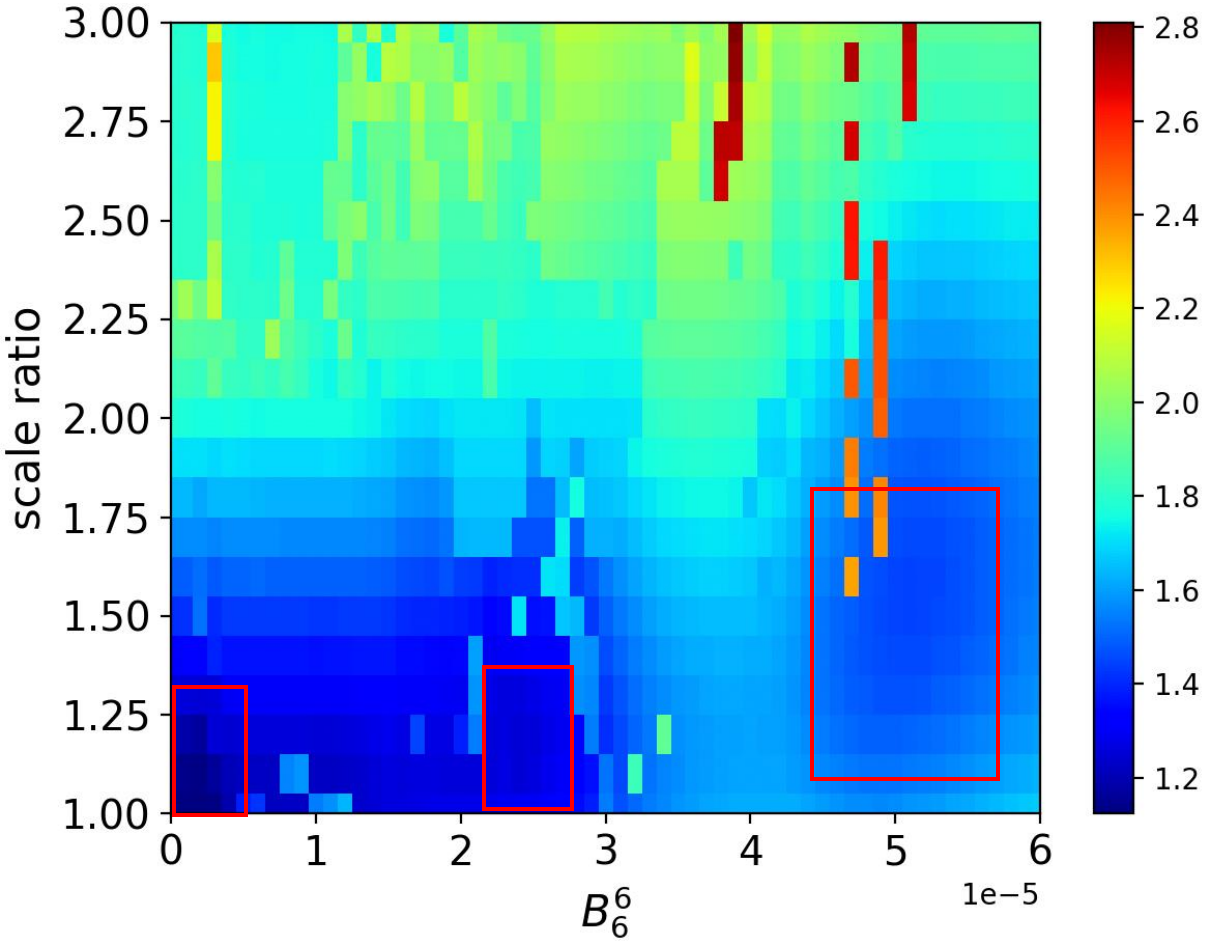
Log scale of the χ^2 is plotted

3 minimum is found:

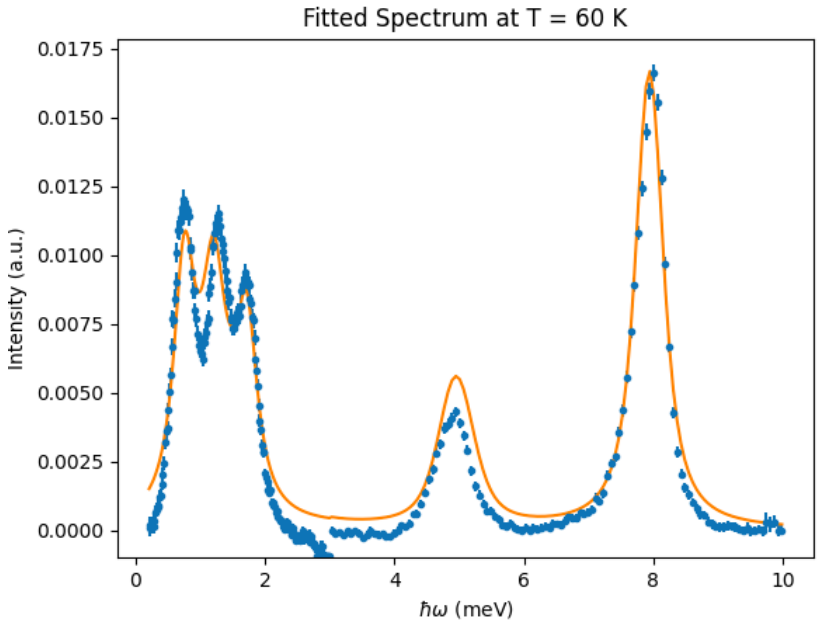
Ratio=1, B66 = 2e-6, χ^2 = 13.26031214920301

Ratio = 1.1, B66 =14e-6, χ^2 = 17.84898674029859

Ratio = 1.5, B66 =51e-6 , χ^2 = 27.806452927379116



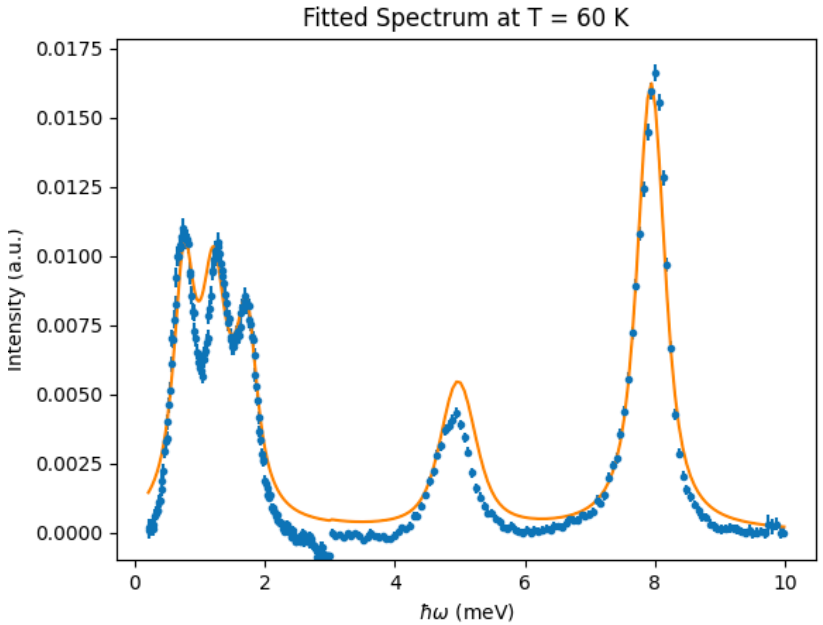
Ratio = 1, B66 =2e-6



Only fix ratio, varying B66 is allowed

[-1.03291671e-01, -5.94158093e-04, 2.31510957e-06, -2.41563119e-06]

$\chi^2 = 13.26$

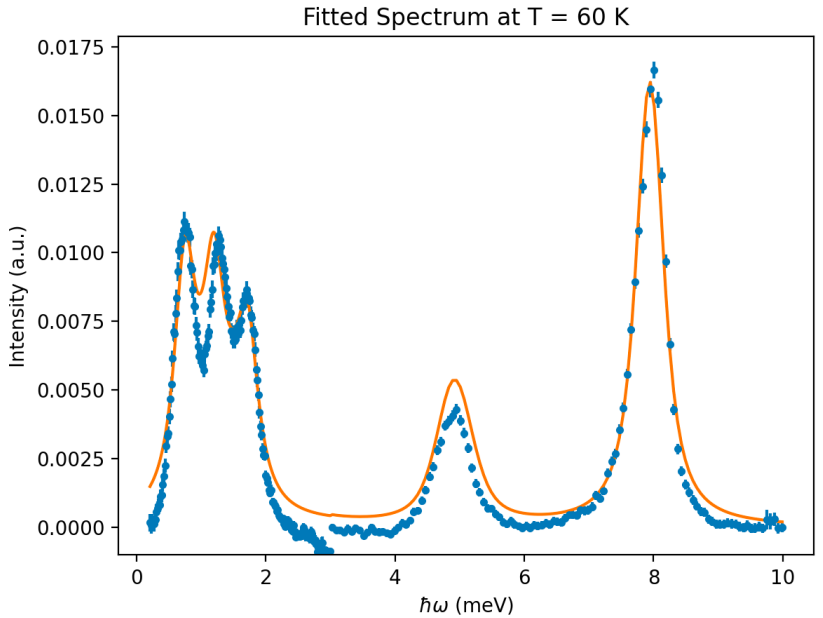


Varying all parameters

[-1.03486638e-01, -5.94945934e-04, 2.33918507e-06, -2.32121687e-06]

Ratio = 1.09384

$\chi^2 = 13.717$



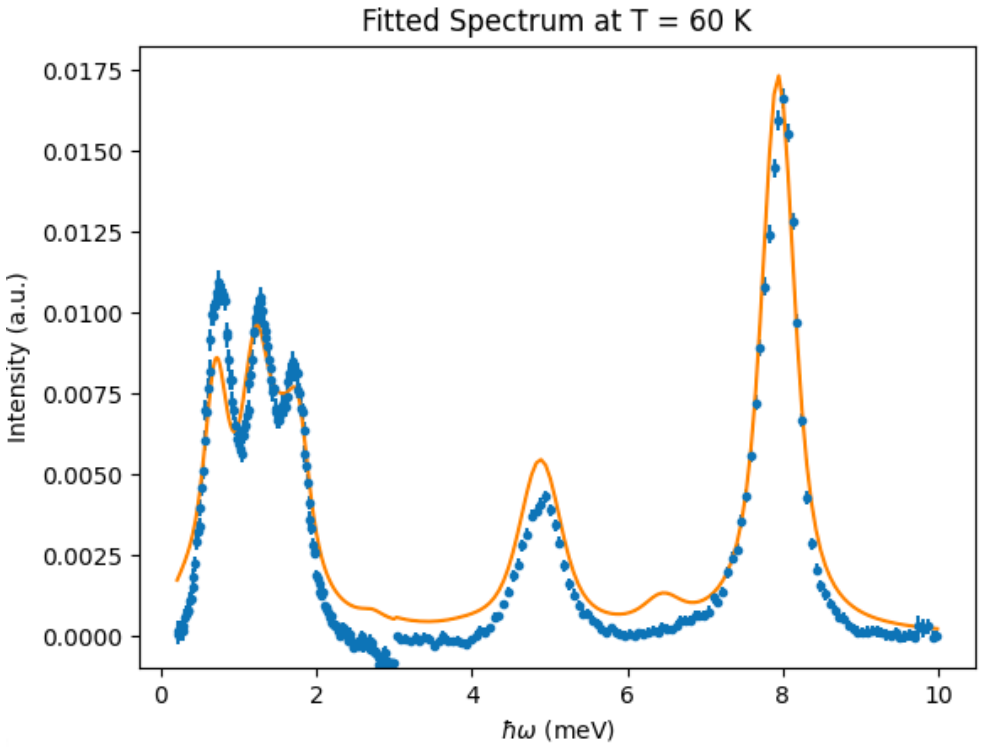
Vary all parameters, and energy @ 4.896 meV

[-1.02826783e-01, -5.93542821e-04, 2.27704290e-06, 2.71793264e-06]

Ratio = 1.0821

$\chi^2 = 13.423$

Ratio = 1.1, B66 =14e-6
small peak ~6.5 meV, possible too weak to see



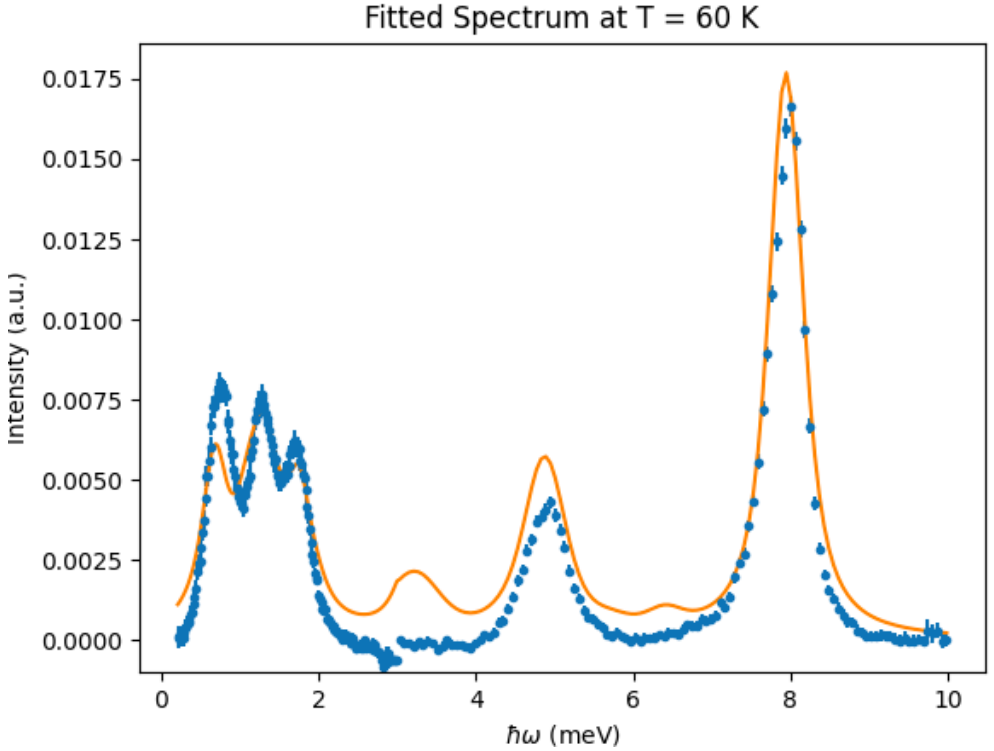
Fix ratio and B66

[-1.15501545e-01,
-5.55693127e-04,
2.27453260e-06,
2.40000000e-05]

Vary all parameters goes to the same result as the previous page

$\chi^2 = 17.848$

Ratio = 1.5, B66 =51e-6
More obvious peak that we didn't see, less possible



Fix ratio and B66

[-1.31170323e-01,
-5.08883804e-04,
2.18840668e-06,
5.10000000e-05]

Vary all parameters, the fitting goes to random results.

$\chi^2 = 27.806$