Neutron and X-ray Scattering of Quantum Materials

PHYS-640

Week 4 exercises

1: Critical magnetic scattering of MnF_2

Task 1: Find the signal of the sample

1.
We wish to find the (100) magnetic Bragg peak which is only present below the transition around 70 K. Usually, the colder, the better in terms of signal strength so measuring at for example at 10 K is a good start. Note that in a real experiment we would initially look for nuclear Bragg peaks while cooling down because the cooling usually takes a couple of hours. Note also that the lowest temperature attainable in an experiment depends on the cryostat but is often around 2 K.

2.
Not knowing at all how the sample is positioned in the cryostat, we will have to do a relatively wide scan in a3 initially to find the sigal. Since MnF_2 is a cubic system, it should be sufficient to scan 90° as shown in Fig. 1(a). There appears to be a signal between $-10°$ and $-5°$ so we performed a scan in this range as shown in Fig. 1(b). Convinced that this really looks like a Bragg peak, we narrow the range a little further to obtain the data shown in Fig. 1(c). Fitting a Gaussian to get the peak position gives a3 $= -7.57°$. We now fix the instrument at a3 $= -7.5°$. Note that $-7.6°$ is also a perfectly valid choice with this instrumental resolution.

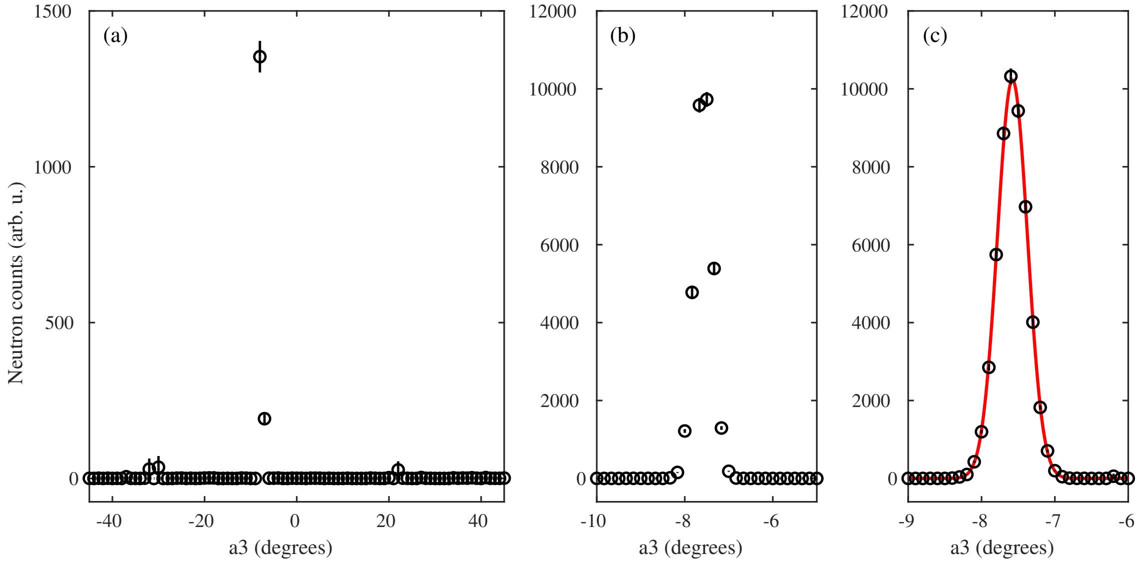

Figure 1: Searching for the sample by doing a3 scans for first a wide range (a), then narrowing down the range (b)-(c). The black points represent the simulation data and the red line in (c) is a fit to a Gaussian with center at $-7.57°$.

Task 2: Find the best configuration for the instrument

1.
The magnetic peaks are $(H0L)$ with $H+L=$ odd according to the Yamani paper. The instrument is setup with $(HK0)$ in the horizontal scattering plane. Since $L=0$ is fixed and even, we need H to be odd to fullfil the selection rule for the magnetic diffraction peaks. To maximize the form factor we choose to measure (100) but could in principle also do (300).

2.
We run a scan of $(H00)$ for $H \in [0.9, 1.1]$ and with 41 steps for the symmetry setting 0 (chair) and 1 (W). The results are shown in Fig. 2. It is clear that the resolution (peak width) is significantly better for the W configuration.

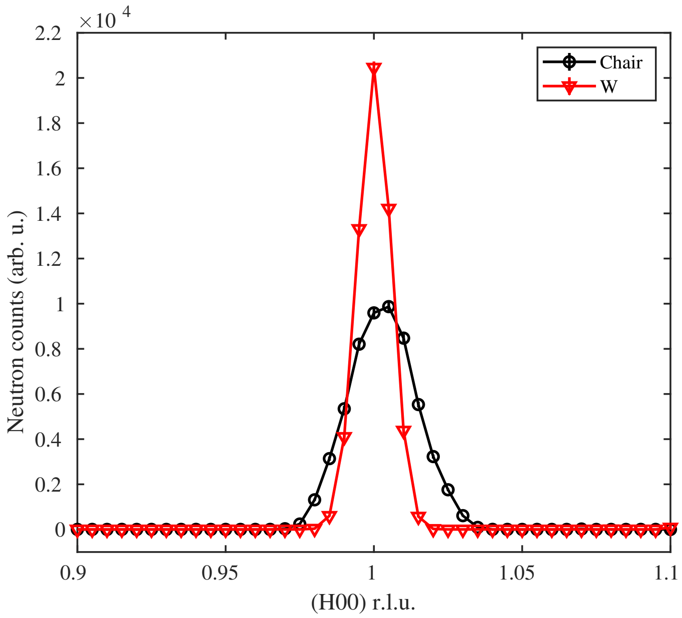

Figure 2: Comparison of scans through (100) performed with the instrument in chair and W configuration.

3.
When the neutrons are always scattered in the same sense (+,+,+) any uncertainty in their direction (divergence) gets amplified and this makes the resolution worse. Contrarily, if the scattering sense alters along the way (+,-,+) any additional uncertainty in the direction picked up on the way may get corrected back and results in a better resolution. For the reminder of the simulations we use the W configuration (sym 1).

Task 3: Improving signal-to noise – slit scans

1.
Scanning the slits from 0 (fully closed) to 5 cm (fully open) with 0.5 cm steps results in the plots shown in Fig. 3. In general one does not run experiments with too tight slits. For example if the sample is a bit off center and we have very tight slits then we risk cutting part of the signal when rotating the sample. In this case, we go for 2 cm on all slits but 1.5 cm would also be alright.

Task 4: Test which scans are the best

1.
Figure 2 shows that scanning $H \in [0.95, 1.05]$ should be enough but we decide to scan a bit wider in order to capture any peak broadening around the transition. We go for $H \in [0.9, 1.1]$. In a real experiment one might do the narrower scans for low and high temperature and the long ones only around the transition.

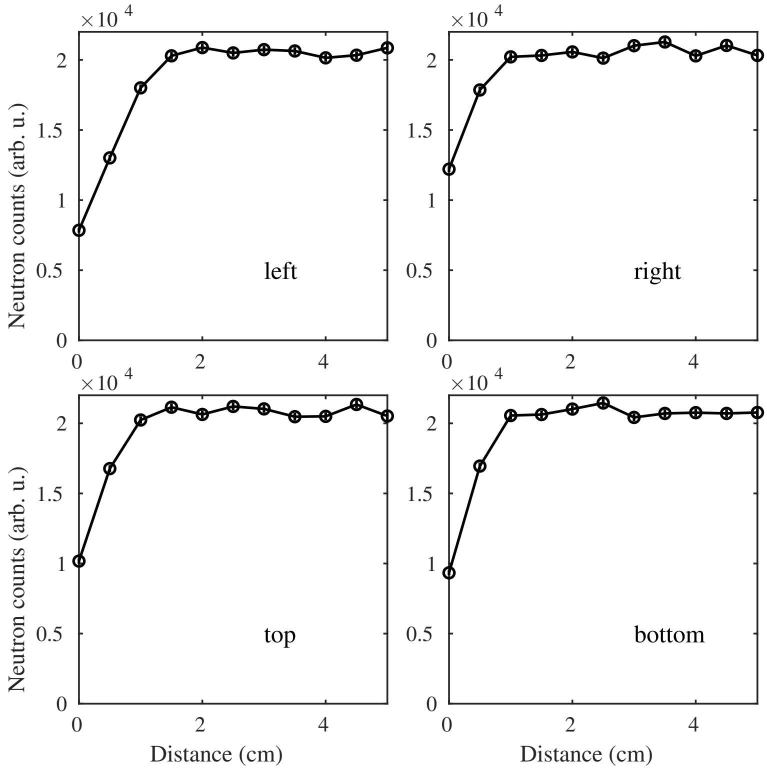

Figure 3: Scans of all four slits.

2.
The step size in Fig. 2 looks OK. The peak is reasonably well described. That means 41 steps.

3.
We can probably get away with a lot less rays. So far we simulated 10^7 for each point. Around the transition where the signal is weaker we might want to keep that but at low temperatures we can probably simulate 10^5 rays per point.

4.
For a relatively rough reproduction of the Yamani figure we could go for something like $T = 80, 75, 70, 69, 68, 67, 66, 65, 64, 63, 62, 61, 60, 55, 50, 45, 40, 35, 30, 20, 10$ K, meaning finer steps around the transition and larger ones and higher and lower temperatures.

5.
That depends on the machine running the code but it took around half an hour to do it on PC17 which sits in the Big Lab.

Task 5: Perform the scans

OK, done that. In the following we use the data set provided on Moodle.

Task 6: Analyze the data

(a) Plot the q-scan at the lowest and highest temperature of your scan in the same plot. What do you notice?

The scans for 20 and 80 K are compared in Fig. 4. At 20 K there is a clear Bragg peak whereas at 80 K it has disappeared. Note that we use the data for 20 K instead of 10 K for no particular reason but it works just the same.

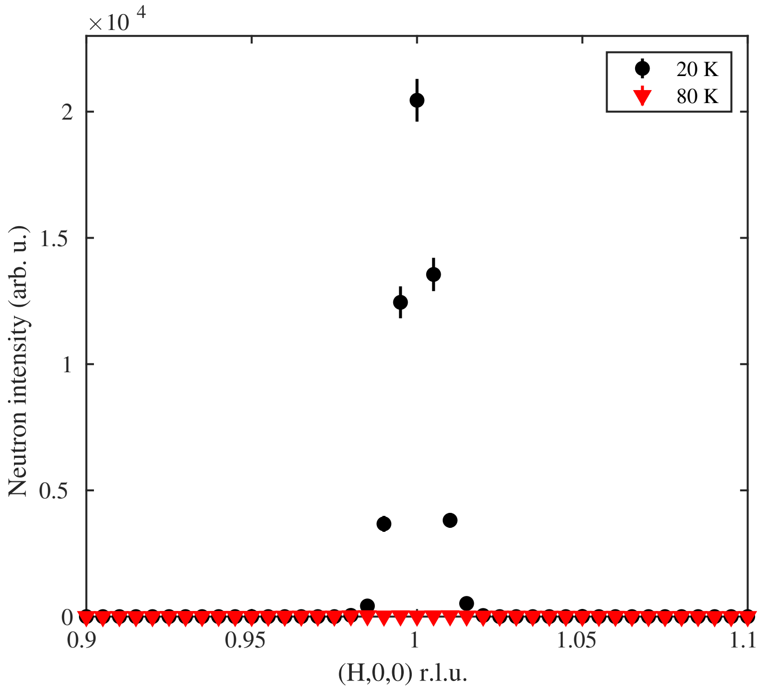

Figure 4: Scans through (100) performed at 20 and 80 K.

(b) Fit a Gaussian function to describe the peak profile at each temperature. You might have to fix the position to $H = 1$ for temperatures close to the transition in order to get meaningful fits.

The fits are shown together with the simulated data in Fig. 5. Note that the neutron counts were normalized to the number of rays used in each simulation in order to be able to compare the relative intensities.

(c) Plot the integrated intensities as a function of temperature. Fit the intensities close to the transition to the piecewise function:

$$I(T) = \begin{cases} I_0|T - T_C|^{2\beta} + C & \text{for} \quad T \leq T_C, \\ C & \text{otherwise,} \end{cases}$$

where I_0, T_C, β and C are all free parameters. Plot the fit on top of the data points. What is the transition temperature?

The area under a Gaussian is $A = \sqrt{2\pi} I_0 \sigma$, where I_0 is the peak height and σ the width. Unless we have to compare the intensity with for example a numerical integration we can leave out the constant $\sqrt{2\pi}$ such that $A = I_0\sigma$. This may appear somewhat lazy but if we are only after the shape of the curve as a function of temperature or determining the transition temperature, it is perfectly sufficient as shown in Fig. 6(a). From the fit we obtain $T_C = 68.4(1)\,\mathrm{K}$ although with 1 K step this is a bit overconfident in terms of precision. It is what the fitting algorithm gives us but we are of course always allowed to give a more realistic error estimate which in this case would be $\pm 0.5\,\mathrm{K}$.

Speaking of errors, in Fig. 6(a), the errors on the integrated intensity, δA, are obtained from propagating the errors, δI_0 and $\delta\sigma$, on the fitted I_0 and σ:

$$\delta A = \sqrt{\left(\frac{\partial A}{\partial I_0}\right)^2 (\delta I_0)^2 + \left(\frac{\partial A}{\partial \sigma}\right)^2 (\delta\sigma)^2} = \sqrt{\sigma^2 (\delta I_0)^2 + I_0^2 (\delta\sigma)^2}.$$

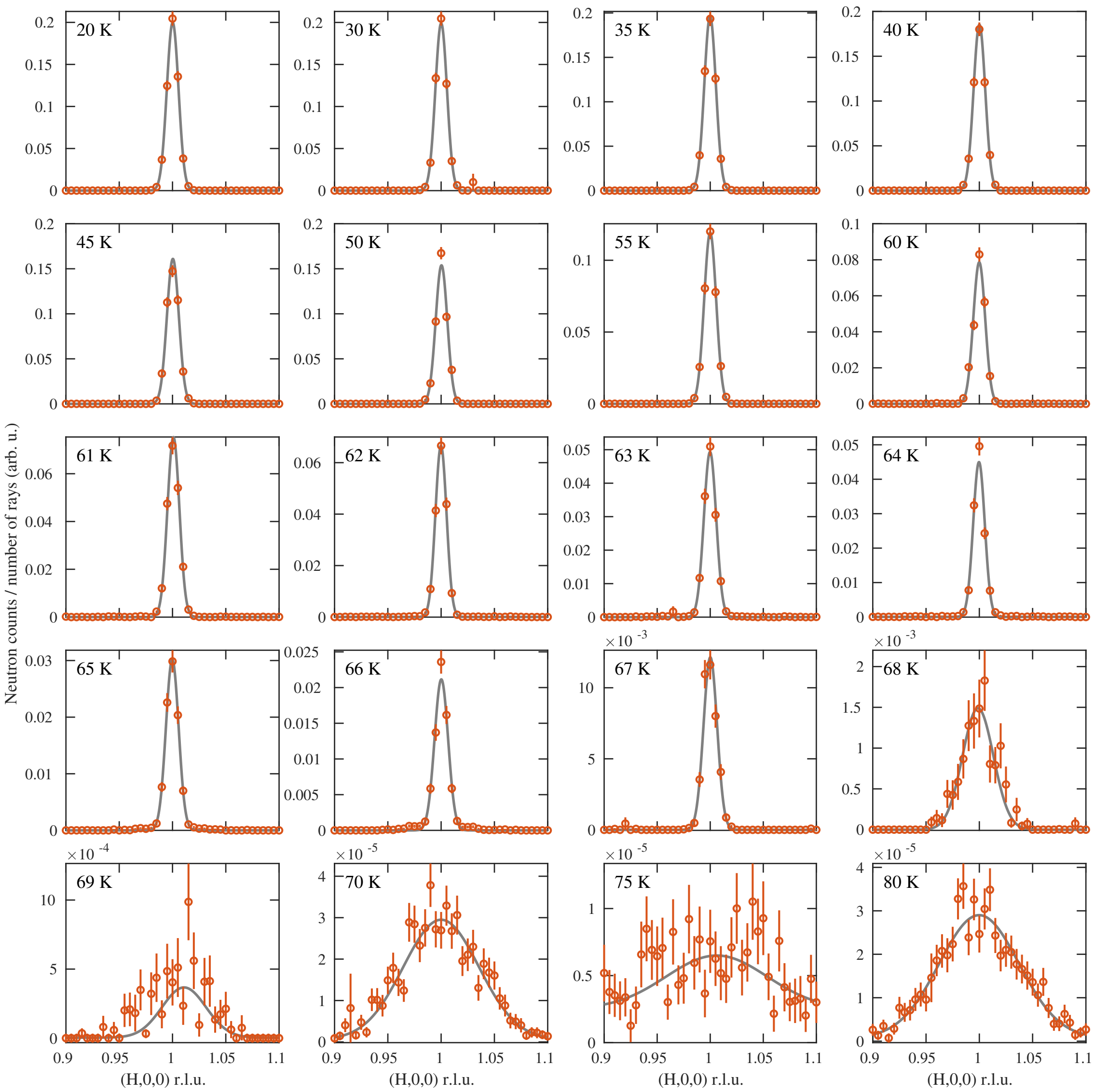

Figure 5: Gaussian fits to the simulated data for all temperatures.

The constant β in the power law function is known as the critical exponent and tells us something about the physics in the system undergoing the magnetic phase transition. You can usually find a table listing the value of this exponent for various universality classes in your favourite statistical physics book. In this particular case, our fit gave $2\beta = 1.01(8)$ and thus $\beta = 0.51(4)$ which is consistent with $\beta = \frac{1}{2}$ from mean-field theory. In the Yamani paper they find $\beta = 0.29(1)$ which close that for a 3D Ising antiferromagnet.

(d) Plot the peak widths as a function of temperature. How can we explain the behavior?

Panel (b) of Fig. 6 shows the Gaussian peak width, σ, as a function of temperature. Note that this is not the same as the FWHM (full width at half maximum) but they are of course related, FWHM $= 2\sqrt{2\ln 2}\sigma$. Figure 6(b) clearly shows that the peak width diverges at the transition. The peak width is related to the magnetic domain sizes in the system. A wider peak means smaller domains and vice versa, a narrow peak means larger domains. Well below the transition temperature, the system is in a fully ordered state and the peak has the width of the instrumental resolution. As the transition is approached the order becomes less stable and smaller domains are formed yielding an increasingly larger peak width. To quantify the domain size (or correlation

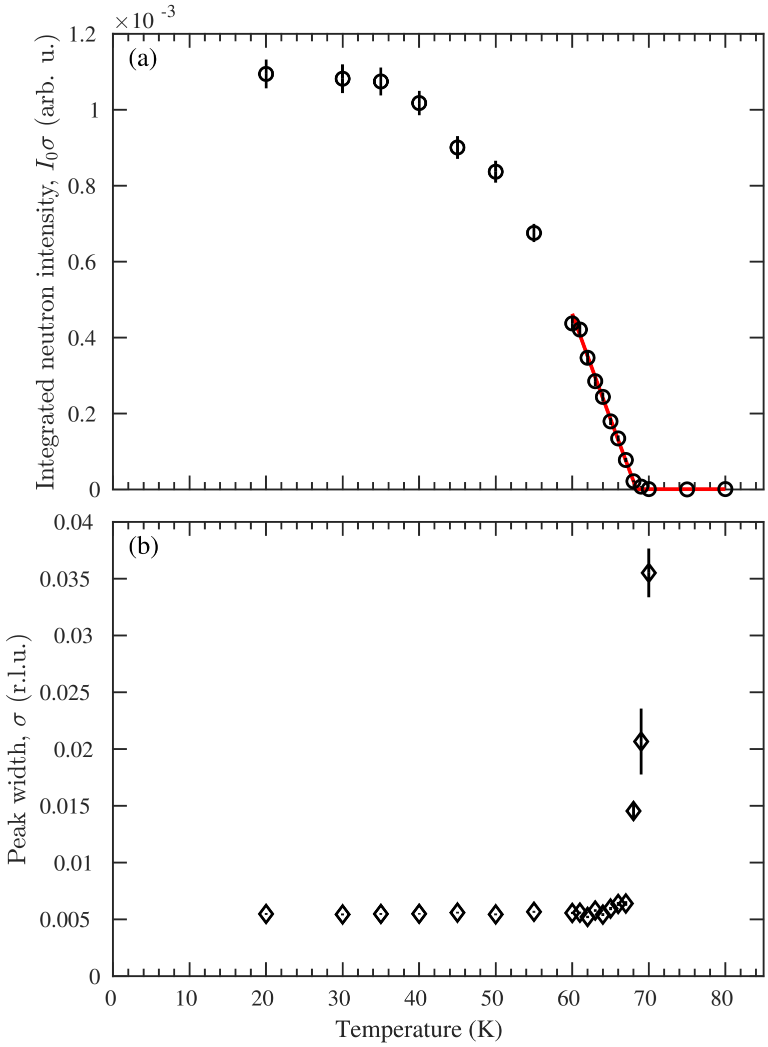

Figure 6: Temperature behavior of the (100) Bragg peak. (a) Integrated neutron intensity as a function of temperature (black circles) with a power law fitted close to the transition (red line). (b) Gaussian peak width as a function of temperature.

length) we would have to do a more careful fit to a Voigt function: a convolution between a Gaussian for the intrumental resolution and a Lorentzian describing the sample signal.