
Neutron and X-ray Scattering of Quantum Materials

PHYS-640

Week 3 exercises

1: The time-of-flight experiment

(a) Derive Eq. (5.15) in the notes. What can be done to improve the wavelength resolution at an instrument?

(b) As seen from Eq. (5.14), we will need long guides to transport neutrons to the sample position, we will need long guides to transport neutrons to the sample position. Calculate the critical angle for a guide with a single Ni layer and neutrons with energy, $E = 5$ meV.

(c) The Spallation Neutron Source at the Oak Ridge National Laboratory in Tennessee, US, has neutron pulse frequency of 60 Hz. The SEQUOIA instrument is placed $L = 25$ m from the moderator and a wavelength band of $[0.2, 0.7]$ Å is needed for an experiment. Is frame overlap going to be a problem in this experiment.

(d) Exercise 5.P.3 in the neutron notes.

2: Critical magnetic scattering of MnF_2

Do the McStass simulation exercise Tasks 0-5. We will save the analysis of the data (Task 6) for next week.

3: The Be filter

Exercise 5.P.5 in the neutron notes.

Critical magnetic scattering of MnF_2

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Introduction

The objective of this exercise is to gain insight into the process of conducting Neutron scattering experiments. By harnessing the power of Monte Carlo ray tracing simulation software, McStas, you will develop a deep understanding of experimental procedures, reaching a level of detail typically only attainable at real research facilities.

This exercise is designed to demonstrate how precise instrumentation can significantly enhance the accuracy of scientific outcomes. It achieves this by optimizing instrument settings and urging you to carefully strategize the most efficient use of your time to obtain the desired measurements.

The scientific foundation for this exercise is rooted in the work of Yamani¹. While the Yamani article serves as a comprehensive reference for various aspects of experimental neutron scattering, our focus here is exclusively on the findings presented in Figure 25, which we work to replicate in this exercise. For a deeper understanding of the scientific context surrounding the MnF_2 sample, I recommend consulting the Yamani article.

The structure of this exercise is designed to provide you with a concise introduction to McStas, offering an overview of key parameters and guidance on running simulations. The assignment itself is divided into distinct tasks, each corresponding to a step in the typical experimental process, allowing you to progress through them realistically.

Setup of the simulation

For this exercise, we are using the GUI (Grafical User Interface) for McStas. Where the initial window is shown below in fig. 1.



Fig. 1: McStas graphical user interface (GUI)

After opening the instrument file in the GUI, you will encounter one of the following windows. It's crucial to ensure that there are no spaces in the file path leading to the location of the instrument file. Otherwise, McStas will return an error.

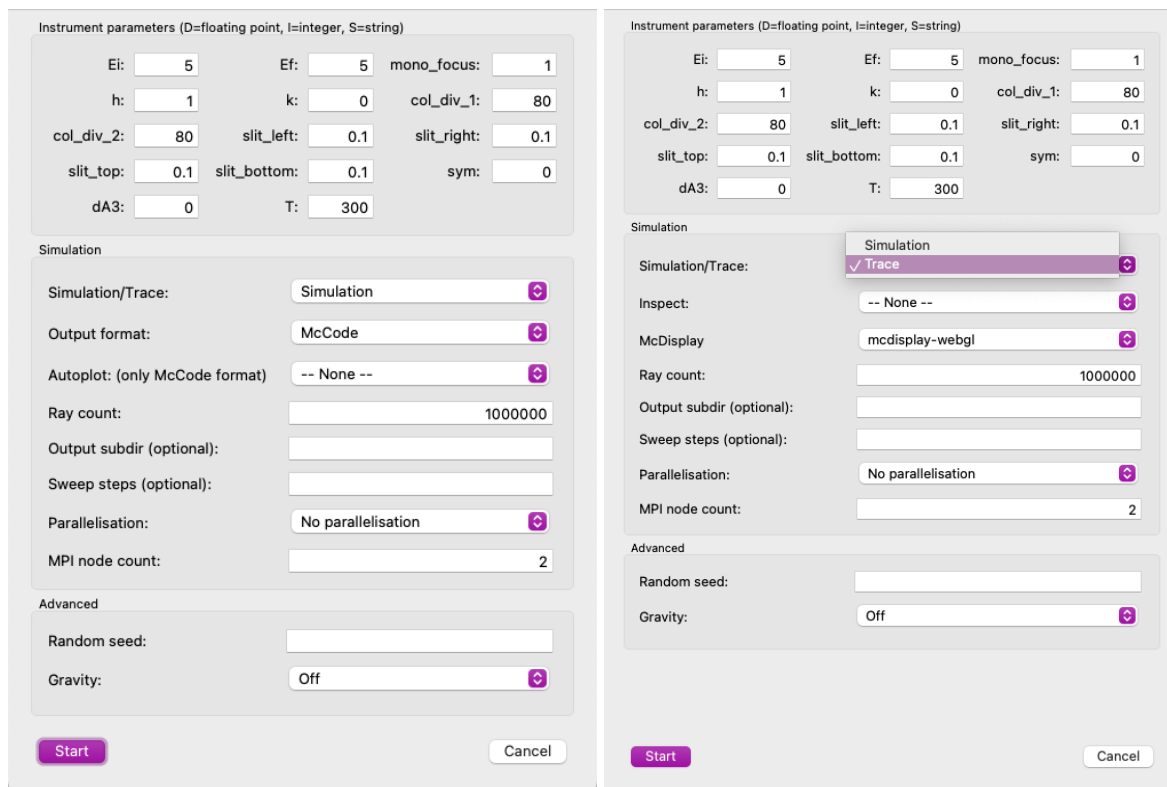


Fig. 2: Two pictures of the simulation control window in the McStas GUI. (Left) the default window that will show up on when the “run” button is pressed in the start window. (Right) Where you can find the setting for doing a trace, thereby visualizing the instrument in 3D.

The top box displays instrument-specific parameters that are customizable for various simulations. It also provides the capability to perform scans across these parameters. For instance, if you wish to perform a scan on the energy (Ei) ranging from 4 to 6 meV, you can simply input [4, 6] within the box and specify the "Sweep step" parameter in the simulation interface to determine the number of steps in your scan.

It's important to note that when scanning from 4 to 6 meV with a step size of 0.1 meV, you should configure your scan to include 21 points. If you set it to 20, you will miss the 4 meV point in your scan.

Explanation of simulation settings:

- **Autoplot**: whether a plot will be automatically generated after the simulation has ended. I recommend `mcplt-matplotlib`.
- **Ray count**: This parameter specifies the number of rays employed for each stage of the simulation. The computation time scales approximately linearly with the number of rays chosen. If you configure a sweep step, the simulation will perform this specified number of rays for each step.

- **Output subdir:** This setting designates the folder name for the simulation you are conducting. If the specified name already exists within the folder, an error will be triggered. If this field is left blank, the system will automatically generate a name based on the instrument's name and timestamp.

McStas automatically generates plots depicting the simulation results. Upon completion, these results are visualized as a series of plots displayed on the monitors positioned throughout the instrument. These plots can represent one-dimensional data or color-coded representations, as illustrated in Figure 3.

This capability exemplifies the utility of simulations for comparing with real experiments. Simulations provide us with a deeper understanding of how the neutron beam is modified as it traverses the instrument. In comparison to real experiments, where we can only detect neutrons once, simulations allow us to place monitors without hindering the continued propagation of the neutron beam. It is therefore important to note that the sole real detector employed in this context is the one labeled 'Detector' in the bottom right corner on Figure 3. All other displayed plots represent aspects of the instrument that are typically inaccessible, but are included here to enhance our understanding of the instrument's inner workings and to facilitate debugging when needed.

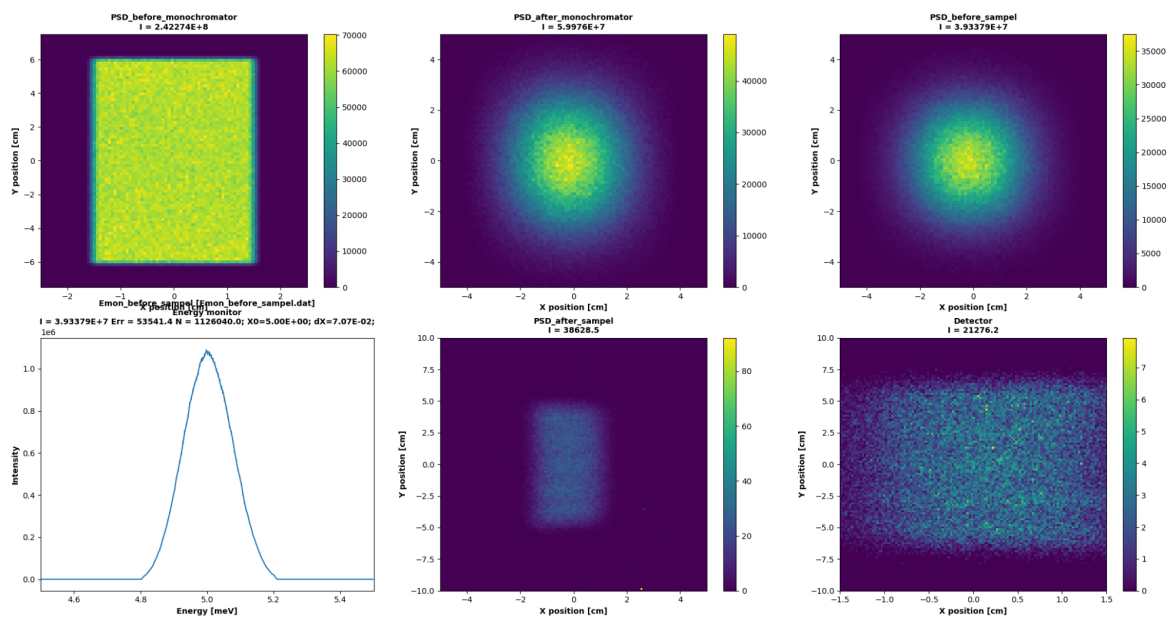


Figure 3: Results of a McStas simulation

In addition to the graphical representations themselves, the results are interactive and provide numerical values that describe the data. By clicking on any of the displayed plots, you can access more detailed information at the top of the plot, which changes slightly for different types of monitors. You can explore various descriptive statistics, such as means, standard deviations, integrated intensities, and the number of detected rays.

To test that McStas is running properly, please complete Task 0.

Task 0: To test whether the simulation is compiling properly, do the following steps.

1. Open the instrument file in the GUI.

2. Press the **run** button, and wait for the pop-up window which is displayed in fig. 2. It is very important that the instrument parameters which are in the top part of the window. If they are not, there is an error with the instrument file in respect to the running McStas version.
3. Perform a **trace** to get a 3D model of the instrument that you can view.

Assignment

Task 1: Find the signal of the sample.

You have prepared the MnF₂ sample, and as a result, you are aware of the orientations of the crystallographic axes relative to the sample itself. In order to explore the phase transition, the sample needs to be securely mounted within a cryostat. This is accomplished by affixing the sample mount onto a specialized rod designed to fit snugly within the cryostat. Subsequently, the rod is firmly secured in place, as demonstrated in the example depicted in Figure 4.



Fig. 4: (Left) Example picture of a sample mounted on the sample stick, (Right) The sample stick being inserted into the cryostat on the neutron instrument.

Figure 4 illustrates the challenges, as there is often an abundance of equipment, such as tubes and hoses, which can limit your maneuverability, particularly when it comes to rotating the cryostat. Additionally, maintaining a precise orientation along the crystal axis can be a challenge when the sample is enclosed within the cryostat, and your sole frame of reference is a rough guideline marked atop the rod. Consequently, the initial step in any experiment involves aligning the sample by identifying the reflections.

1. When inserting your sample, it starts at a temperature of 300 K, and at this temperature, there is no detectable magnetic signal. You need to consider at which temperature the sample should be at for you to be able to see the magnetic signal.
2. Perform sample rotation scans to find the angel offset of the orientation (**dA3**). The offset that you find should be kept to that value for all other simulations in this exercise.

Hint: You want to start to scan wide, and then do more focused scans around the peak.

Task 2: Find the best configuration for the instrument.

In neutron experiments, it is common for the instruments you use to offer multiple settings or configurations that can be chosen to enhance your experiment. The specific types of configurations available can vary significantly from one instrument to another, as each instrument is unique in its design and capabilities. To gain a deeper insight, it's essential to determine the optimal configuration for the instrument that will best suit your experimental needs.

There are two main configurations what we can choose our TAS to be in, as shown in Figure 5.

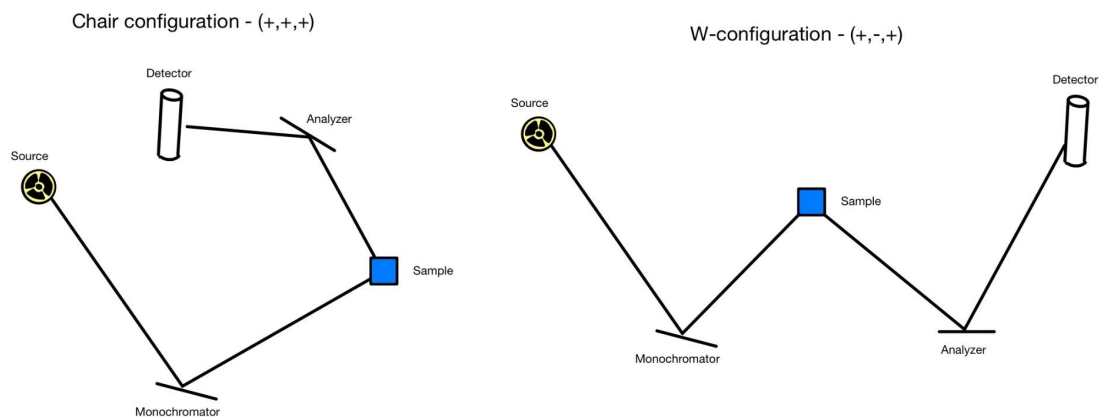


Fig. 5:(Left) Chair configuration of a TAS. (Right) w-configuration of a TAS

1. From Yamani [1], find which h, k-point you want to scan to see the magnetic phase transition, and perform it in McStas.
2. Perform the q-scan with the sym=0 and again with the sym=1 and compare the results.
3. Think about why the signals are different and choose a configuration to use, moving forward.

Task 3: Improving signal-to-noise - slit scans

A widely adopted procedure across various instrument types involves enhancing the signal-to-noise ratio on the detector signal. This is achieved by narrowing down the neutron beam, focusing it more precisely on the sample, while minimizing the impact of background radiation from the surrounding sample environment. To accomplish this, neutron-absorbing slits are strategically placed before the sample. The procedure for configuring these slits is as follows:

- Set all slits open (5 cm in this case).
- Choose one slits and make a scan of its opening from 0 mm to open.
- Look at the 'Detector' signal at the different positions and find the best position for the slit and note down the result.
- Repeat for all slits till the setting for all of them have been performed. (top, bottom, right and left)

1. Perform the slit scans.

Task 4: Test which scans are the best

In every experiment, it is important to assess the duration allocated for data collection across different scans. A critical trade-off becomes evident: you must weigh the quality of the statistical data, often measured by the number of counts within your peak, against the time needed to accumulate this data. Conversely, extending the data collection period for a single scan may only marginally enhance the quality of that specific scan while restricting your capacity to conduct additional scans.

To recreate the plot from the Yamani article, you now need to consider the following:

1. How wide should the q-scan be?
2. How many points should be in the q-scan?
3. How many rays should be simulated for each point?
4. Which temperatures do you want to measure?
5. Come with an estimate on how long time it will take to perform the entire experiment.

Task 5: perform the scans

You have made a plan, and you should now execute it. You can take two approaches to make all the different scans. 1) Do it manually by typing in the GUI. 2) Use a shell script to execute the simulations through terminal commands.

I recommend starting with the second option and testing if that works, and then move on to method 1 if that is not the case.

1. Modify the `run_multiples.sh` code to cover the scan that you want.
2. Make sure the file is an executable and navigate to the folder location through the terminal. The script can be executed through `./run_multiples.sh`. You can check that the simulation is running by seeing the same messages in the terminal as is normally seen in the GUI

Note: This simulation can potentially take hours to run, depending on the amount of scans you are performing. You can tell the simulation to run on multiple cores simultaneously, which will speed up the computing time significantly. This is however limited by the number of cores that you have on your computer.

Task 6: Analyze the data

The next important thing is to analyze the data. For each scan performed, the collected data across each scan is found in the `mccode.dat` file.

1. Discuss what information from the scan you need to recreate the red curve on fig. 5

References:

1. Yamani, Z., Tun, Z. & Ryan, D. H. Neutron scattering study of the classical antiferromagnet MnF_2 : a perfect hands-on neutron scattering teaching course Special issue on Neutron Scattering in Canada. *Can. J. Phys.* **88**, 771–797 (2010).