
Neutron and X-ray Scattering of Quantum Materials

PHYS-640

Week 12 exercises

The following instructions are for the course excursion to the Paul Scherrer Institute on Dec 9-10, 2024. You have two tasks:

- Identify the orientation of a LiNbO_3 single crystal using the two-axis neutron diffractometer, Orion, shown in Fig 1(left).
- Analyze inelastic neutron scattering data measured on $\text{K}_2\text{Ni}_2(\text{SO}_4)_3$ at the CAMEA spectrometer, shown in Fig 1(right).

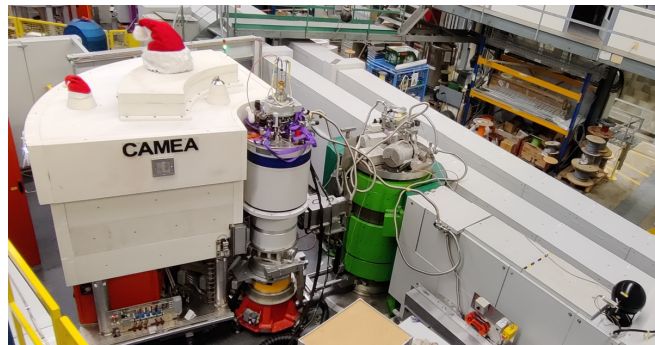
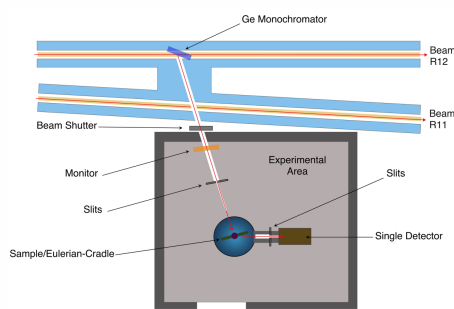


Figure 1: (left) Drawing of the two-axis diffractometer Orion. (right) Photo of the CAMEA neutron spectrometer in Christmas mode.

1: Preparation

For investigating the inelastic neutron data collected at CAMEA we will need to install some analysis software. **Please do so before we go!**

We will use a jupyter notebook so if you don't have one installed on your computer, you can do so following these steps:

- (1) Installing a software called anaconda
(<https://www.anaconda.com/products/individual#Downloads>)
- (2) Create a new anaconda environment, via either via an anaconda terminal: `conda create --name MJOLNIR python=3.8` or by using the anaconda navigator
- (3) Activate the MJOLNIR environment in the terminal with `conda activate MJOLNIR`, or through the navigator
- (4) Install the JupyterLab or the JupyterNotebook. Alternatively you can open a terminal and type: `pip install notebook`

In addition we will need a customised software package called MJOLNIR to look at our inelastic neutron data. In order to install it:

- (1) Activate the newly created anaconda environment if not done already through the terminal by typing: `conda activate MJOLNIR`
- (2) Install the MJOLNIR package through the terminal typing: `pip install MJOLNIR`. If you have problems try: `pip install PyQt5==5.15.2 --user` and then retry `pip install MJOLNIR`
- (3) Install the graphical user interface via `pip install MJOLNIRGui`

Finally test whether the installations worked

- (1) Open the anaconda terminal in the MJOLNIR environment
- (2) Type: `conda activate MJOLNIR`
- (3) Type: `MJOLNIRGui` this should open a graphical interface
- (4) Close the graphical interface and try to open a jupyter notebook in the conda environment via typing: `jupyter notebook`
- (5) In the first cell write: `import MJOLNIR`, make a new line and type: `MJOLNIR.__version__`. Press Ctrl+Enter and check the output just below the cell. It should give the version of MJOLNIR, which is currently 1.3.4.

The next part concerns the alignment exercise on Orion and can be done on the train Monday morning or at home before going.

(a) What are the crystal structure and lattice parameters of LiNbO_3 ? Which nuclear Bragg peaks would be suitable to identify the crystal orientation? *Hint: You probably already did something similar for the Week 2 exercises.*

(b) Given a neutron wavelength of $\lambda = 3.3 \text{ \AA}$ at Orion, which scattering angles do we need to measure the peaks suggested in question (a)?

(c) Think about how you would go about finding a Bragg peak.

2: Sample alignment

(a) Mount the sample on the diffractometer. Make sure that the beam is actually hitting it (well centered + correct height).

(b) Look for Bragg peaks and determine the crystal orientation.

(c) Does the intensity ratio of the different peaks correspond to the calculated structure factor?

(d) Quantify the tilt out of the horizontal plane of the identified crystallographic axes.

3: Data analysis

Since we will be following a real experiment on CAMEA, for this part we adapt. It will quite possibly be the most exciting part.