FOPRA - 61 Praktikumsversuch Inelastische Neutronenstreuung am PANDA (FRM II)

Lösch Augustin, Matthias Quintern, Bauer Lukas

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Contents

1 Introduction

The goal of this internship is to gain an insight into the world of neutron research and in this course to create a dispersion relation of a lead sample with the help of the virtual PANDA experiment.

2 Theory

2.1 Bragg's law

This equation gives the angles for coherent scattering of waves from a crystal lattice, it is the most important formula by far for this kind of experiment:

$$2d_{hkl}sin\Theta = \lambda n \quad \text{whereby} \quad d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}} \tag{1}$$

In our example this expression will simplify because we are looking at $[0, 0, 2]$. Meaning $h, k = 0; l = 2$. Here h, k, l are called Miller indices.

2.2 Laue equation

The Laue equation is aquivalent to Bragg's law:

$$\boldsymbol{Q} = \boldsymbol{G} = h\boldsymbol{g_1} + k\boldsymbol{g_2} + \boldsymbol{g_3}, \tag{2}$$

where $\boldsymbol{g_i}$ are basis vectors of the reciprocal lattice. Wave-vectors satisfying this equation from the Bragg reflections in the spectra of the sample.
While we look into inelastic scattering one has to modify the laue euqation:

$$\boldsymbol{Q} = \boldsymbol{k_i} - \boldsymbol{k_f} = \boldsymbol{G} \mp \boldsymbol{q}, \tag{3}$$

where $\boldsymbol{k_i}$ is the incoming wave vector, $\boldsymbol{k_f}$ is the outgoing wave vector after inelastic scattering, $\boldsymbol{G}$ is the reciprocal lattice vector and $\boldsymbol{q}$ is called a Phonon.

2.3 Dispersion relation

The connection between frequency and wave vector is known as a dispersion relation. The dispersion relation contains in principle all information about the dynamic properties of the sample, such as specific heat capacity or the speed of sound. The goal of this experiment is to conduct a phonon dispersion relation of a lead sample.

3 Experimental setup

3.1 Experimental Setup

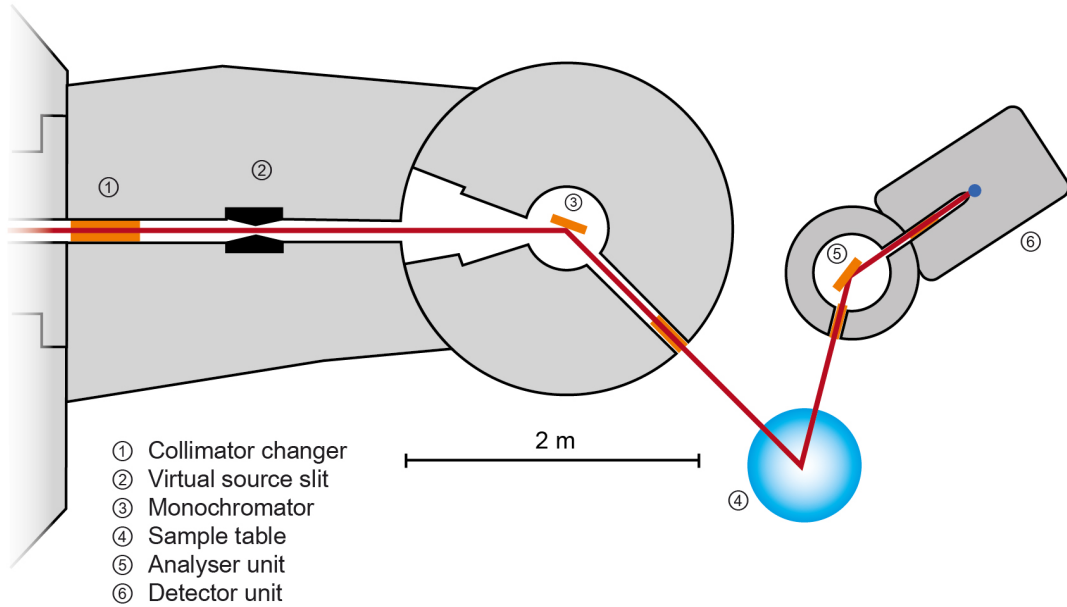

Figure 1: Setup of the PANDA Experiment which is a triaxial spectrometer.

3.2 Procedure and Results

First of all, we began with the program "Takin" which is an open-source software for experiment planning, visualisation, and data analysis. With this tool, we were able to visualize a 2D plane of the reciprocal lattice with an Ewald-construction for the chosen wave vector k_f of the scattered neutrons on the left side. On the right side there was a schematic sketch of the three axis spectrometer setup with the angles at all three axis corresponding to the Ewald-construction on the left. For the experiment a 2D plane of the reciprocal lattice of lead (Pb) spanned by the vectors (1,1,0) and (0,0,1) was chosen so that the points (0,0,2) and (1,1,1) became visible.

Next, we started "Nicos". It is also a free to use software used to control the lab instrument. To control the PANDA setup we needed to load the setup for it and set some parameters (see figure 2) so that we were able to get measuring done.

Figure 2: Information on the examined Pb-sample

Before the necessary scans could be carried out, the spectrometer had to be calibrated. In order to know which spatial direction corresponds to which 2θ angle, we needed to determine the orientation of our sample. To do so, we identified the 2θ angle of the [002] elastic-peak in Takin and then performed a scan to see at which angle the peak actually occurs. The difference is the rotation offset of the sample. The next step was to get the translation of the sample right, for which we scanned at the [002] peak while varying x/y translation. After the calibrations it was possible to start with basic scans, where either the Energy E or the momentum transfer $Q = k_i - k_f$ are kept constant and the other one is changed in fixed steps over a certain range in order to find a peak. With the help of a few of these preliminary scans it was possible to get a basic idea of where the different peaks are located.

With that information it was now practicable to measure the whole dispersion relation for the lead sample. For that a small and simple code (see figure 3) was run overnight to collect all the data in several different scans.

```python
1   kf(1.55)
2   for i in range(7):
3       qcscan((0,0,2,i),(0,0,0.01,0), 220, 5)
4   kf(2.66)
5   for i in range(5,9):
6       qcscan((0,0,2,i),(0,0,0.01,0), 220, 5)
7   for i in range(5,12):
8       qscan((0,0,2+i/10,0),(0,0,0,0.05), 170, 5)
9   for i in range(5,12):
10      qscan((0,0,2-i/10,0),(0,0,0,0.05), 170, 5)
11
```

Figure 3: Python Code that includes E- and Q-scans for the dispersion relation

These measurements included scans with constant E and scans with constant Q. The whole dispersion was measured with constant E scans while one measurement series ranged from $1\,\mathrm{meV}$ to $6\,\mathrm{meV}$ with $k_f = 1{,}55\,\frac{1}{\text{Å}}$ (example in figure 4) and another one ranged from $5\,\mathrm{meV}$ up to $8\,\mathrm{meV}$ with $k_f = 2{,}66\,\frac{1}{\text{Å}}$.
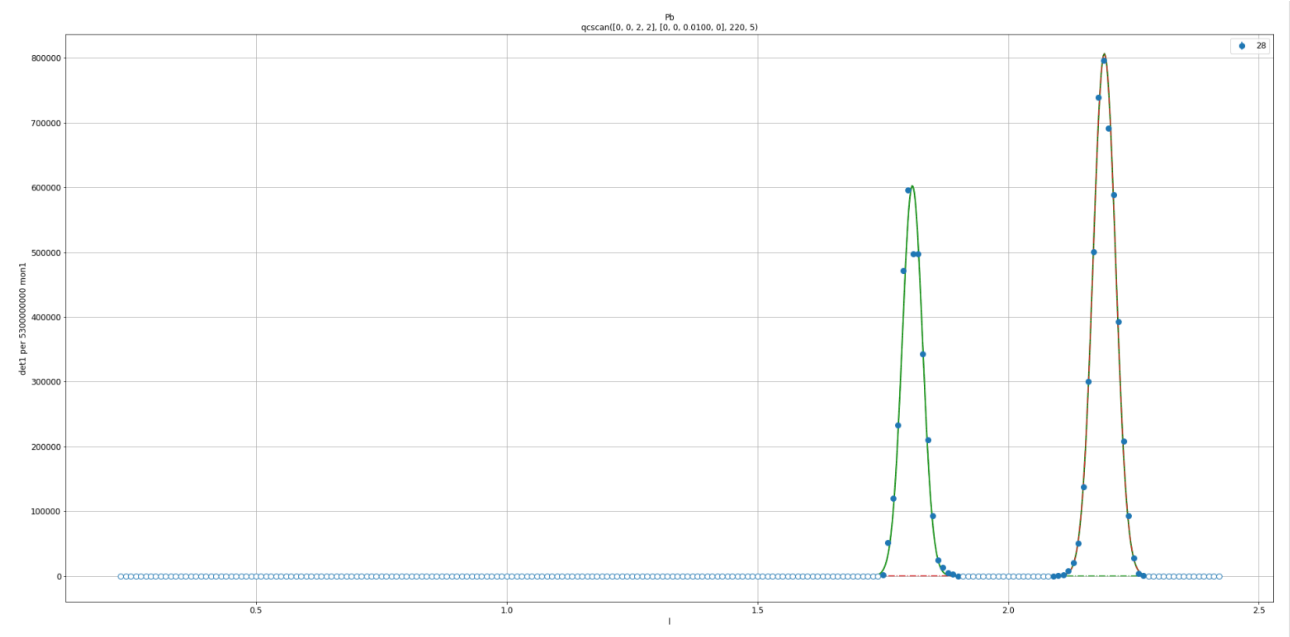
Figure 4: Example for a q-scan at $k_f = 1{,}55\,\frac{1}{\text{Å}}$

Closer to the edge of the Brillouin zone additional scans with constant Q were carried out (example in figure 5), because the dispersion relation flattens out on the edge of the zone. That leads to broader peaks when varying Q in this area, because the Energy is nearly constant for a certain range of Q values, therefore making scans with constant Q more precise. Those scans were measured ranging from $l = 0{,}9\,\frac{1}{\text{Å}}$ to $1{,}5\,\frac{1}{\text{Å}}$ and from $l = 2{,}5\,\frac{1}{\text{Å}}$ to $3{,}1\,\frac{1}{\text{Å}}$.
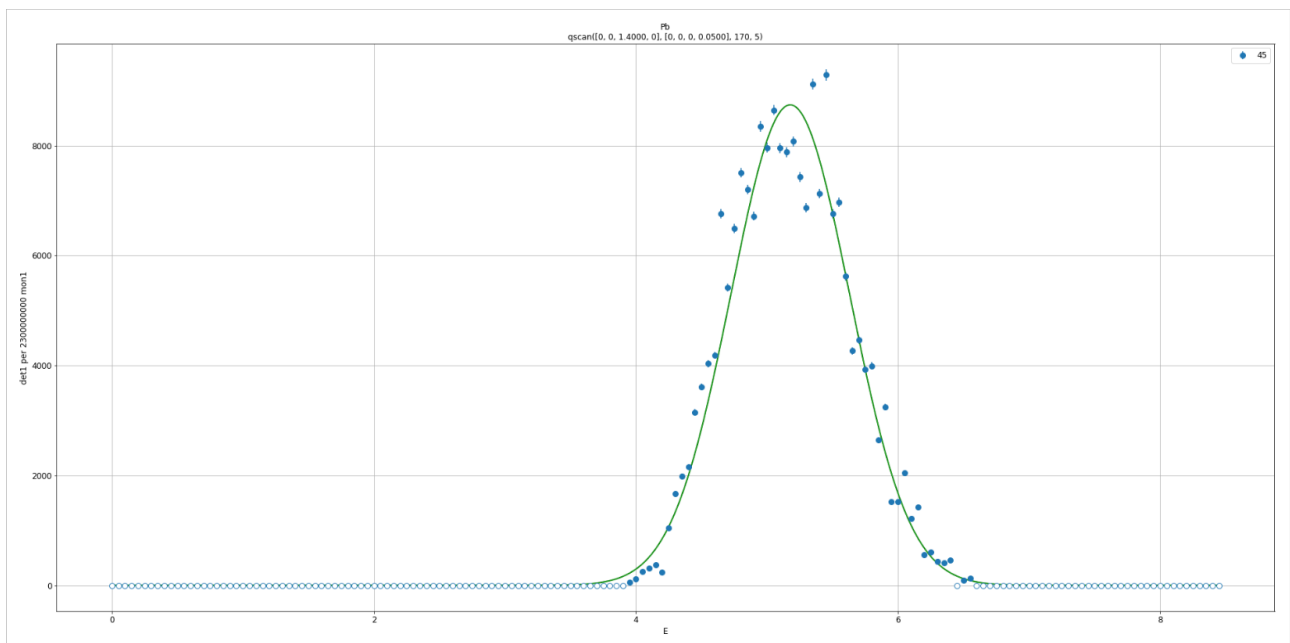

Figure 5: Example for an E-scan at $k_f = 1{,}55\,\frac{1}{\text{Å}}$

After all the scans were completed all the different intensity peaks were fitted with Gauss curves using "ufit" which is also an in-house software for data analysis. The fitting software then provided the necessary information on peak location and FWHM which was used to calculate the errors.

3.3 Dispersion Relation

With another feature of the "ufit" software it was possible to create a mapping of all the measurements and create a 2D colour map, where the dispersion relation, that we expected to get from the scans, was quite obvious to see.
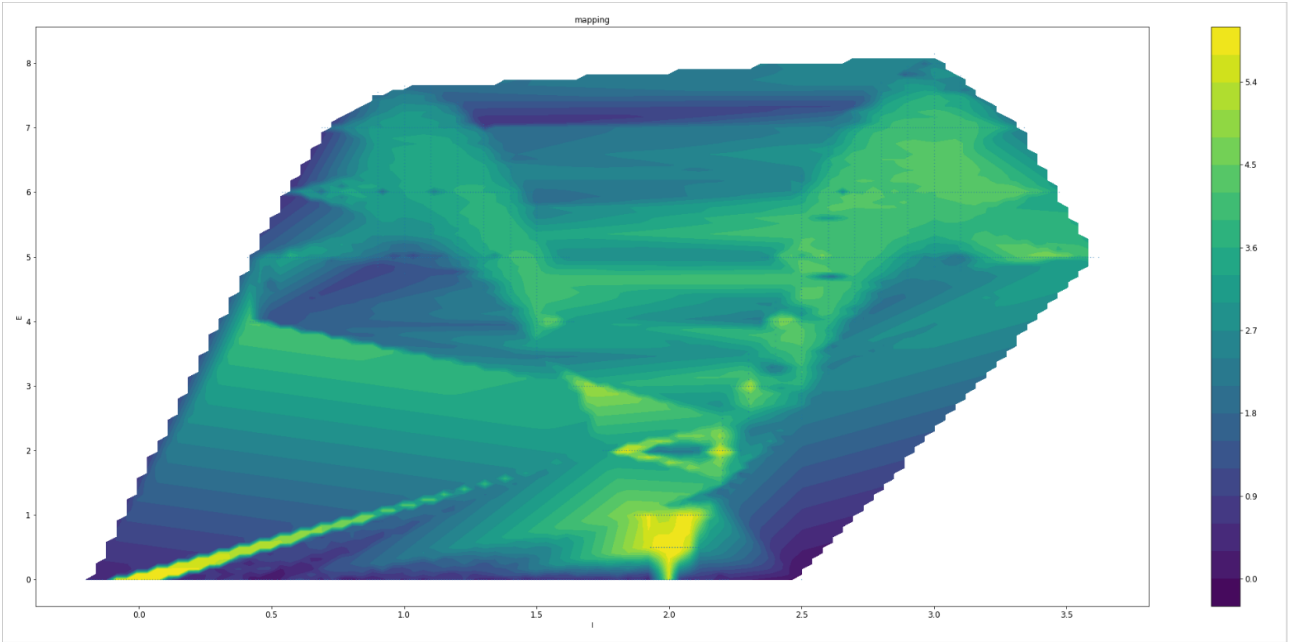

Figure 6: mapping of all the measurement that were executed

With all the Gauss fit done, the necessary information for the dispersion relation (figure 7) was gathered from the fit results and could be fitted with a sinus function:

$$E = a \cdot |sin(b \cdot l + c)| \tag{4}$$

The Graph shows that the sinus function describes the dispersion relation very good, similar to the
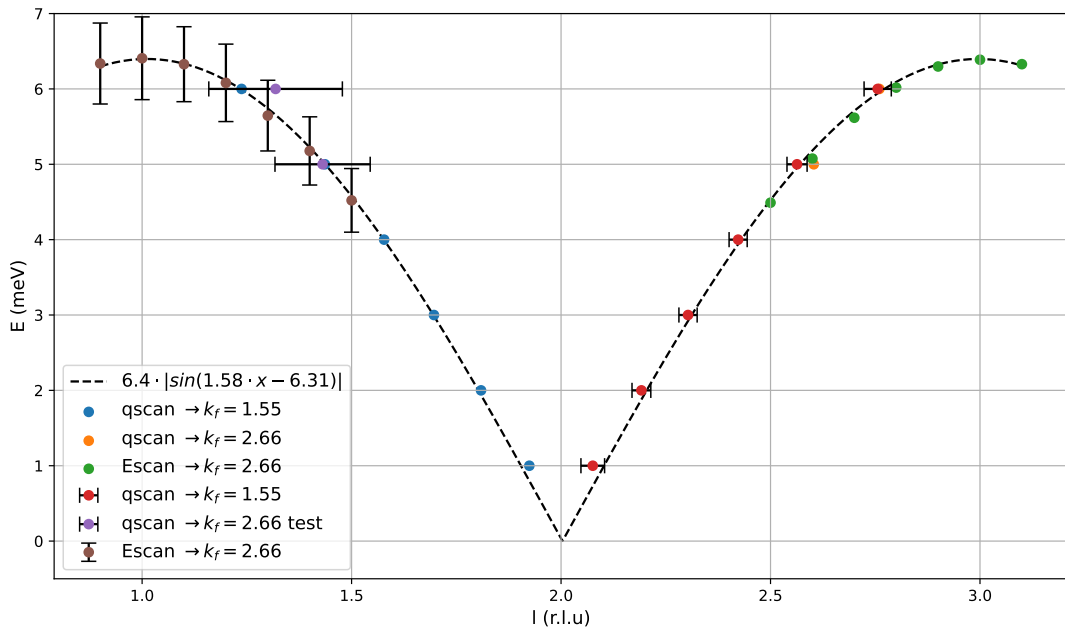

Figure 7: Fitted dispersion relation for the virtual lead sample.

dispersion model of a linear chain. We can also see that the peaks measured at constant energy with

$k_f = 1{,}55 \frac{1}{\text{Å}}$ at lower Energies are much sharper and have smaller errors than the peaks measured at higher constant energies with $k_f = 2{,}66 \frac{1}{\text{Å}}$. That is why additional scans with constant Q at the border of the Brillouin zone were performed to get a good dispersion curve at the higher energies.

3.4 Speed of sound

The speed of sound is related to the energy by $\omega = \frac{E}{\hbar} = v \cdot q$. Using a linear approximation for the dispersion relation at [002], we can derive

$$v = a \cdot b / \hbar, \tag{5}$$

where a, b are the fit parameters for the dispersion relation. $v_{\text{lead}} = (1536{,}28 \pm 40{,}68) \frac{\text{m}}{\text{s}}$. Whereas other sources like Wikipedia suggest a value around: $1200 \frac{\text{m}}{\text{s}}$. When we compare both values one gets to the conclusion that our result is compromised due to errors which were made in the process while simulating the experiment.

3.5 Resolution Ellipsoid
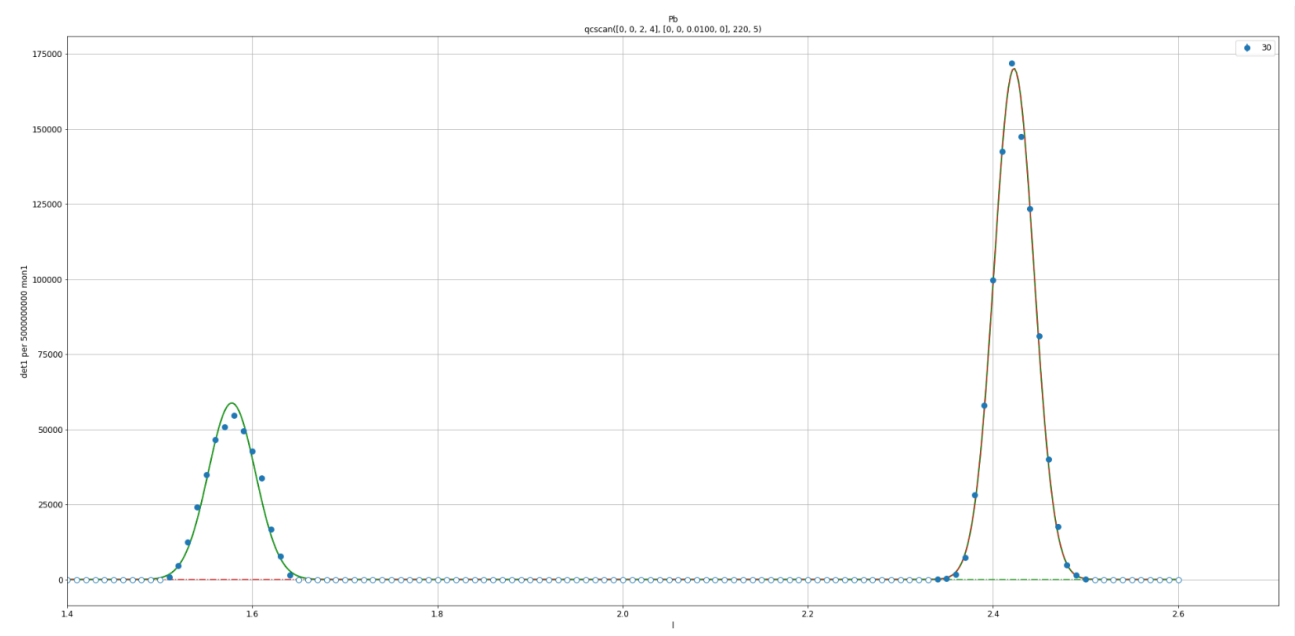
Peaks for resolution ellipsoid:
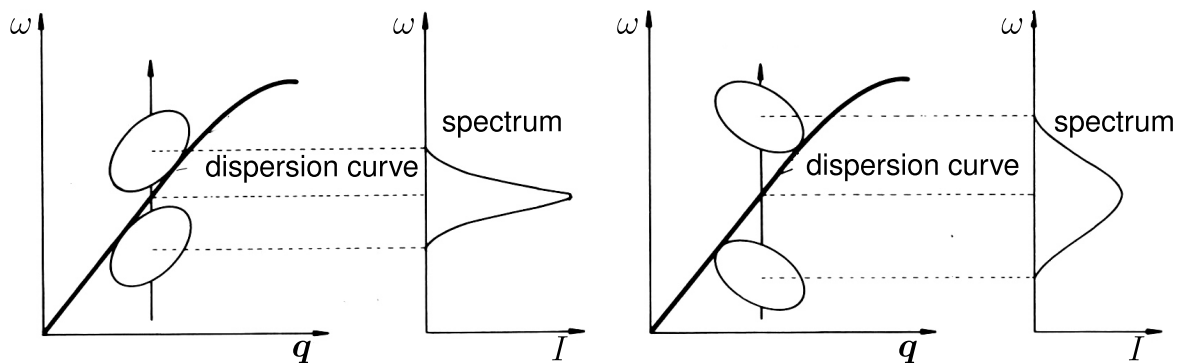

Figure 8

Erklärung?

Figure 9: Focused vs. unfocused measurement (source: instruction manual)