

Physics with Neutrons I

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Exercise sheet 3

<https://wiki.mlz-garching.de/n-lecture06:index>

Solutions

1. Python

Some exercises require the use of some program for numerical computation, such as Matlab, Mathematica or some programming language. Several exercises will require the use of a computer. The solutions will always be given in the language python. Although you are not forced to, it might be a good idea to install the requirements to run these programs on your computer:

- python, the language interpreter <http://www.python.org/download/>
- ipython, a nice command line <http://ipython.scipy.org/dist/>
- numpy & scipy, packages for numerical and scientific computing
<http://www.scipy.org/Download/>
- matplotlib, a package for 2D-plotting <http://matplotlib.sourceforge.net/>

Personally, I use the ANACONDA distribution of python which comes with the developing environment SPYDER <https://www.anaconda.com/download/>

2. Coherent and Incoherent scattering cross section

In most cases, real materials do not have a single scattering length, but a distribution of several values. This could be due to different elements, isotopes or a non-zero nuclear spin. In case of a nuclear spin, the isotope has two scattering lengths, one for parallel spin alignment of nucleus and neutron b^+ and one for antiparallel alignment b^-

- In the experiment, we use cross sections σ instead of scattering lengths b to describe a sample and especially distinguish between coherent and incoherent scattering. How are those quantities related? Is there a fundamental difference for a mixture of elements, isotopes or spin-states?
- What extreme cases of scattering can happen in any system?
- Calculate the coherent and incoherent scattering cross sections for an element with n isotopes. Assume that each isotope has a relative abundance f_i
- Calculate the coherent and incoherent scattering cross sections for a single isotope with nuclear spin I .
- Determine the coherent and incoherent scattering cross sections of pure Hydrogen and Deuterium with the following values:

Nuclide	I	b (fm)	Nuclide	I	b (fm)
^1H	$1/2$	$b^+ = 10.85$ $b^- = -47.50$	^2H	1	$b^+ = 9.53$ $b^- = 0.98$

Solution

- In the derivation of the double differential cross section, the sum can be splitted in two parts. The first considers all pairs of atoms and results in the collective or coherent scattering, while the second only sums over individual atoms and gives the incoherent scattering. In the prefactor of both sums we find the scattering cross sections given by:

$$\sigma_{coh} = 4\pi (\bar{b})^2$$

$$\sigma_{inc} = 4\pi (\overline{b^2} - (\bar{b})^2) = 4\pi \overline{(\Delta b)^2}$$

Here, each atom has an individual scattering length b_i and can be written as $b_j = \bar{b} + \Delta b$ with the expectation value $\bar{b} = \langle b_i \rangle_i$. In the calculation, only the distribution of different scattering lengths is important regardless of their origin. Accordingly, there is no difference between the coherent and incoherent scattering due to different spin states, isotopes or elements.

- The extreme cases are summarized in the table below:

\bar{b}	Δb	Remarks
0	0	no scattering at all
0	large	only incoherent scattering, positive and negative b_i
large	0	only coherent scattering, all b_i are identical
large	large	coherent and incoherent scattering

- In order to calculate the scattering cross sections we need the statistical quantities \bar{b} and $\overline{b^2}$. For a mixture of different isotopes with relative abundance f_i this gives the following expressions which can be inserted in the above definitions of σ_{coh} and σ_{inc} :

$$\sum_{i=1}^N f_i = 1$$

$$\bar{b} = \langle b_i \rangle_i = \sum_{i=1}^N f_i \cdot b_i$$

$$\overline{b^2} = \langle b_i^2 \rangle_i = \sum_{i=1}^N f_i \cdot b_i^2$$

- In case of a single isotope with nuclear spin, we can basically use the same expressions but we can express the relative abundance f_i in terms of the spin. In any scattering event, the spins of neutron and nucleus can be aligned either parallel (with scattering length b^+) or anti parallel (with scattering length b^-). This is expressed in the value of the total spin of the system neutron-nucleus which is either

$$S^+ = I + 1/2, \text{ for parallel alignment or}$$

$$S^- = I - 1/2, \text{ for anti parallel alignment}$$

With each total Spin S , a number N of possible states is associated, representing the value of one selected component of the spin vector:

$$N^+ = 2S^+ + 1 = 2I + 2, \text{ for parallel alignment}$$

$$N^- = 2S^- + 1 = 2I, \text{ for anti parallel alignment}$$

With this, the relative abundance f of spin configurations can be calculated as:

$$f^+ = \frac{f^+}{f^+ + f^-} = \frac{I + 1}{2I + 1}, \text{ for parallel alignment}$$

$$f^- = \frac{f^-}{f^+ + f^-} = \frac{I}{I + 1}, \text{ for anti parallel alignment}$$

Finally, arbitrary mixtures of isotopes, elements and spin states can be combined in the following way:

$$\bar{b} = \langle b_{i,+/-} \rangle_{i,+/-} = \sum_{i=1}^N f_i \cdot (f_i^+ b_i^+ + f_i^- b_i^-)$$

$$\bar{b}^2 = \langle b_{i,+/-} \rangle_{i,+/-}^2 = \sum_{i=1}^N f_i \cdot (f_i^+ (b_i^+)^2 + (f_i^- b_i^-)^2)$$

- With the above equations we get for hydrogen or deuterium:

Nuclide	\bar{b} (fm)	\bar{b}^2 (fm ²)	σ_{coh} (b)	σ_{inc} (b)	σ_{abs} (b)
¹ H	-3.74	652	1.76	80.2	0.333
² H	6.68	60.9	5.61	2.04	0.000519

The absorption cross section is listed additionally, to illustrate, why heavy water is often used as a moderator, even though scattering is stronger and more efficient for hydrogen (normal water).

3. Bragg Scattering II

Consider a similar setup of exercise 4 on sheet 2 (Bragg Scattering) with neutron wavelength $\lambda = 2.0\text{\AA}$, lattice parameter $d = 3.2\text{\AA}$ and $n = 100$ scattering planes. Assume, that each scatterer (scattering plane) has its own scattering length b_j and compute the scattering pattern for the following cases:

1.

$$b_j = \begin{cases} 0 & \text{if } j \text{ is even,} \\ 1 & \text{if } j \text{ is odd.} \end{cases}$$

2.

$$b_j = \begin{cases} 1 & \text{if } j \text{ is even,} \\ 2 & \text{if } j \text{ is odd.} \end{cases}$$

3.

$$b_j = \begin{cases} -1 & \text{if } j \text{ is even,} \\ 1 & \text{if } j \text{ is odd.} \end{cases}$$

4. Choose b_j randomly for each scatterer (plane) : $b_j = 0$ or $b_j = 1$

5. Choose b_j randomly for each scatterer (plane) : $b_j = 1$ or $b_j = 2$

6. Choose b_j randomly for each scatterer (plane) : $b_j = -1$ or $b_j = 1$

7. Feel free to play around!

Solution

The solution of this exercise is mostly equivalent to exercise 4 on sheet 2. Hence, only the new parts and results are presented here.

The scattering length is the amplitude b of a scattered wave. So, in order to account for different values b_j at different scattering planes we take this into account when summing up all contributing scattered waves. The previous expression:

$$I_{tot} = (A_0 + A_1 + \dots + A_{N-1})^2 = \left(\begin{array}{c} \cos(0 \cdot \phi) + \cos(1 \cdot \phi) + \dots + \cos((N-1) \cdot \phi) \\ \sin(0 \cdot \phi) + \sin(1 \cdot \phi) + \dots + \sin((N-1) \cdot \phi) \end{array} \right)^2$$

which has the same scattering length everywhere is changed to:

$$I_{tot} = (A_0 + A_1 + \dots + A_{N-1})^2 = \left(\begin{array}{c} b_0 \cdot \cos(0 \cdot \phi) + b_1 \cdot \cos(1 \cdot \phi) + \dots + b_{N-1} \cdot \cos((N-1) \cdot \phi) \\ b_0 \cdot \sin(0 \cdot \phi) + b_1 \cdot \sin(1 \cdot \phi) + \dots + b_{N-1} \cdot \sin((N-1) \cdot \phi) \end{array} \right)^2$$

In the Python script, this has to be implemented as well. The previous computation read:

```
# add up all contributing waves
for n in range(N):
    x += np.cos(n*phi)
    y += np.sin(n*phi)
```

This is extended by the scattering length as well. There are several ways how to express b_j and the following is just one possibility.

```
# add up all contributing waves
for n in range(N):
    b = (...) # see the following cases
    x += b*np.cos(n*phi)
    y += b*np.sin(n*phi)
```

```
Case 1. : b = np.mod(n,2)
Case 2. : b = np.mod(n,2)+1
Case 3. : b = 2*np.mod(n,2)-1
Case 4. : b = np.random.choice([0,1])
Case 5. : b = np.random.choice([1,2])
Case 6. : b = np.random.choice([-1,1])
```

For cases 4. to 6. the result will be different for each computation. However, this will only show for small numbers N of scattering planes as for large N statistics take over.

- Case 0 : No distribution of b . This is just a reference for the scattering pattern without disorder.
- Case 1 : Every second atom is missing, which means that we are looking at a scattering planes with double the distance. accordingly, the distance between scattering peaks in k -space is halved.
- Case 2 : the lattice can be split into a superposition of two parts, one with $b = 1.5$ (see Case 0) for all planes, and another one with alternating $b_j = \pm 0.5$ (see Case 3). The resulting scattering function is again the superposition of these two contributions. The first part creates the large peaks, while the second one creates the smaller peaks in between.

- Case 3 : A negative scattering length means that the neutron gets a phase shift of π when it is scattered, which is not the case for positive b . If we add this additional phase shift to the Bragg equation, any case of constructive interference (a phase shift between two adjacent planes of $n2\pi \hat{=} 2\pi$) will become a destructive interference instead (phase shift of $n2\pi + \pi \hat{=} \pi$), and vice versa. Hence, the Bragg peak positions are shifted by half the periodicity in k-space.
- Case 4 : The random distribution in the next three cases allow us to think about the signal in terms of coherent and incoherent scattering. For Case 4, the relative difference between the b_j is very large which is why we see a strong incoherent contribution in the noisy background in between Bragg peaks. The effect of Case 1, that we have additional Bragg peaks, is not visible for this random distribution of the same b_j .
- Case 5 : Essentially identical to Case 4, but since the relative difference between the b_j is smaller, and the mean value is larger, we observe higher intensity Bragg peaks with lower background.
- Case 6 : In this last case, the mean of the b_j is zero. Accordingly we observe no coherent scattering (Bragg peaks) at all and only see background noise due to incoherent scattering. (note the scale of the plot)

