Physics with neutrons 2

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Exercise sheet 6
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EXERCISE 6.1

Calculate $\langle u^2\rangle_T$ and f^2_{DWF} for lead ($\theta_D = 88\,\mathrm{K}$), copper ($\theta_D = 315\,\mathrm{K}$), and diamond ($\theta_D = 1860\,\mathrm{K}$) at $T = 10\,\mathrm{K}$ and $T = 1000\,\mathrm{K}$ with the low and high temperature approximations. Which material is most useful as a monochromator? What can be done to improve the reflectivity of copper monochromators?

Solution. The DWF form-factor contribution is given by

$$f^2_{DWF} = e^{-2W(Q)} = e^{-\frac{1}{6}Q^2\langle\zeta^2\rangle}$$

with the mean square atomic displacement $\langle\zeta^2\rangle$, which of course depends on the temperature of the material, and can be approximated with different models.
One model is the Debye model, assuming a spectrum of excitation frequencies for N atoms given by

$$Z(\omega) = \frac{9N\omega^2}{\omega^3_{max}},$$

where the cutoff frequency is expressed in terms of the Debye temperature Θ_D:

$$\omega_{max} = \frac{k_b\Theta_D}{\hbar}.$$

For this model we get a mean square displacement of (EXERCISE 9)

$$\langle\zeta^2\rangle = \frac{9\hbar^2}{2k_b\Theta_D M}P(T) = \frac{9k_b\Theta_D}{2M\omega^2_{max}}P(T),$$

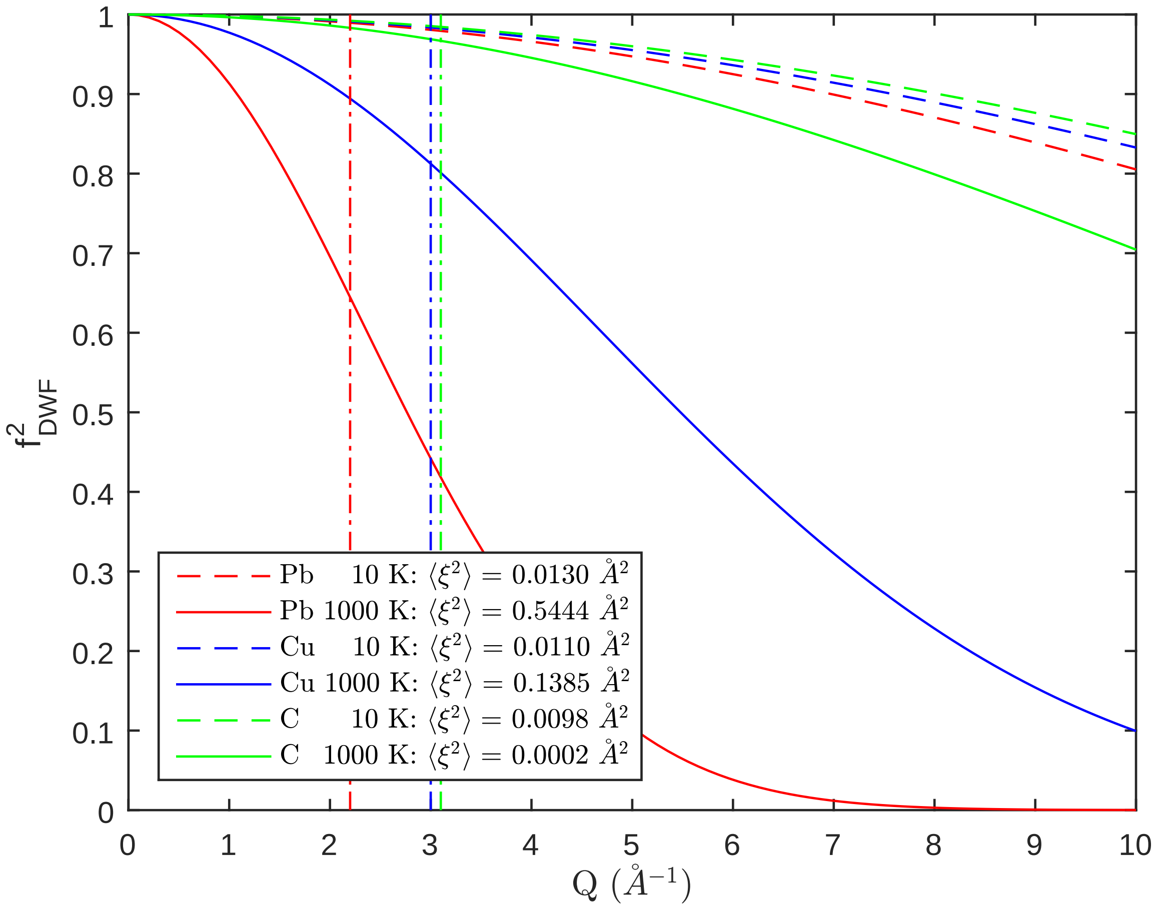
with a function $P(T)$ that depends on the temperature relative to Θ_D.
In the high-temperature regime, $T \gg \Theta_D$, it is simply given by

$$P(T) = 4\frac{T}{\Theta_D} \Longrightarrow \langle\zeta^2\rangle = \frac{18\hbar^2 k_b T}{k_b^2\Theta_D^2 M}.$$

In the low-temperature regime, $T \ll \Theta_D$, we get

$$P(T) = 1 + 4\frac{\pi^2}{6}\left(\frac{T}{\Theta_D}\right)^2 \Longrightarrow \langle\zeta^2\rangle = \frac{9\hbar^2}{2k_b\Theta_D M} + \frac{3\pi^2\hbar^2k_b^2T^2}{k_b^3\Theta_D^3 M}.$$

The figure shows the DWF for the given materials and temperatures:



The vertical lines indicate the first allowed Bragg reflexion, which can be used for monochromatizing neutrons. The most useful monochromator material obviously would be diamond. Lead, on the other hand, is quite unsuitable. The reflectivity of copper, which is a commonly used monochromator because it is easy to produce large good quality single crystals, benefits strongly from cooling it down. □

EXERCISE 6.2

Prove that spin-incoherent scattering is $\frac{2}{3}$ spin-flip scattering and $\frac{1}{3}$ non-flip scattering. This can be done by the following steps:

1. Start with the expression given in the lecture for $\overline{b}$ in (A.2.10), assuming a single isotope with nuclear spin I. Express b^+ and b^- in the form

$$b^+ = \overline{b} + g^+(I)\cdot B \qquad \text{and}$$
$$b^- = \overline{b} + g^-(I)\cdot B \qquad \text{with} \quad B = \frac{b^+ - b^-}{2I+1},$$

   i. e. find $g^+(I)$ and $g^-(I)$.

2. Now we want to unify $g^+(I)$ and $g^-(I)$ so that we can give a single expression for b. Do so using the projection operator P that projects the spin of the neutron from its initial quantization axis onto a new quantization axis in direction of $\vec{I} = (I_x, I_y, I_z)$, which is

$$P(\vec{I}) = 1 + I_x\sigma_x + I_y\sigma_y + I_z\sigma_z = 1 + \vec{I}\cdot\sigma.$$

   The new axis $\vec{I}$ is the quantization axis of the nucleus (neutron and nucleus have to have the same quantization axis to decide if they are parallel or antiparallel). $\sigma_{x,y,z}$ are the Pauli matrices and σ is a vector of the Pauli matrices.

3. This yields an expression for the scattering length of a nucleus using the mean value of parallel and antiparallel neutron-nucleus spin alignment and the deviation thereof. Which part of this scattering length will give rise to incoherent scattering? Write the incoherent cross section.

4. We are now not only interested in the probability that there is *some* incoherent scattering event but want to split it up in probabilities for scattering events where the neutron has a spin when incoming $|s_i\rangle$ and when outgoing $|s_f\rangle$. These spin states are prepared / measured in polarizers / detectors that are sensitive in the laboratory z-direction. Therefore the two spin states can both be either up $\binom{1}{0}$ or down $\binom{0}{1}$. The probabilities (cross sections) can be calculated using

$$\sigma_{|s_i\rangle\to|s_f\rangle} = 4\pi\left|b_{|s_i\rangle\to|s_f\rangle}\right|^2 \propto \left|\langle s_f|\vec{I}\sigma|s_i\rangle\right|^2 = \left|\langle s_f|I_x\sigma_x|s_i\rangle + \langle s_f|I_y\sigma_y|s_i\rangle + \langle s_f|I_z\sigma_z|s_i\rangle\right|^2.$$

   Calculate $b_{|\uparrow\rangle\to|\uparrow\rangle}$, $b_{|\uparrow\rangle\to|\downarrow\rangle}$,$b_{|\downarrow\rangle\to|\uparrow\rangle}$, and $b_{|\downarrow\rangle\to|\downarrow\rangle}$ as functions of the nuclear spin components I_x, I_y, and I_z.

5. Assume that the nuclei are not aligned, therefore $I_x^2 = I_y^2 = I_z^2$ to calculate the relative frequencies of spin flip and non spin flip scattering.

Solution. 1. We start with

$$\overline{b} = \frac{I+1}{2I+1}\cdot b^+ + \frac{I}{2I+1}\cdot b^-,$$

solve for $b^{+/-}$, write $x\cdot\overline{b}$ as $\overline{b} + (x-1)\cdot\overline{b}$, express $(x-1)\cdot\overline{b}$ by b^+ and b^-:

$$b^+ = \overline{b} + I\cdot B \qquad b^- = \overline{b} + (-I-1)\cdot B$$

2. We know that there are $2I+2$ possibilities for the projection which yields b^+ and $2I$ for the one which yields b^-. As we are interested in relative frequencies, they reduce to $I+1$ and I. The projection gives an additional

   − for the antiparallel alignment. Therefore we rewrite:

$$b^+ = \overline{b} + (\underbrace{I+1}_{P(+)} - 1)\cdot B \qquad b^- = \overline{b} + (\underbrace{-I}_{P(-)} - 1)\cdot B$$

   and arrive at the unified expression

$$b = \overline{b} + \vec{I}\sigma \cdot B.$$

3. The incoherent scattering is only due to the second part. As a side note, isotope-incoherent scattering would turn up as

$$b = \sum_j c_j \cdot \left(\overline{b_j} + \vec{I}_j \sigma \cdot B_j\right)$$

   and is therefore non-flip. The incoherent cross section is

$$\sigma_{\text{inc}} = 4\pi \left|\vec{I}\sigma \cdot B\right|^2 = 4\pi B^2 \cdot \left|\vec{I}\sigma\right|^2.$$

   Note the similarity to the expression for the spin-dependent cross section given on the exercise sheet! (No, this is no coincidence. . .)

4. The Pauli matrices are

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

   Multiplying these matrices with the up (+) and down (−) vectors gives $\sigma_z(\pm) = \pm(\pm)$, $\sigma_x(\pm) = +(\mp)$, and $\sigma_y(\pm) = \pm i(\mp)$. As up and down are orthotogonal, only a few terms survive:

$$\begin{aligned} b_{|\uparrow\rangle\to|\uparrow\rangle} &= +I_z & \qquad b_{|\uparrow\rangle\to|\downarrow\rangle} &= I_x + iI_y \\ b_{|\downarrow\rangle\to|\downarrow\rangle} &= -I_z & \qquad b_{|\downarrow\rangle\to|\uparrow\rangle} &= I_x - iI_y \end{aligned}$$

5. The relative frequencies are given by the respective sums of the cross sections:

$$\sigma_{\text{nf}} = \sigma_{|\uparrow\rangle\to|\uparrow\rangle} + \sigma_{|\downarrow\rangle\to|\downarrow\rangle} \propto |I_z|^2 + |I_z|^2 = 2I_z^2$$

$$\sigma_{\text{sf}} = \sigma_{|\uparrow\rangle\to|\downarrow\rangle} + \sigma_{|\downarrow\rangle\to|\uparrow\rangle} \propto |I_x + iI_y|^2 + |I_x - iI_y|^2 = 2(I_x^2 + I_y^2)$$

   It follows that

$$\sigma_{\text{sf}} = 2 \cdot \sigma_{\text{nf}}.$$

   We have seen that the spin-flip is a phenomenon caused by two subsequent projections of the spin of the neutron: from the lab z axis onto the polarization axis of the nucleus and then back on the lab z axis. The scattering event itself does not flip the spin.

   This makes sense as the particle we identified for the neutron-nucleus interaction, the π^0, has spin 0 and can therefore not transmit angular momentum. The lightest meson with spin 1 is the ρ^0 which is however much heavier than the pion (770 MeV compared to 135 MeV). This should result in a weaker interaction which is not observed.

□

EXERCISE 6.3

Derive the representation

$$G(\mathbf{r},t) = \frac{1}{N}\sum_{j,j'}\int \langle \delta\Big(\mathbf{R}-\mathbf{r}_{j'}(0)\Big)\delta\Big(\mathbf{R}+\mathbf{r}-\mathbf{r}_j(t)\Big)\rangle dR$$

from the expression for the intermediate scattering function

$$I(\mathbf{Q},t) = \frac{1}{N}\sum_{j,j'}\langle e^{-i\mathbf{Q}\cdot\mathbf{r}_{j'}(0)} e^{i\mathbf{Q}\cdot\mathbf{r}_j(t)}\rangle_T$$

using the substitution

$$e^{-i\mathbf{Q}\cdot\mathbf{r}_{j'}(0)} = \int e^{-i\mathbf{Q}\cdot\mathbf{r}'}\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)d\mathbf{r}'.$$

Solution. $G(\mathbf{r},t)$ is the so called space-time pair correlation function, transforming the reciprocal spatial space coordinates $\mathbf{Q}$ to real space $\mathbf{r}$. With this ansatz we calculate

$$\begin{aligned}
G(\mathbf{r},t) &= \frac{1}{(2\pi)^3}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}} I(\mathbf{Q},t) = \frac{1}{(2\pi)^3}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}}\frac{1}{N}\sum_{j,j'}\langle e^{-i\mathbf{Q}\cdot\mathbf{r}_{j'}(0)} e^{i\mathbf{Q}\cdot\mathbf{r}_j(t)}\rangle_T \\
&= \frac{1}{N}\sum_{j,j'}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}}\Big\langle\frac{1}{(2\pi)^3}\int d\mathbf{r}' e^{-i\mathbf{Q}\cdot\mathbf{r}'}\,\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)\, e^{i\mathbf{Q}\cdot\mathbf{r}_j(t)}\Big\rangle_T \\
&= \frac{1}{N}\sum_{j,j'}\int d\mathbf{r}'\,\Big\langle\frac{1}{(2\pi)^3}\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot(\mathbf{r}+\mathbf{r}'-r_j(t))}\,\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)\Big\rangle_T \\
&= \frac{1}{N}\sum_{j,j'}\int d\mathbf{r}'\,\Big\langle\delta\left(\mathbf{r}'+\mathbf{r}-\mathbf{r}_j(t)\right)\,\delta\Big(\mathbf{r}'-\mathbf{r}_{j'}(0)\Big)\Big\rangle_T,
\end{aligned}$$

where we used

$$\int d\mathbf{Q}\, e^{-i\mathbf{Q}\cdot\mathbf{r}} = (2\pi)^3\delta(\mathbf{r})$$

in the last step. $G(\mathbf{r},t)$ describes the correlation between the atom j' at time $t=0$ at position $\mathbf{r}'$ and the atom j at a later time t at another position $\mathbf{r}'+\mathbf{r}$, i.e. the probability of having two atoms j and j' in a well defined spatial and temporal correlation. $G(\mathbf{r},t)$ may therefore be considered as the most general description of the statics and dynamics of condensed matter on an atomic scale. □