Physics with neutrons 2

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Exercise sheet 9
To be discussed 2017-07-11, room C.3203

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EXERCISE 9.1

Derive the Lorentz factor

$$L(\theta) = \frac{1}{\sin\theta \sin 2\theta}$$

The origin of the Lorentz factor is twofold:

1. The statistical distribution of the crystallites in a polycrystalline sample has to be considered.
2. The detector covers only part of the Debye-Scherrer cone, which describes the Bragg scattering from polycrystalline materials. As sketched in Figure 1, the wavevector $\mathbf{k}'$ of the scattered neutrons lies on a cone, known as Debye-Scherrer cone, where the axis of the cone is along the wavevector $\mathbf{k}$ of the incoming neutrons and θ is the Bragg angle.

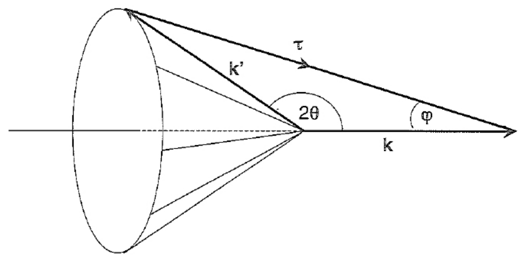

Figure 1: Debye-Scherrer cone for Bragg scattering from polycrystalline materials.

Solution. First we consider the statistical distribution of the crystallites in a polycrystalline sample. The fraction of microcrystals oriented to fulfill Bragg's law $\lambda = 2d\sin\theta$ can be obtained by considering Figure 2. All crystallites with reciprocal lattice vectors lying in the dotted surface area of a sphere with radius τ contribute to the scattering. The active surface area amounts to $2\pi\tau^2 \cos\theta d\theta / 4\pi\tau^2$. Hence, the total scattering for the Debye-Scherrer cone is given by

$$\sigma_{\text{cone}} \propto \int_0^{\pi/2} \delta(k' - k) cos\theta d\theta, \tag{1}$$

where $\delta(k' - k)$ confines the integration to elastic scattering. Using the geometry sketched in Figure 1 we find

$$k'^2 - k^2 = \tau^2 - 2\tau k \cos\phi = \tau^2 - 2\tau k \sin\theta = (k' + k)(k' - k),$$

where we used the relation $\theta = \pi/2 - \phi$. Setting $k' \approx k$ yields

$$k' - k = \frac{1}{2k}(\tau^2 - 2\tau k \sin\theta). \tag{2}$$

Combining Eqs. (1) and (2) yields

$$\sigma_{\mathbf{cone}} \propto \int_0^{\pi/2} \delta(\tau^2 - 2\tau k \sin\theta)\cos\theta d\theta. \tag{3}$$

We solve the integral in Eq. (3) by the substituion $x = 2\tau k \sin\theta$:

$$\sigma_{\mathbf{cone}} \propto \int_0^{\pi/2} \delta(\tau^2 - x)\frac{1}{2\tau k}dx = \frac{1}{2\tau k}.$$

Setting $\tau = 2k\sin\theta$ from Bragg's law we find

$$\sigma_{\text{cone}} \propto \frac{1}{\sin\theta}. \tag{4}$$

If the neutron detector with diameter d is at a distance r from the sample, it intercepts a fraction $q = d/2\pi r \sin(2\theta)$ of the neutrons in the cone. Multiplying σ_{cone} of Eq. (3) with the θ-dependent term of q yields the final result for the Lorentz factor:

$$L(\theta) = \frac{1}{\sin(\theta)\sin(2\theta)}$$

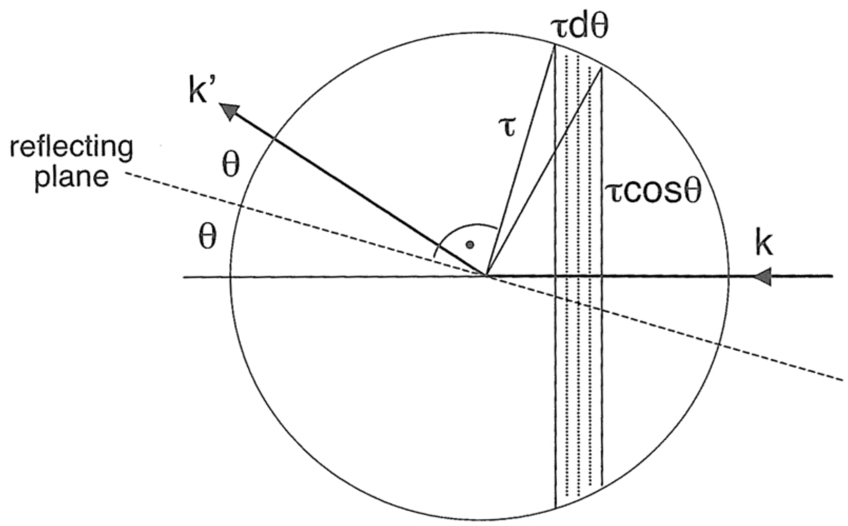

Figure 2: Sketch showing the fraction of crystallites satisfying the Bragg condition.

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EXERCISE 9.2

Consider the localized ferromagnet EuO and the itinerant ferromagnet Ni with their properties given in the table. Calculate the intensity ratio of magnetic scattering and nuclear scattering from the (111) Bragg peak in powder samples.

	EuO	Ni
crystal structure	fcc	fcc
lattice constants	$a = 5.13\,\text{Å}, \alpha = 90°$	$a = 3.52\,\text{Å}, \alpha = 90°$
magnetic moments	$7\mu_B$	$0.6\mu_B$

Shull and Smart, Phys. Rev. 76, 1256 (1949).

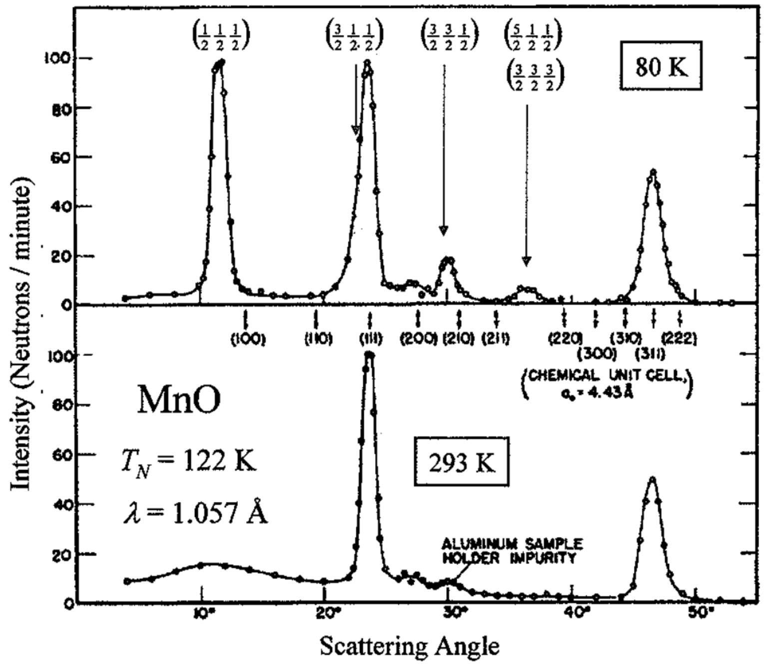

Figure 3: Neutron diffraction patterns for MnO above and below the Néel temperature.

EXERCISE 9.3

By comparing the intensity of the magnetic $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)$ with the nuclear (111) Bragg reflection from power diffraction measurements estimate the magnetic moment of the Mn^{2+} ions in the antiferromagnet MnO. Do you need to take the Lorentz factor into account? As discussed last week, the magnetic form factors can be found at
`https://www.ill.eu/sites/ccsl/ffacts/`.

Solution. From the measurement shown in Fig. 3[1], we can see that the nuclear (111) reflection (at $2\theta_{nucl} \simeq 24°$ and the magnetic $\left(\frac{1}{2}\frac{1}{2}\frac{1}{2}\right)$) reflection (at $2\theta_{nucl} \simeq 12°$ are of about the same intensity at $T = 80\,\mathrm{K}$.

For this problem, we can start from the expression for the intensity of powder peaks:

$$I \propto \frac{1}{8\pi}\frac{d}{r}\frac{V\lambda^3}{V_{UC}^2}\frac{P_{hkl}F_{hkl}^2}{\sin\theta\sin(2\theta)}, \tag{5}$$

where d, r and λ are instrument parameters, V the sample volume, V_{UC} the unit cell volume, P_{hkl} the multiplicity of the (hkl) reflection, S_{hkl} the structure factor and 2θ is the scattering angle (the factor 1/sin.. is the geometrical Lorentz factor calculated in the previous exercise).

For the magnetic peak, we have to replace the scattering amplitude F_{hkl} (which contains the

[1]**C. Shull et al., Phys. Rev. 76 (1949) 1256**.

nuclear scattering length and the structure factor) by an equivalent for magnetic scattering

$$F_{mag,hkl}^2 = (\gamma_n r_0)^2 f_{mag}^2 \langle S_z \rangle^2 (1 - (\hat{Q} \cdot \hat{e}^2)) S_{mag}^2, \tag{6}$$

with the magnetic form factor f, the spin S_z and the structure factor S_{mag}.

Therefore, cancelling all constant parameters, the ratio of nuclear to magnetic scattering will be

$$1 = \frac{I^{nucl}}{I^{mag}} = \frac{F_{nucl,hkl}^2}{(\gamma_n r_o)^2 f_{mag}^2 \langle S_z \rangle_T^2 (1 - (\hat{Q} \cdot \hat{e})^2) S_{mag}^2} \frac{V_{UC,mag}^2 \sin\theta_{mag} \sin 2\theta_{mag}}{V_{UC,nucl}^2 \sin\theta_{nucl} \sin 2\theta_{nucl}}. \tag{7}$$

Now we can look at the individual terms:

- For the FCC NaCl structure $F_{nucl,111} = 4(b_{Mn} - b_O) = -4 \cdot 0.953 \cdot 10^{-12}$ cm. Note that b_{Mn} is negative, so that the minus sign produces a larger amplitude than a plus sign would.
- The magnetic momentum transfer is $Q = 4\pi \sin(\theta_{mag})/\lambda \simeq 1.25 \text{Å}^{-1}$, so the magnetic form factor, determined from the graph, is $f \simeq 0.85$ (To evaluate the graph, look on the given ILL website).
- The magnetic unit cell parameter is twice as large as the chemical cell parameter, therefore $V_{UC,mag} = 8V_{UC,nucl}$. (with this unit cell, the magnetic reflection we are looking at is not indexed as $(\frac{1}{2}\frac{1}{2}\frac{1}{2})$), but (111).)
- The most tricky part is the magnetic structure factor. In[2] the magnetic structure is explained in detail - ferromagnetically coupled sheets parallel to (111), with the moments aligned in-plane - and the structure factor is calculated as 32 for (111) and $(\overline{111})$, but zero for all other equivalent diretions. Therefore, $S_{mag} = \frac{1}{4} \cdot 32^2$.
- As given in[3], the Mn spins are oriented in (111) planes. For the reflections with structure factor $\neq 0$, i.e. (111) and $(\overline{111})$, the spins are perpendicular to Q, so that $(1 - (\hat{Q} \cdot \hat{e})^2) = 1$.
- The ratio of sines is approximately 0.257.
- $\gamma_n r_0$ is approximately $0.54 \cdot 10^{-12}$ cm.

With this information, we can calculate $\langle S_z \rangle$:

$$\langle S_z \rangle = \sqrt{\frac{4^2 \cdot 0.953^2}{0.54^2 \cdot 0.85^2 \cdot 0.25 \cdot 32^2} \cdot 8^2 \cdot 0.247} \simeq 2.11. \tag{8}$$

That would indicate a magnetic moment of $\mu = gS_z \simeq 4.2\mu_B$ at 80K. Indeed, in saturation (i.e. at very low temperature), we expect a Mn moment of $5\mu_B$, so that our calculation seems to be quite reasonable.

[2] **W.L. Roth**, **Phys. Rev. 110 (1958) 1333**.
[3] **W.L. Roth**, **Phys. Rev. 110 (1958) 1333**.

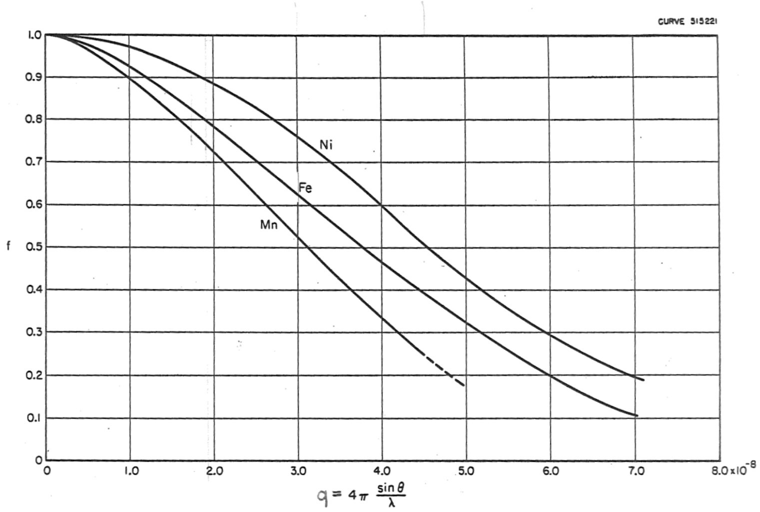

Fig. I — Form factors for Manganese, Iron and Nickel

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EXERCISE 9.4

From your solid state physics course you should remember the dispersion relation for phonons. Calculate the dispersion of an acoustic phonon of a linear chain of atoms with a lattice constant of $a = 2$Å. The measured velocity of sound is assumed to be 2300 m/s. Draw the scattering diagram for an inelastic neutron scattering experiment with $k_f = 2.57\,\text{Å}^{-1}$ at the boundary of the 2^{nd} Brioullin zone using energy and momentum conservation. Consider phonon creation and annihilation.

Solution. The phonon dispersion of a linear chain of equal atoms is:

$$\omega(k) = 2\sqrt{\frac{D}{m}}\left|\sin\frac{ka}{2}\right|, \tag{9}$$

with an effective spring constant D, the atom mass m and the lattice constant a. (If we only take positive k into account, we can omit the absolute value.)
The velocity of sound is defined as the slope around $k = 0$:

$$v_s = \frac{d\omega}{dk}\Big|_{k=0} = 2\sqrt{\frac{D}{m}}\frac{a}{2}\cos\frac{ka}{2}\Big|_{k=0} = \sqrt{\frac{D}{m}}a, \tag{10}$$

so we can calculate the prefactor of the dispersion for the values given in the exercise:

$$\omega(k) = \frac{2v_s}{a}\sin\frac{ka}{2}\Big|_{k=0} = 23\text{THz}\cdot\sin(k\cdot 1\text{Å}) \tag{11}$$

, or, in terms of energy,

$$E(k) = 15\,\text{meV}\cdot\sin(k\cdot 1\text{Å}). \tag{12}$$

For inelastic scattering, we need to know both q and $\hbar\omega$ of the excitation: the boundary of the second Brillouin zone is defined by $Q = 3\pi/a = 4.71$Å, and $E(3\pi/a) = 15$ meV as calculated above.

The finale wavevector is given as $k_f = 2.57\text{Å}^{-1}$. For calculation of the incident wavevector we use conservation of energy:

$$\frac{\hbar^2 k_i^2}{2m} = \frac{\hbar^2 k_f^2}{2m} \pm \hbar\omega \rightarrow k_i = \sqrt{k_f^2 \pm \frac{2m\omega}{\hbar}}. \tag{13}$$

For the '+' sign we get $k_i = 3.73\text{Å}^{-1}$, while for the '-' sign the radicant is negative. In other words, only phonon creation can be observed with this fixed k_f.
The scattering angle can be calculated from the cosine theorem (see scattering diagram):

$$Q^2 = k_i^2 + k_f^2 - 2k_i k_f \cos\theta \rightarrow \theta = 94.5°. \tag{14}$$

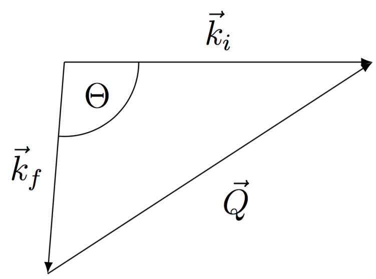

Figure 4:

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