Physics with neutrons 2

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Exercise sheet 8
To be discussed 2017-06-27, room C.3203

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Exercise 8.1

Derive the equation

$$\vec{M}_\perp^* \cdot \vec{M}_\perp = \sum_{\alpha,\beta} \left(\delta_{\alpha\beta} - \hat{Q}_\alpha \hat{Q}_\beta\right) \cdot M_\alpha^* M_\beta \tag{1}$$

Solution.

$$\vec{M}_\perp = \hat{Q} \times \left(\vec{M} \times \hat{Q}\right)$$

$$\vec{M}_{\perp,i} = \epsilon_{ijk} Q_j (\epsilon_{klm} M_l Q_m) = \epsilon_{kij}\epsilon_{klm} Q_j M_l Q_m$$

$$\vec{M}_{\perp,i} = (\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}) Q_j M_l Q_m = M_i \underbrace{Q_m Q_m}_{=1,|\hat{Q}|=1} - Q_i Q_j M_j,$$

where we used $\epsilon_{kij}\epsilon_{klm} = \delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}$ (Proof e.g. at `https://de.wikiversity.org/wiki/Kurs.Theoretische_Mechanik/Lösungen`).
Calculating the dot product:

$$\vec{M}_\perp^* \vec{M}_\perp = (M_i^* - Q_i Q_j M_j^*)(M_i - Q_i Q_k M_k)$$

$$\vec{M}_\perp^* \vec{M}_\perp = M_i^* M_i - M_i^* Q_i Q_k M_k \underbrace{- Q_j M_j^* Q_i M_i + \overbrace{Q_i Q_i}^{=1} Q_j M_j^* Q_k M_k}_{=0}$$

$$\vec{M}_\perp^* \vec{M}_\perp = M_i^* M_i - Q_i Q_k M_i^* M_k = \sum_{ik} (\delta_{ik} - Q_i Q_k) M_i^* M_k$$

□

Exercise 8.2

1. Consider magnetic scattering on a single crystal of Ni (fcc). Evaluating equation (C.5.20) from the lecture for a ferromagnet and using eq. 1, the ferromagnetic cross-section reads

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = N \frac{(2\pi)^3}{v_0} (\gamma r_0)^2 e^{-2W(\vec{Q})} F^2((\vec{Q})) \langle \hat{S}^z \rangle^2 \sum_{\vec{G}} \langle 1 - \left(\hat{\vec{Q}} \cdot \hat{\vec{M}}\right)^2 \rangle \delta(\vec{Q} - \vec{G}). \tag{2}$$

   Calculate the contributions of the magnetic domains, which are aligned along the <111> directions, to the (111) Bragg peak. What are the contributions to the (111) peak for a completely isotropic distribution of the spins?

2. For the orthorhombic UGe_2 the magnetic moments are all aligned along the [100] direction. Considering a powder sample: Which lines contain magnetic contributions and are most suitable for magnetic scattering?

Solution. 1.

$$\vec{M}_\perp = \hat{Q} \times \left(\vec{M} \times \hat{Q}\right)$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\omega} = N\frac{(2\pi)^3}{v_0}(\gamma r_0)^2 e^{-2W(\vec{Q})}F^2((Q))\langle \hat{S}^z\rangle^2 \sum_{\vec{G}} \langle 1 - \left(\hat{\vec{Q}} \cdot \hat{\vec{M}}\right)^2 \rangle \delta(\vec{Q} - \vec{G})$$

$$\propto \sum_{\vec{G}} \left[1 - \left(\hat{\vec{G}} \cdot \hat{\vec{M}}\right)^2\right] \delta\left(\vec{Q} - \vec{G}\right).$$

Here, with $\hat{G} = \frac{1}{3}(1,1,1)$ and 8 domains $(1,1,1),(-1,1,1),(1,-1,1),(1,1,-1),(-1,-1,1),$ $(-1,1,-1),(1,-1,-1),(-1,-1,-1)$:

$$\left(\frac{d\sigma}{d\Omega}\right)_{mag.} \propto \frac{1}{8}\sum_{i=1}^{8}\left(1 - \left(\hat{\vec{G}} \cdot \hat{\vec{M}}\right)^2\right) = \frac{2}{3}$$

For isotropic spin distribution:

$$\frac{d\sigma}{d\Omega}^{iso}_{mag} \propto \int_{\vec{G}} d\vec{G} \left[1 - \left(\underbrace{\hat{\vec{G}} \cdot \hat{\vec{M}}}_{=GM\cos\theta}\right)^2\right] \delta(\vec{Q} - \vec{G})$$

$$\left(\frac{d\sigma}{d\Omega}\right)^{iso}_{mag} \propto \frac{1}{4\pi}\underbrace{\int d\phi}_{2\pi}\int_0^\pi d\theta \left[1 - \left(\underbrace{GM}_{=1}\cos\theta\right)^2\right] = \frac{2}{3}$$

2. No contributions for $\vec{Q} = (h00)$, since the cross-product with $\vec{M}$is zero. All $\vec{Q} = (0kl)$ allowed → choose lowest due to decreasing magnetic form factor with increasing Q. (Note the difference to phonons where you want Q as large as possible)

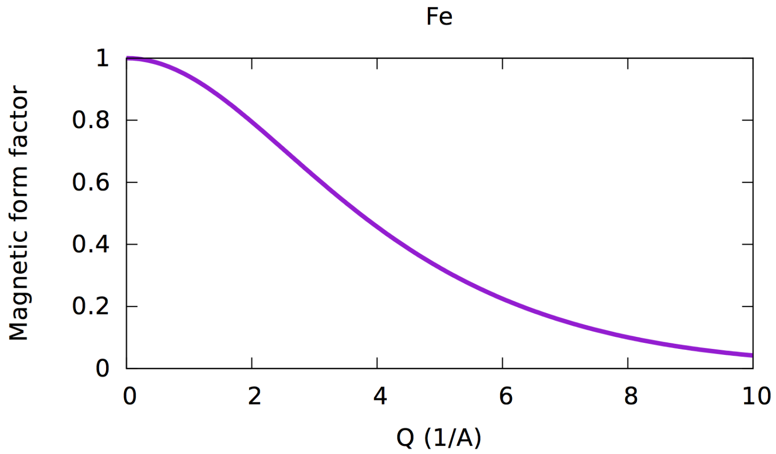
□

EXERCISE 8.3

1. Plot the magnetic form factors for 3d (e.g. Fe) and 4f electrons.

2. How much does the magnetic form factor diminish the magnetic scattering in the (110) peak of Fe?

Solution. 1. The electron configuration of Fe is [Ar] $3d^6 4s^2$. With Hund's rule we get $S = 2$, $L = 2$, $J = 4$. Magnetic form factors are calculated in the dipole approximation using tabulated spherical Bessel functions, which dan be found e.g. at `https://www.ill.eu/sites/ccsl/ffacts/`. Note the different definition of the scattering wavenumber $s = \frac{Q}{4\pi}$, where Q is the usual neutron scattering wavenumber.
For Fe we get the following plot:



2. Fe crystallises in a bcc structure with $a = 2.87\,\text{Å}$. The (110) peak appears at $Q = \frac{2\pi}{a}\sqrt{1^2+1^2+0^2} = 3.1\,\text{Å}^{-1}$. For the intensity we get, using the plot:

$$I \propto f^2(Q = 3.1\,\text{Å}^{-1}) = 0.6^2 = 0.36^2$$

□