Notes for exercise sheet 5

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Exercise 1

Only the magnetisation perpendicular to the scattering vector contributes:

$$\vec{M}_\perp = \hat{Q} \times \left(\vec{M} \times \hat{Q}\right) \tag{1}$$

a) Contributions of the 8 <111> domains

$$\vec{M}_{\perp,1} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}1\\1\\1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \begin{pmatrix}0\\0\\0\end{pmatrix} \tag{2}$$

$$\vec{M}_{\perp,2} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}-1\\1\\1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \frac{1}{3}\begin{pmatrix}-4\\2\\2\end{pmatrix} \tag{3}$$

$$\vec{M}_{\perp,3} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}1\\-1\\1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \frac{1}{3}\begin{pmatrix}2\\-4\\2\end{pmatrix} \tag{4}$$

$$\vec{M}_{\perp,4} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}1\\1\\-1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \frac{1}{3}\begin{pmatrix}2\\2\\-4\end{pmatrix} \tag{5}$$

$$\vec{M}_{\perp,5} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}-1\\-1\\1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \frac{1}{3}\begin{pmatrix}-2\\-2\\4\end{pmatrix} \tag{6}$$

$$\vec{M}_{\perp,6} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}-1\\1\\-1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \frac{1}{3}\begin{pmatrix}-2\\4\\-2\end{pmatrix} \tag{7}$$

$$\vec{M}_{\perp,7} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}1\\-1\\-1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \frac{1}{3}\begin{pmatrix}4\\-2\\-2\end{pmatrix} \tag{8}$$

$$\vec{M}_{\perp,8} = \frac{1}{3}\begin{pmatrix}1\\1\\1\end{pmatrix} \times \left(\begin{pmatrix}-1\\-1\\-1\end{pmatrix} \times \begin{pmatrix}1\\1\\1\end{pmatrix}\right) = \begin{pmatrix}0\\0\\0\end{pmatrix} \tag{9}$$

The ferromagnetic cross-section is given by (see e.g. Squires p. 147):

$$\left(\frac{d\sigma}{d\Omega}\right)_{mag.} = \underbrace{\frac{N\left(2\pi\right)^3}{V_0}}_{\text{unit cell}} \left(\gamma \overbrace{r_0}^{\text{e}^-\text{radius}}\right)^2 \underbrace{\left\langle S_{\vec{M}}\right\rangle^2}_{\text{spin avg.}} \overbrace{e^{-2W}}^{\text{Debye}-\text{Waller}} \sum_{\vec{G}} \left| \frac{1}{2} g \underbrace{F_m\left(\vec{G}\right)}_{\text{structure factor}} \right|^2 \left[1 - \left(\hat{\vec{G}} \cdot \hat{\vec{M}}\right)^2\right] \delta\left(\vec{Q} - \vec{G}\right) \tag{10}$$

$$\propto \sum_{\vec{G}} \left[1 - \left(\hat{\vec{G}} \cdot \hat{\vec{M}}\right)^2\right] \delta\left(\vec{Q} - \vec{G}\right) \tag{11}$$

Here, with $\hat{G} = \frac{1}{3}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ and the contributing domains 2-7:

$$\left(\frac{d\sigma}{d\Omega}\right)_{mag.} \propto \frac{1}{8}\sum_{i=2}^{7} 1 - \left(\hat{\vec{G}} \cdot \hat{\vec{M}}_i\right)^2 = \frac{2}{3} \tag{12}$$

For isotropic spin distribution:

$$\left(\frac{d\sigma}{d\Omega}\right)_{mag.}^{iso.} \propto \int_{\vec{G}} d\vec{G} \left[1 - \left(\underbrace{\hat{\vec{G}} \cdot \hat{\vec{M}}}_{=GM\cos\vartheta}\right)^2\right] \delta\left(\vec{Q} - \vec{G}\right) \tag{13}$$

$$\left(\frac{d\sigma}{d\Omega}\right)_{mag.}^{iso.} \propto \frac{1}{4\pi}\underbrace{\int d\phi}_{2\pi} \int_{-1}^{1} d\cos\vartheta \left[1 - \left(\underbrace{GM}_{=1}\cos\vartheta\right)^2\right] = \frac{2}{3} \tag{14}$$

b) Orthorhombic cell with M along [001]

No contributions for $Q = (00l)$, since the cross-product in equation 1 is zero. All $Q = (hk0)$ allowed $\Rightarrow$ 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 2

The perpendicular component of the magnetisation is given by:

$$\vec{M}_\perp = \hat{Q} \times \left(\vec{M} \times \hat{Q}\right) \tag{15}$$

$$M_{\perp,i} = \epsilon_{ijk} Q_j \left(\epsilon_{klm} M_l Q_m\right) = \epsilon_{kij}\epsilon_{klm} Q_j M_l Q_m \tag{16}$$

$$M_{\perp,i} = \left(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}\right) Q_j M_l Q_m = M_i \underbrace{Q_m Q_m}_{=1,\,|\hat{Q}|=1} - Q_i Q_j M_j \tag{17}$$

Calculating the dot product:

$$M^*_{\perp,i} M_{\perp,i} = \left(M^*_i - Q_i Q_j M^*_j\right)\left(M_i - Q_i Q_k M_k\right) \tag{18}$$

$$M^*_{\perp,i} M_{\perp,i} = M^*_i M_i - M^*_i Q_i Q_k M_k \underbrace{- Q_j M^*_j Q_i M_i + \overbrace{Q_i Q_i}^{=1} Q_j M^*_j Q_k M_k}_{=0} \tag{19}$$

$$M^*_{\perp,i} M_{\perp,i} = M^*_i M_i - Q_i Q_k M^*_i M_k = \sum_{ik}\left(\delta_{ik} - Q_i Q_k\right) M^*_i M_k \tag{20}$$

Exercise 3

The form factor is defined as

$$f\left(\vec{Q}\right) = \int d^3r\, \rho\left(\vec{r}\right) \exp\left(i\vec{Q}\vec{r}\right) \tag{21}$$

In spherical coordinates:

$$f\left(Q\right) = 2\pi \int drr^2 \int d\cos\left(\vartheta\right)\ \rho\left(r\right) \exp\left(iQr\cos\left(\vartheta\right)\right) \tag{22}$$

$$f\left(Q\right) = 2\pi \int drr^2 \rho\left(r\right) \left[-\frac{i}{Qr} \cdot \exp\left(iQr\cos\left(\vartheta\right)\right)\right]_{\cos(\vartheta)=-1}^{\cos(\vartheta)=1} \tag{23}$$

$$f\left(Q\right) = 2\pi \int drr^2 \rho\left(r\right) \left[\frac{i}{Qr} \cdot \exp\left(-iQr\right) - \frac{i}{Qr} \cdot \exp\left(iQr\right)\right] \tag{24}$$

With $\sin x = \frac{i}{2}\left(e^{-x} - e^{x}\right)$:

$$f\left(Q\right) = 4\pi \int dr\, \frac{r}{Q} \sin\left(Qr\right) \cdot \rho\left(r\right) \tag{25}$$

a) Shell of radius R_0, using delta function:

$$f\left(Q\right) = 4\pi \int dr\, \frac{r}{Q} \sin\left(Qr\right) \cdot \frac{\delta\left(R_0 - r\right)}{4\pi R_0^2} \tag{26}$$

$$f\left(Q\right) = \frac{1}{QR_0} \sin\left(QR_0\right) \tag{27}$$

b) Sphere of radius R_0, using Heaviside step function:

$$f\left(Q\right) = 4\pi \int dr\, \frac{r}{Q} \sin\left(Qr\right) \cdot \frac{\vartheta\left(R_0 - r\right)}{4\pi R_0^3} \tag{28}$$

$$f\left(Q\right) = \int_0^{R_0} dr\, \frac{r}{Q} \sin\left(Qr\right) \cdot \frac{1}{R_0^3} \tag{29}$$

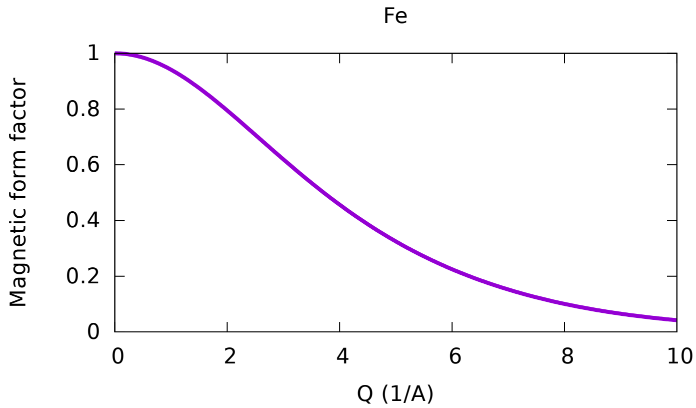
$$f\left(Q\right) = \frac{\sin\left(QR_0\right)}{\left(QR_0\right)^3} - \frac{\cos\left(QR_0\right)}{\left(QR_0\right)^2} \tag{30}$$

c) Fe form factor

The electron configuration of Fe is [Ar] $3d^6 4s^2$. With Hund's rules we get $S = 2,\ L = 2,\ J = 4$.

Magnetic form factors are calculated in the dipole approximation using tabulated spherical Bessel functions, which can be found – for example – here: `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:



d) (110) peak of Fe

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:

$$I \propto f^2(Q = 3.1\text{Å}^{-1}) = 0.6^2 = 0.36 \tag{31}$$