Notes for exercise sheet 6

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Exercise 1

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

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

The nuclear cross-section is given by (see e.g. Squires p. 37):

$$\left(\frac{d\sigma}{d\Omega}\right)_{nuc.} = \underbrace{N \frac{(2\pi)^3}{V_0}}_{\text{unit cell}} \overbrace{e^{-2W}}^{\text{Debye-Waller}} \sum_{\vec{G}} \left|\underbrace{F_n\left(\vec{G}\right)}_{\text{structure factor}}\right|^2 \delta\left(\vec{Q} - \vec{G}\right) \tag{2}$$

At $\vec{Q} = \vec{G}$ the ratio is:

$$\frac{(d\sigma/d\Omega)_{mag.}}{(d\sigma/d\Omega)_{nuc.}} = (\gamma r_0)^2 \langle S_{\vec{r}}\rangle^2 \left|\frac{1}{2} g F_m\left(\vec{Q}\right)\right|^2 \frac{2}{3} \cdot \left|F_n\left(\vec{Q}\right)\right|^{-2} \tag{3}$$

Exercise 2

The Landau-Lifshitz equation describes the precession movement of the magnetic moment $\vec{\mu}$ in an effective field $\vec{B}$:

$$\frac{d\vec{\mu}}{dt} = -\gamma \vec{\mu} \times \vec{B}. \tag{4}$$

Expressions for potential energy of magnetic moment i:

$$U = -\vec{\mu_i} \cdot \vec{B}, \qquad U = -\frac{1}{\gamma^2} \vec{\mu_i} \cdot \sum_{j \varepsilon NN} J_j \vec{\mu_j} \tag{5}$$

$$\Rightarrow\ \vec{B} = \frac{1}{\gamma^2} \sum_{j \varepsilon NN} J_j \vec{\mu_j} \tag{6}$$

The equation of motion now reads:

$$\frac{d\vec{\mu_i}}{dt} = -\frac{1}{\gamma} \vec{\mu_i} \times \left(\sum_{j \varepsilon NN} J_j \vec{\mu_j}\right). \tag{7}$$

Inserting the ansatz for the solution:

$$\vec{\mu_i} = \begin{pmatrix} const \cdot \exp\left[i\left(\vec{q} \cdot \vec{r_i} - \omega t\right)\right] \\ const \cdot \exp\left[i\left(\vec{q} \cdot \vec{r_i} - \omega t + \pi/2\right)\right] \\ \mu \end{pmatrix} \tag{8}$$

we get the dispersion:

$$\omega = \underbrace{-\frac{\mu}{\gamma}}_{=2S} \left[\sum_{j \varepsilon NN} J_j \left(1 - e^{-i\vec{q}\cdot(\vec{r}_j - \vec{r}_i)} \right) \right]. \tag{9}$$

fcc

In an fcc lattice the 12 nearest neighbours with the coupling J_n are at the positions (lattice constant a):

$$\vec{n}_1 = \begin{pmatrix} a/2 \\ a/2 \\ 0 \end{pmatrix}, \vec{n}_2 = \begin{pmatrix} a/2 \\ -a/2 \\ 0 \end{pmatrix}, \vec{n}_3 = \begin{pmatrix} -a/2 \\ a/2 \\ 0 \end{pmatrix}, \vec{n}_4 = \begin{pmatrix} -a/2 \\ -a/2 \\ 0 \end{pmatrix} \tag{10}$$

$$\vec{n}_5 = \begin{pmatrix} 0 \\ a/2 \\ a/2 \end{pmatrix}, \vec{n}_6 = \begin{pmatrix} 0 \\ -a/2 \\ a/2 \end{pmatrix}, \vec{n}_7 = \begin{pmatrix} 0 \\ a/2 \\ -a/2 \end{pmatrix}, \vec{n}_8 = \begin{pmatrix} 0 \\ -a/2 \\ -a/2 \end{pmatrix} \tag{11}$$

$$\vec{n}_9 = \begin{pmatrix} a/2 \\ 0 \\ a/2 \end{pmatrix}, \vec{n}_{10} = \begin{pmatrix} -a/2 \\ 0 \\ a/2 \end{pmatrix}, \vec{n}_{11} = \begin{pmatrix} a/2 \\ 0 \\ -a/2 \end{pmatrix}, \vec{n}_{12} = \begin{pmatrix} -a/2 \\ 0 \\ -a/2 \end{pmatrix}. \tag{12}$$

The 6 next-nearest neighbours with the coupling J_m are at:

$$\vec{m}_1 = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}, \vec{m}_2 = \begin{pmatrix} 0 \\ a \\ 0 \end{pmatrix}, \vec{m}_3 = \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix} \tag{13}$$

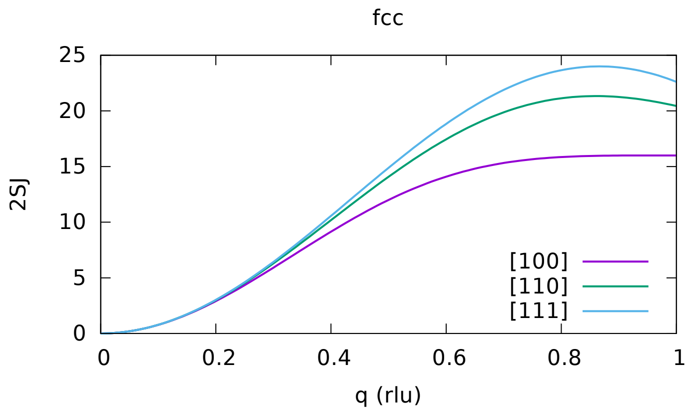
$$\vec{m}_4 = \begin{pmatrix} -a \\ 0 \\ 0 \end{pmatrix}, \vec{m}_5 = \begin{pmatrix} 0 \\ -a \\ 0 \end{pmatrix}, \vec{m}_6 = \begin{pmatrix} 0 \\ 0 \\ -a \end{pmatrix}. \tag{14}$$

The dispersion relation is:

$$E_{fcc}(\vec{q}) = 2S \left(\underbrace{12J_n - J_n \cdot \sum_{j\varepsilon\{1,2,..,12\}} e^{-i\vec{q}\cdot\vec{n}_j}}_{nearest} + \underbrace{6J_m - J_m \cdot \sum_{j\varepsilon\{1,2,..,6\}} e^{-i\vec{q}\cdot\vec{m}_j}}_{next-nearest} \right) \tag{15}$$

Assuming $J_n = J_m$:

$$E_{fcc}(\vec{q}) = 2SJ_n \left(18 - \sum_{j\varepsilon\{1,2,..,12\}} e^{-i\vec{q}\cdot\vec{n}_j} - \sum_{j\varepsilon\{1,2,..,6\}} e^{-i\vec{q}\cdot\vec{m}_j} \right) \tag{16}$$



bcc

In a bcc lattice the 8 nearest neighbours with the coupling J_n are at the positions (lattice constant a):

$$\vec{n}_1 = \begin{pmatrix} a/2 \\ a/2 \\ a/2 \end{pmatrix}, \vec{n}_2 = \begin{pmatrix} -a/2 \\ a/2 \\ a/2 \end{pmatrix}, \vec{n}_3 = \begin{pmatrix} a/2 \\ -a/2 \\ a/2 \end{pmatrix}, \vec{n}_4 = \begin{pmatrix} a/2 \\ a/2 \\ -a/2 \end{pmatrix} \tag{17}$$

$$\vec{n}_5 = \begin{pmatrix} -a/2 \\ -a/2 \\ a/2 \end{pmatrix}, \vec{n}_6 = \begin{pmatrix} -a/2 \\ a/2 \\ -a/2 \end{pmatrix}, \vec{n}_7 = \begin{pmatrix} a/2 \\ -a/2 \\ -a/2 \end{pmatrix}, \vec{n}_8 = \begin{pmatrix} -a/2 \\ -a/2 \\ -a/2 \end{pmatrix}. \tag{18}$$

The 6 next-nearest neighbours with the coupling J_m are at:

$$\vec{m}_1 = \begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}, \vec{m}_2 = \begin{pmatrix} 0 \\ a \\ 0 \end{pmatrix}, \vec{m}_3 = \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix} \tag{19}$$

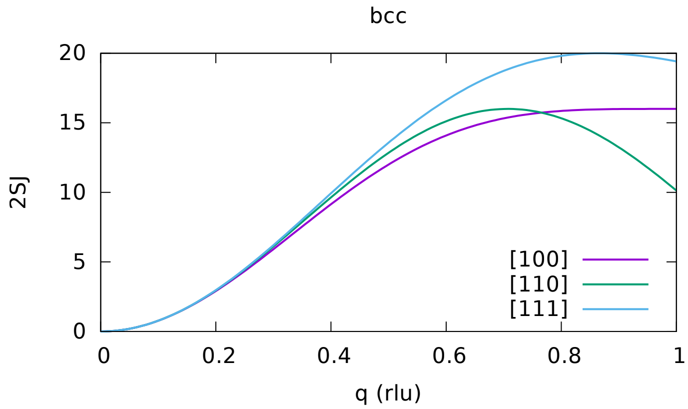
$$\vec{m}_4 = \begin{pmatrix} -a \\ 0 \\ 0 \end{pmatrix}, \vec{m}_5 = \begin{pmatrix} 0 \\ -a \\ 0 \end{pmatrix}, \vec{m}_6 = \begin{pmatrix} 0 \\ 0 \\ -a \end{pmatrix}. \tag{20}$$

The dispersion relation is:

$$E_{bcc}(\vec{q}) = 2S \left(\underbrace{8J_n - J_n \cdot \sum_{j\varepsilon\{1,2,..,8\}} e^{-i\vec{q}\cdot\vec{n}_j}}_{nearest} + \underbrace{6J_m - J_m \cdot \sum_{j\varepsilon\{1,2,..,6\}} e^{-i\vec{q}\cdot\vec{m}_j}}_{next-nearest} \right) \tag{21}$$

Assuming $J_n = J_m$:

$$E_{bcc}(\vec{q}) = 2SJ_n \left(14 - \sum_{j\varepsilon\{1,2,..,8\}} e^{-i\vec{q}\cdot\vec{n}_j} - \sum_{j\varepsilon\{1,2,..,6\}} e^{-i\vec{q}\cdot\vec{m}_j} \right) \tag{22}$$



Exercise 3

The inner energy of the magnons is given by:

$$U = \int d^3q \frac{E(q)}{\exp\left(\frac{E(q)}{k_B T}\right) - 1} = \int d^3q \frac{Dq^2}{\exp\left(\frac{Dq^2}{k_B T}\right) - 1}. \tag{23}$$

Changing to spherical coordinates and integrating out the angular parts:

$$U = 4\pi \int dq q^2 \frac{Dq^2}{\exp\left(\frac{Dq^2}{k_B T}\right) - 1}. \tag{24}$$

Substituting $s = \frac{Dq^2}{k_B T}$, $q = \sqrt{\frac{k_B T}{D}}$, $dq = \frac{k_B T}{2Dq} ds$:

$$U = 2\pi \int ds \frac{(s/D)^{3/2} (k_B T)^{5/2}}{\exp(s) - 1}. \tag{25}$$

The specific heat is given by:

$$C_v = \left(\frac{\partial U}{\partial T}\right)_V = 2\pi \frac{\partial}{\partial T} \int ds \frac{(s/D)^{3/2} (k_B T)^{5/2}}{\exp(s) - 1} \propto T^{3/2}. \tag{26}$$