Physics with neutrons 2

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Exercise sheet 11
To be discussed 2017-07-25, room C.3203

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EXERCISE 11.1

Calculate the spin wave dispersion for an fcc lattice with nearest and next-nearest neighbor interactions J_1 and J_2, respectively. The spin-wave dispersion is given by (Wagner (1972))

$$\hbar\omega(\mathbf{q}) = 2S(J(0) - J(\mathbf{q})) + g\mu_B H_a \tag{1}$$

with the Fourier transformed exchange function

$$J(\mathbf{q}) = \sum_{j,j'} J_{jj'} e^{i\mathbf{q}\cdot(\mathbf{R}_j - \mathbf{R}_{j'})} \tag{2}$$

as e.g. given in 'Neutron Scattering in Condensed Matter Physics' by A. Furrer page 145ff (the book also gives a good introduction to magnetic excitations). Knowing the exchange constants of EuO and EuS[1], discuss their dispersion near the zone boundaries.

Solution. In an fcc lattice with lattice parameter a, the nearest-neighbor distance is $a/\sqrt{2}$, of which there are 12 neighbors per atom (along [110] directions), and next-nearest-neighbor distances a, of which there are 5 neighbors (along [100] directions). From the lecture, the dispersion is given by

$$\hbar\omega_{\mathbf{q}} = 2S(J(0) - J(\mathbf{q})),$$

with

$$J(\mathbf{q}) = \sum_{j,j'} J_{j,j'} \exp\left[i\mathbf{q}(\mathbf{R}_j - \mathbf{R}_{j'})\right].$$

Considering only n.n. and next-n.n. interactions with couplings J_1 and J_2, we get

$$J(\mathbf{q}) = J_1\Big(e^{i(q_x+q_y)a/2} + e^{-i(q_x+q_y)a/2} + e^{i(q_x-q_y)a/2} + e^{-i(q_x-q_y)a/2} +$$

$$e^{i(q_x+q_z)a/2} + e^{-i(q_x+q_z)a/2} + e^{i(q_x-q_z)a/2} + e^{-i(q_x-q_z)a/2} +$$

$$e^{i(q_y+q_z)a/2} + e^{-i(q_y+q_z)a/2} + e^{i(q_y-q_z)a/2} + e^{-i(q_y-q_z)a/2}\Big) +$$

$$J_2(e^{iq_xa} + e^{-iq_xa} + e^{iq_ya} + e^{-iq_ya} + e^{iq_za} + e^{-iq_za})$$

The latter part should be familiar from the lecture. Similarly, we replace the exponentials by cosines and get

$$J(\mathbf{q}) = 2J_1\Big(\cos\Big(\frac{a}{2}(q_x+q_y)\Big) + \cos\Big(\frac{a}{2}(q_x-q_y)\Big) + \cos\Big(\frac{a}{2}(q_x+q_z)\Big) + \cos\Big(\frac{a}{2}(q_x-q_z)\Big) +$$

[1] L. Passell et al., Phys. Rev. B 14 (1976) 4897

$$\cos\left(\frac{a}{2}(q_y+q_z)\right)+\cos\left(\frac{a}{2}(q_y-q_z)\right)\Bigg)+2J_2(\cos q_x a+\cos q_y a+\cos q_z a).$$

Thus, the dispersion is

$$\hbar\omega_{\mathbf{q}} = 4SJ_1\Bigg(6-\cos\left(\frac{a}{2}(q_x+q_y)\right)-\cos\left(\frac{a}{2}(q_x-q_y)\right)-\cos\left(\frac{a}{2}(q_x+q_z)\right)-\cos\left(\frac{a}{2}(q_x-q_z)\right)-$$

$$\cos\left(\frac{a}{2}(q_y+q_z)\right)-\cos\left(\frac{a}{2}(q_y-q_z)\right)\Bigg)+4SJ_2\big(3-\cos q_x a-\cos q_y a-\cos q_z a\big).$$

Near the zone center, we can expand the cosine and get an isotropic, very similar law as for simple cubic systems:

$$\hbar\omega_{\mathbf{q}} \approx 4SJ_1\cdot\frac{1}{2}\frac{a^2}{4}\left((q_x+q_y)^2+(q_x-q_y)^2+(q_x+q_z)^2+(q_x-q_z)^2+(q_y+q_z)^2+(q_y-q_z)^2\right)$$

$$+4SJ_2\cdot\frac{1}{2}a^2q^2=\frac{1}{2}SJ_1a^2(4q_x^2+4q_y^2+4q_z^2)+2SJ_2a^2q^2=2Sa^2q^2(J_1+J_2).$$

In the high symmetry directions, we get:

- along [100], $q_x = q$, $q_y = q_z = 0$:

$$\hbar\omega_{\mathbf{q}} = 4SJ_1(6-\cos\frac{aq}{2}-\cos\frac{aq}{2}-\cos\frac{aq}{2}-\cos\frac{aq}{2}-2)+4SJ_2(3-\cos(aq)-2)$$

$$=16SJ_1\left(1-\cos\frac{aq}{2}\right)+4SJ_2\big(1-\cos(aq)\big).$$

- along [110], $q_x = q_y = q' = q/\sqrt{2}$, $q_z = 0$:

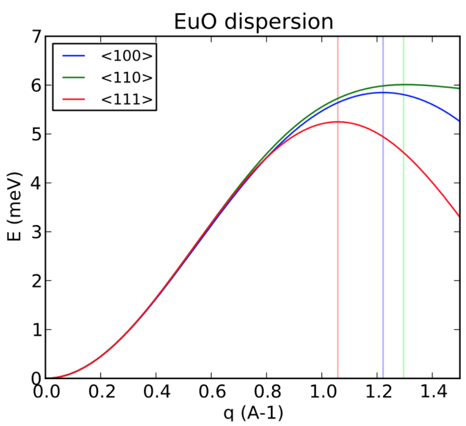
$$\hbar\omega_{\mathbf{q}} = 4SJ_1\left(6-\cos(aq')-1-\cos\frac{aq'}{2}-\cos\frac{aq'}{2}-\cos\frac{aq'}{2}-\cos\frac{aq'}{2}\right)+4SJ_2\big(3-2\cos(aq')-1\big)$$

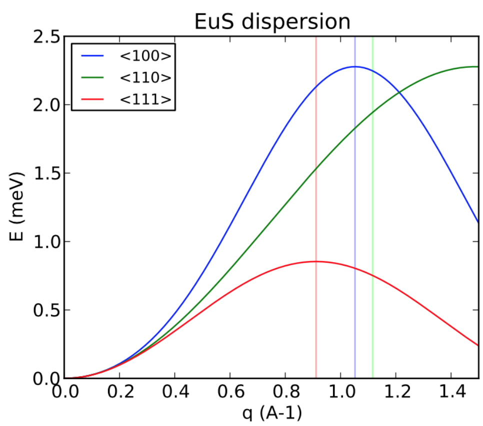
$$=16SJ_1\left(1-\cos\frac{aq'}{2}\right)+4S(J_1+2J_2)\big(1-\cos(aq')\big).$$

- along [111], $q_x = q_y = q_z = q'' = q/\sqrt{3}$:

$$\hbar\omega_{\mathbf{q}} = 4SJ_1\big(6-3\cos(aq'')-3\big)+4SJ_2\big(3-3\cos(aq'')\big)=12S(J_1+J_2)\big(1-\cos(aq'')\big).$$

The following graphs show the dispersions calculated as above for EuO (a = 5.14 Å) and EuS (a = 5.97 Å) using the exchange constants given by [**?**], which were also shown in the lecture. The zone boundaries are shown as vertical lines:





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