University of Zurich[UZH]

PHY585 Exercises
Sheet 2

FS 23
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Exercise 1 *Spin waves in a two-dimensional antiferromagnet*

La_2CuO_4 is a nice example for a two-dimensional Heisenberg antiferromagnet consisting of CuO_2 plains, see Fig. 1. The dispersion-relation of the spin waves is given by

$$\hbar\omega(\vec{Q}) = 2J\sqrt{1 - \cos^2\left(\frac{a}{2}Q_x\right)\cos^2\left(\frac{a}{2}Q_y\right)}. \tag{1}$$

Calculate the exchange coupling J by using the experimental data along $\vec{Q} = (Q_x, 0, 0)$ shown in Fig. 1.

Exercise 2 *Spin waves in a three-dimensional antiferromagnet*

In $YBa_2Cu_3O_{6.15}$ it is possible to observe spin-waves due to the coupling between two CuO_2 planes, see Fig. 2. The Heisenberg Hamiltonian can be written as

$$H = \sum_{i,j} J_{\parallel} S_i S_j + \sum_{i,k} J_{\perp} S_i S_k. \tag{2}$$

Because we have two Cu spins per unit cell, we will observe two spin-wave branches, an an acoustic and an optical branch. The dispersion relation is given by:

$$\hbar\omega\left(\vec{Q}\right) = 2J_{\parallel}\sqrt{1 - \gamma^2\left(\vec{Q}\right) + \frac{J_{\perp}}{2J_{\parallel}}\left(1 \pm \gamma\left(\vec{Q}\right)\right)}, \tag{3}$$

$$\gamma\left(\vec{Q}\right) = \frac{\cos\left(aQ_x\right) + \cos\left(aQ_y\right)}{2}, \tag{4}$$

where $+$ is the acoustic branch and $-$ is the optical branch. Calculate the exchange couplings $J_{\perp}$ and $J_{\parallel}$ using the experimental data shown in Fig. 2. (Hint: It is best to look at the maximum and the minimum of the optical branch.)

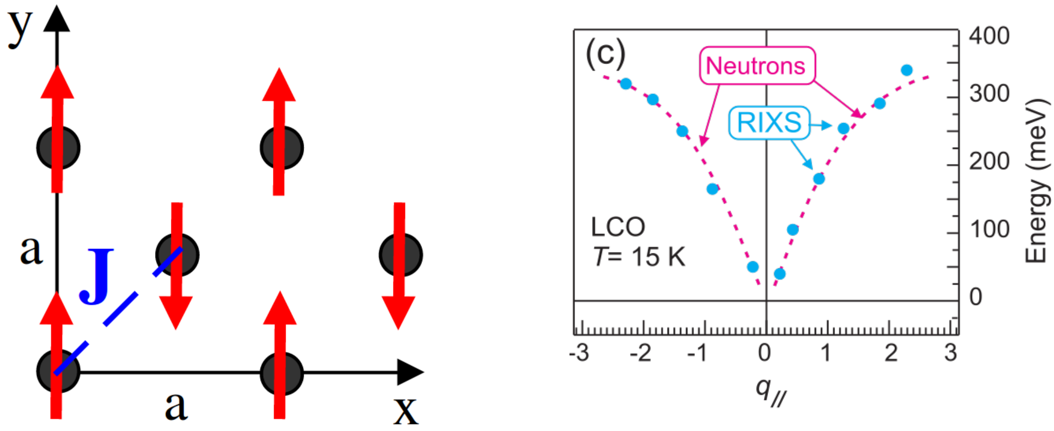

Figure 1: (Left) The arrangement of the spins in the CuO_2 plane of high T_c superconductors. (Right) The dispersion relation of the spin waves in the CuO_2 planes of La_2CuO_4. From S. M. Hayden et al., Phys. Rev. Lett. **67**, 3622 (1991).

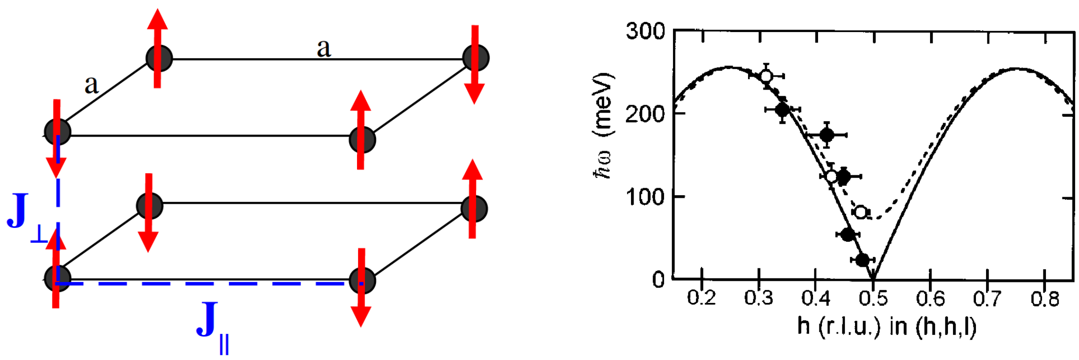

Figure 2: (Left) The arrangement of the spins in the CuO_2 plane of YBCO. (Right) The dispersion relation of the acoustic (solid line) and optical (dashed line) spin waves in the CuO_2 planes of $YBa_2Cu_3O_{6.15}$. From S. M. Hayden et al., Phys. Rev. B **54**, R6905(R) (1996).

Exercise 3 *Heusler alloy as polarizing neutron monochromator*

Heusler alloys are a class of crystals that have the chemical formula X_2YZ ordered in a common L21 face centered cubic crystal structure with the following unit cell:

$$X1 : (0, 0, 0)$$
$$X2 : (0.5, 0.5, 0.5)$$
$$Y : (0.75, 0.75, 0.75)$$
$$Z : (0.25, 0.25, 0.25)$$

These systems have a particular use in neutron instrumentation as some of these crystals have magnetic atoms that lead to a difference between the spin-up and spin-down Bragg-scattering that can be used to polarize the neutron beam. As the Bragg condition has to be fulfilled, the crystal can be used as monochromator and polarizer at the same time.

a) Calculate the selection rules and structure factors from the nuclear scattering length b_X, b_Y, b_Z of the three atomic species.

b) Consider a Heusler alloy with ferromagnetic order of the Y atom. The magnetic form factor shall be $f_M(q) = f_m(|q|) * \mu_y$. The shape of the form factor vanishes with increasing |q|. Modify the structure factor from (a) to retrieve the spin-up and spin-down structure factors.

c) Beam polarization is defined as $P = 2(I_{up}\text{-}I_{down})/(I_{up}+I_{down})$ so a beam with equal intensity of spin-up and spin-down neutrons would have P=0 and a perfectly polarized beam with only spin-up neutrons P=1. Which condition would a Heusler alloy need to fulfil to provide optimal polarization at the [111] Bragg reflection?

Expected results (please check):

a) $h + k + l = 2n + 1 \Rightarrow |b_Y - b_Z|$, $h + k + l = 4n + 2 \Rightarrow |b_Y + b_Z - 2b_X|$, $h + k + l = 4n \Rightarrow |b_Y + b_Z + 2b_X|$

b) Replace b_Y with $b_Y + / - f_M(|q|)$.

c) Selection rule for 2n+1, gives a relation between b_Y, b_Z and $f_m(|q|) * \mu_y$ for spin-up and spin-down that can be put in P.

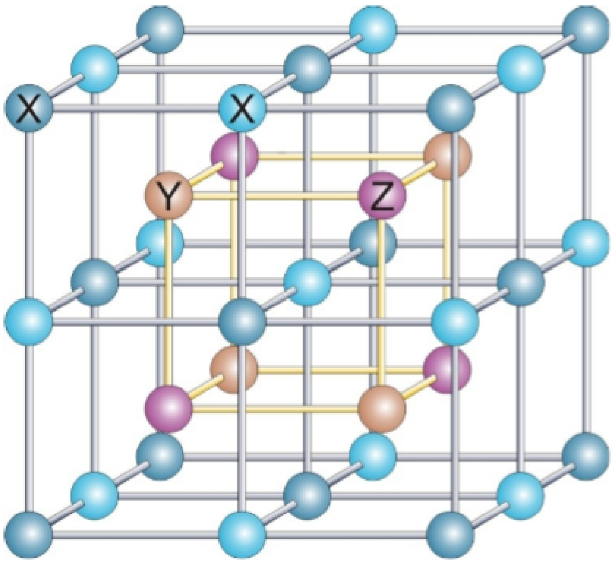

Figure 3