Magnetism in materials

Week 06

1. Show that the Hamiltonian for the Heisenberg model

$$\hat{\mathcal{H}} = -\sum_{<ij>} J\mathbf{S}_i \cdot \mathbf{S}_j \tag{1}$$

can be rewritten as

$$\hat{\mathcal{H}} = -\sum_{<ij>} J\left[\hat{S}_i^z \hat{S}_j^z + \frac{1}{2}(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+)\right] \tag{2}$$

Hence show that for a Heisenberg ferromagnet ($J > 0$) the state $|\Phi\rangle$, which consists of spins on every site pointing up (say), is an eigenstate of the Hamiltonian and has energy E_0 given by

$$E_0 = -NS^2J \tag{3}$$

Consider the Heisenberg antiferromagnet ($J < 0$) with the spins residing on two sublattices, each spin interacting only with those on the other sublattice. Show that the 'obvious' ground state, namely one with each sublattice ferromagnetically aligned but with oppositely directed sublattice magnetizations is not an eigenstate of the Hamiltonian. This emphasizes that the Heisenberg antiferromagnet is a complex and difficult problem.

2. Consider a chain of spins with nearest neighbor exchange constant J_1 and next nearest neighbor exchange constant J_2. The spins lie in planes perpendicular to the chain direction, as can be the case in rare earth metals with a crystal structure such that the atoms lie in layers and the moments within each layer are ferromagnetically aligned in the plane of the layer. Show that the energy per spin in the chain in the ferromagnetic, antiferromagnetic, and helical order are given by

$$E_{FM} = -2S^2(J_1 + J_2) \tag{4}$$

$$E_{AFM} = -2S^2(J_1 + J_2) \tag{5}$$

$$E_H = -2S^2\left(\frac{-J_1^2}{8J_2} - J_2\right) \tag{6}$$

identify in the $J_1 - J_2$ plane the regions in which the chain will order ferromagnetically, antiferromagnetically, or with helical order.

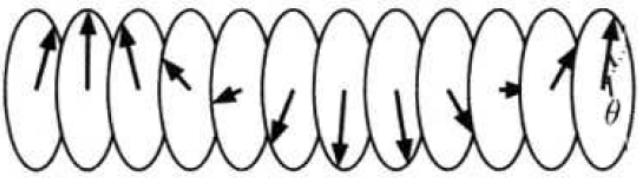

Figure 1:

3. Use the script Curie_Weiss_fit_Ni3TeO6.ipynb to load the data for Ni_3TeO_6 and plot M vs T, the data are in the file 081101-02.dat.

   - Estimate the transition temperature from the plot. Try using the maximum of dM/dT.
   - Choose an appropriate temperature interval where the data can be fitted with a Curie-Weiss law

   $$\chi = \frac{C}{T - T_C} + \chi_0 \tag{7}$$

   Using the Curie-Weiss fit try to estimate the spin state of each Ni ion, taking into account the following: sample mass = 52.2 mg; molar mass/formula unit = 399.68 g/mol; H = 1000 Oe; When the magnetization is expressed in cgs units and is normalized to the number of moles of magnetic ions the Curie constant is given by 8C = g2S(S+1), g=2.
   - What is the direction of the applied field with respect to the direction of spin alignment in the ordered state?

4. When a magnetic field is applied to an antiferromagnet transverse to the direction in which the spins are aligned, the energy of the system takes the form

   $$E = C(J)M^2\cos(2\phi) - 2MB\cos(\phi) + \Delta\cos^2(\phi) \tag{8}$$

   Where ϕ is the angle between the spins and the field, M is the magnitude of the magnetization on the two sublattices, the constant $C(J)$ depends on the exchange interaction strength and the geometry, B is the applied field and Δ parametrize the magnetic anisotropy.

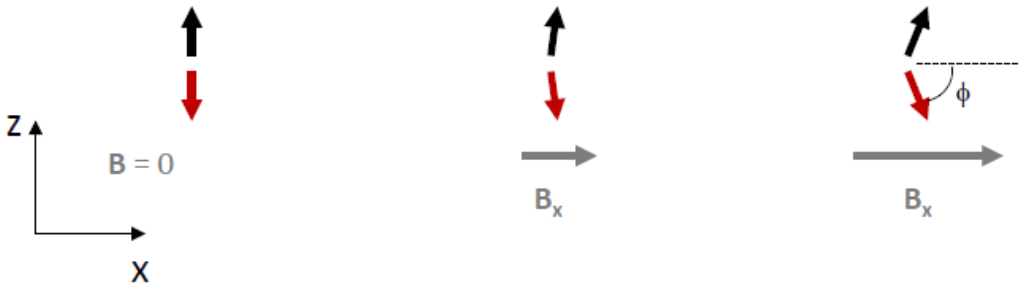

Figure 2:

   The script antiferromagnet.ipynb allows you to plot this function and use the sliders to evaluate how the three contributions change as you vary the parameters.

5. In a Ferrimagnet the spins on two different sublattices are oriented antiparallel to each other but the magnetization on one sublattice is bigger than on the other so that the

sample has a net magnetization. If below the Curie temperature the magnetization scales with respect to the temperature in different ways on the two sublattices one can have a compensation point, that consists in a temperature at which the total magnetization vanishes. Assume that the magnetization on the two sublattices behaves as

$$\begin{cases} M_{\text{up}} = M_{\text{max,up}}(1 - T/T_C)^{\alpha_{\text{up}}} \\ M_{\text{down}} = M_{\text{max,down}}(1 - T/T_C)^{\alpha_{\text{down}}} \end{cases} \tag{9}$$

Use the script Ferrimagnet.ipynb to plot the magnetization as a function of T, and vary the magnetization saturation value and the exponent on the two sublattices to determine when a compensation point can appear.

6. The script point_charge.ipynb performs a point charge calculation of the crystal field levels in the ground $^5I_8$ manifold of Ho^{3+} ions in $LiY_{1-x}Ho_xF_4$.
   Use the script to modify the unit cell parameters and see how this affects the crystal field levels, focus for instance on which levels forms singlets or doublets.

   note: to run the script script you will need to load the LiHoF4.cif that you can find on Moodle. The point charge calculation is done by PyCrystalField. To download and use PyCrystalField, run the following command in a prompt/terminal window:

   pip install git+https://github.com/asche1/PyCrystalField.git@master