Magnetism in materials

Solutions 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.

solution

$$\mathbf{S}_i \cdot \mathbf{S}_j = \hat{S}_i^x\hat{S}_j^x + \hat{S}_i^y\hat{S}_j^y + \hat{S}_i^z\hat{S}_j^z \tag{4}$$

$$= \frac{1}{2}(\hat{S}_i^+ + \hat{S}_i^-)\frac{1}{2}(\hat{S}_j^+ + \hat{S}_j^-) + \frac{1}{2i}(\hat{S}_i^+ - \hat{S}_i^-)\frac{1}{2i}(\hat{S}_j^+ - \hat{S}_j^-) + \hat{S}_i^z\hat{S}_j^z \tag{5}$$

$$= \hat{S}_i^z\hat{S}_j^z + \frac{1}{2}(\hat{S}_i^+\hat{S}_j^- + \hat{S}_i^-\hat{S}_j^+) \tag{6}$$

The Ferromagnetic state $|\Psi\rangle = |\uparrow\uparrow\uparrow ...\rangle$ is an eigenstate of the Hamiltonian since $\forall \quad ij$

$$\hat{S}_i^z\hat{S}_j^z |\Phi\rangle = S^2 |\Phi\rangle \tag{7}$$

$$\hat{S}_i^+ |\Phi\rangle = 0 \tag{8}$$

so that

$$\hat{\mathcal{H}} |\Phi\rangle = -S^2NJ |\Phi\rangle \tag{9}$$

with N the total number of spins. For the antiferromagnetic state $|\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow ...\rangle$ instead we have

$$\hat{S}_i^+\hat{S}_{i+1}^- |... \uparrow_{i-1}\downarrow_i\uparrow_{i+1}\downarrow_{i+2} ...\rangle \propto |... \uparrow_{i-1}\uparrow_i\downarrow_{i+1}\downarrow_{i+2} ...\rangle \tag{10}$$

So the terms $\hat{S}_i^+\hat{S}_j^-$ and $\hat{S}_i^-\hat{S}_j^+$ in the Hamiltonian introduce contributions from states in which a pair of spins are flipped respect to the antiferromagnetic state, this contributions can not cancel each other since the therms comparing in the sum the Hamiltonian 2 each acts on a different pair of spins.

2. Consider a chain of spins with nearest neighbor exchange constant J_1 and next nearest neighbor exchange constant J_2. The spins lays 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

$$E_{FM} = -2S^2(J_1 + J_2) \tag{11}$$
$$E_{AFM} = -2S^2(J_1 + J_2) \tag{12}$$
$$E_H = -2S^2\left(\frac{-J_1^2}{8J_2} - J_2\right) \tag{13}$$

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

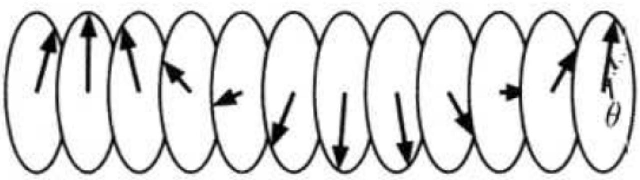

Figure 1:

solution considering the general case in which there is angle θ between a spin and the next in the chain, each spin gives an energy contribution $-2S^2J_1\cos(\theta)$ from the interaction with its two nearest neighbors and a contribution $-2S^2J_2\cos(2\theta)$ from the interaction with its two next nearest neighbors, so

$$E(\theta) = -2S^2(J_1\cos(\theta) + J_2\cos(2\theta)) \tag{14}$$

The Ferromagnetic and antiferromagnetic order corresponds to $\theta = 0$ and $\theta = \pi$ respectively, so

$$E_{FM} = -2S^2(J_1 + J_2) \tag{15}$$
$$E_{AFM} = -2S^2(J_1 + J_2) \tag{16}$$
$$\tag{17}$$

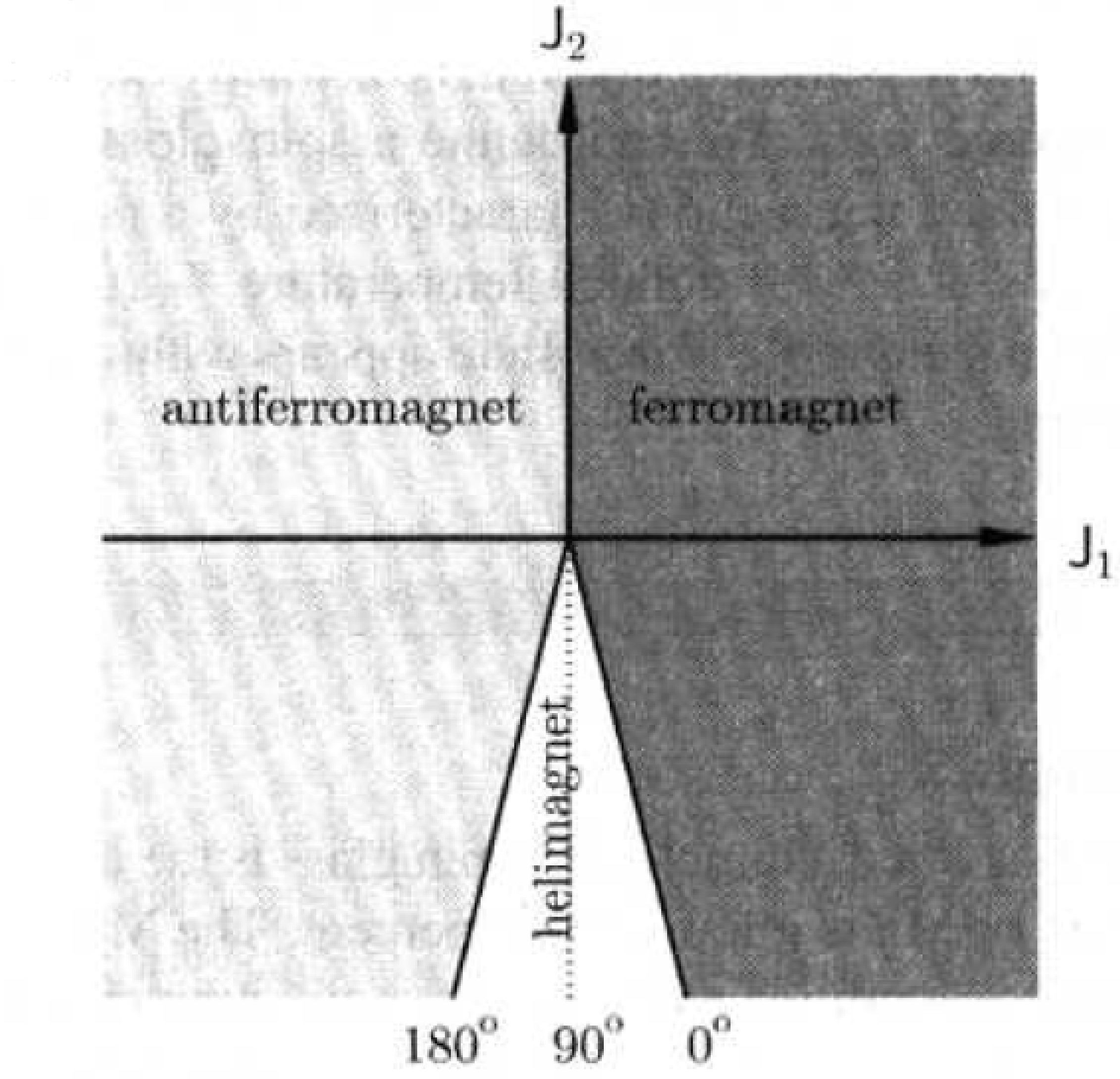

Figure 2:

To find the energy of the helical state we look for the extremal points of the energy

$$\frac{dE(\theta)}{d\theta} = 2S^2(J_1\sin(\theta) + 2J_2\sin(2\theta)) \tag{18}$$

$$= 2S^2\sin(\theta)(J_1 + 4J_2\cos(\theta)) = 0 \tag{19}$$

the solutions $\sin(\theta) = 0$ gives the ferromagnetic or antiferromagnetic order, the helical order is given by $\cos(\theta) = -\frac{J_1}{4J_2}$, substituting it into Equation 14 we get

$$E_H = -2S^2\left(\frac{-J_1^2}{8J_2} - J_2\right) \tag{20}$$

comparing the energies of the three states, we find that the ferromagnetic state has the lower energy when $J_1 > 0$ and $J_2 > -J1/4$, the antiferromagnetic order is favored when $J_1 < 0$ and $J_2 > J1/4$ while the helical order is favored for $J_1 > 0$ and $J_2 < -J1/4$ or $J_1 < 0$ and $J_2 < J1/4$.