Physics 223b: Problem Set 3

due 10am, February 11, 2014 in Prof. Balents' mailbox at the KITP

1. **EuO:** Europium oxide is a black, ferromagnetic insulator with the "rock salt" structure, i.e. with Eu and O occupying the two interpenetrating fcc sublattices of a simple cubic lattice. One expects the Eu atoms to be in a Eu^{2+} state.

   (a) Show that Hunds rules predict the total angular momentum $J = S$ for the Europium atom. What is S? Eu^{2+} loses its two 6s electrons, so it has 7 4f electrons, i.e. the configuration [Xe]$4f^7$. This exactly half-fills the 4f shell, so we follow Hund's first rule and get S=7/2, and L=0 since we have one electron in every orbital.

   (b) The Eu spins interact via ferromagnetic exchange interactions $J_1 = 2.4K$ between true nearest neighbors, and $J_2 = 0.48K$ between second neighbors (i.e. between Eu atoms separated by an O atom along one of the principle axes of the conventional simple cubic lattice). Apply MFT to estimate the Curie point T_c of EuO. Compare to the true $T_c = 69.4K$. We must determine the effective field on a site. Since we consider a ferromagnet, the average spin on all sites is the same, $\langle \vec{S}_i \rangle = \vec{m}$ independent of i. Then the field on a given site is given by $J_1\vec{m}$ times the number of nearest neighbors plus $J_2\vec{m}$ times the number of second neighbors, i.e.

   $$\vec{h} = (z_1 J_1 + z_2 J_2)\,\vec{m}, \tag{1}$$

   where $z_1 = 12$ and $z_2 = 6$ are the number of first and second neighbors. The magnitude of the magnetization m is just given by the usual Brillouin function,

   $$m = SB_S(\beta S h), \tag{2}$$

   so we have the self-consistent equation

   $$h = (z_1 J_1 + z_2 J_2) S B_S(\beta S h). \tag{3}$$

   As in class, the solution with $h \neq 0$ first appears for this equation at $T = T_c$. This corresponds to the condition of equality of slopes of the left and right hand side of Eq. (3). Using the slope of the Brillouin function, we then get

   $$1 = (z_1 J_1 + z_2 J_2)\frac{S(S+1)}{3k_B T_c} \Rightarrow T_c^{MF} = (z_1 J_1 + z_2 J_2)\frac{S(S+1)}{3k_B}. \tag{4}$$

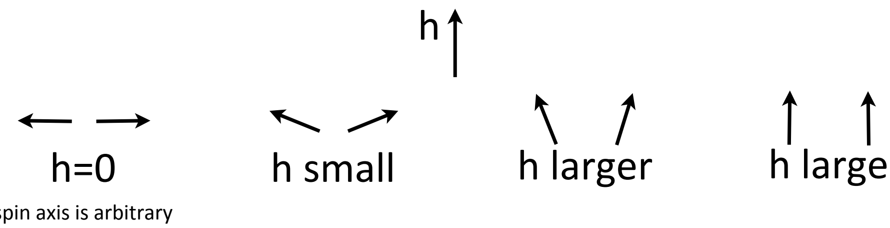
   Now we take $J_1 = 2.4K$ and $J_2 = 0.48K$ and we obtain $T_c^{MF} = 166K$. Unfortunately, I made a mistake in the convention for the exchange constants, and gave values 2 times too large in the homework. It should have been $J_1 = 1.2K$ and $J_2 = 0.24K$, which would give $T_c^{MF} = 83.2K$, which is 20 percent larger than the experimental $T_c^{\text{expt}} = 69.4K$. An overestimate of this amount is typical for mean field theory.

2. **Antiferromagnet in a field:** Consider the antiferromagnetic spin Hamiltonian on the square lattice:

   $$H = J\sum_{\langle ij\rangle} \vec{S}_i \cdot \vec{S}_j - h\sum_i S_i^z, \tag{5}$$

   where $J > 0$ is the exchange coupling between nearest-neighbor spins, and h is an external magnetic field (measured in energy units) which couples to the spins through the Zeeman interaction.

(a) In the classical limit, you may treat $\vec{S}_i$ as a vector of length S. Describe (by a few sketches, no need for extensive quantitative calculations) the classical ground state spin configuration as a function of $0 < h/J < \infty$. Show that for $h > h_{sat} = 8JS$, the spins are "saturated", i.e. fully aligned along the z axis. At zero field, $h = 0$,



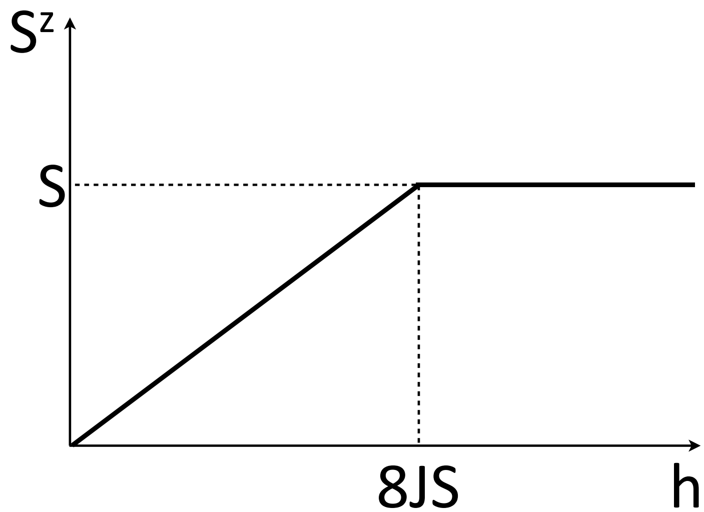
the spins are just antiparallel on the two sublattices. When we turn on a weak field, the best configuration is just to make the spins mostly antiparallel but "canted" a bit in the direction of the field. So one still has the two sublattice structure. In the figure, I have drawn the spins on the two sublattices, which simply tilt more and more toward the field direction with increasing field.

For large enough field, we expect the spins to have fully aligned along the field (z) axis. To work out how large this field is, let us consider the spins to be canted slightly away, and see if this raises or lowers the energy. Take $S_i^z = S\sqrt{1-u^2}$, $S_i^x = \pm Su$, with opposite signs for S_i^x on the two sublattices. Then the energy per site is

$$E/N = 2JS^2\left[(1-u^2) - u^2\right] - hS\sqrt{1-u^2} \approx 2JS^2 + (\frac{hS}{2} - 4JS^2)u^2, \qquad (6)$$

where we expanded to quadratic order in u. We see that the energy has a minimum at $u = 0$ when $h > 8JS$. Thus they are saturated (fully aligned) in this case.

(b) Sketch the magnetization (average values of S^z) versus h/J.



Without any further calculation, we know that $S^z = 0$ for $h = 0$ and reaches S for $h \geq 8JS$. Nearly any sketch that does this is ok. But let's go ahead and get the exact classical form. If we take the energy in Eq. (6) (without the expansion), we can minimize it with respect to u to get

$$u = \pm\sqrt{1 - \frac{h}{8JS}}, \tag{7}$$

for $h < 8JS$. Plugging this back into the formula $S_i^z = \sqrt{1-u^2}$, we find simply $S_i^z = h/(8J)$ for $h < 8JS$ and $S_i^z = S$ for $h > 8JS$. This is just a "ramp".

(c) Now let us treat the problem quantum mechanically, with each $\vec{S}_i$ as a spin operator of spin S. For large values of h/J, we may again assume the ground state is the fully aligned one. Calculate the excitation energy of single magnons above this state. From this calculation, predict the saturation field h_{sat} expected in the quantum model, and compare to the classical limit.

We consider the single spin-flip state, $|i\rangle = S_i^-|FM\rangle$, where $|FM\rangle = \otimes_i |S_i^z = S\rangle$. As in class, if we let H act on $|i\rangle$, we get

$$H|i\rangle = (E_{FM} - JSz + h)|i\rangle + JS \sum_{j\ nn\ i} |j\rangle, \tag{8}$$

where E_{FM} is total energy of the $|FM\rangle$ state. Note the change of sign of the exchange terms relative to what we wrote in class for the ferromagnet (because here the exchange is antiferromagnetic) and the extract $-h$ term in the energy due to the field. From this, taking a plane-wave state, we get the excitation energy $\epsilon(\mathbf{k}) = E - E_{FM}$,

$$\epsilon(\mathbf{k}) = h - JSz + 2JS \sum_{\alpha=1}^{d} \cos k_\alpha. \tag{9}$$

For the square lattice $d = 2$, $z = 4$, and the energy is minimized when $k_\alpha = \pi$, so

$$\epsilon(\pi, \pi) = h - 4JS - 4JS = h - 8JS. \tag{10}$$

This means the excitation energy is positive for $h > h_{sat} = 8JS$, exactly the same as in the classical limit.