Physics 211B : Assignment #3

[**1**] *Atomic physics* – Consider an ion with a partially filled shell of angular momentum J, and Z additional electrons in filled shells. Show that the ratio of the Curie paramagnetic susceptibility to the Larmor diamagnetic susceptibility is

$$\frac{\chi^{\rm para}}{\chi^{\rm dia}} = -\frac{g_{\rm L}^2\, J(J+1)}{2Zk_{\rm B}T}\,\frac{\hbar^2}{m\langle r^2\rangle} \ .$$

where $g_{\rm L}$ is the Landé g-factor. Estimate this ratio at room temperature.

[**2**] *Adiabatic demagnetization* – In an ideal paramagnet, the spins are noninteracting and the Hamiltonian is

$$\mathcal{H} = \sum_{i=1}^{N_{\rm p}} \gamma_i\, \boldsymbol{J}_i \cdot \boldsymbol{H}$$

where $\gamma_i = g_i\mu_i/\hbar$ and $\boldsymbol{J}_i$ are the gyromagnetic factor and spin operator for the $i^{\rm th}$ paramagnetic ion, and $\boldsymbol{H}$ is the external magnetic field.

(a) Show that the free energy $F(H,T)$ can be written as

$$F(H,T) = T\,\Phi(H/T) \ .$$

If an ideal paramagnet is held at temperature $T_{\rm i}$ and field $H_{\rm i}\,\hat{\boldsymbol{z}}$, and the field $H_{\rm i}$ is *adiabatically* lowered to a value $H_{\rm f}$, compute the final temperature. This is called "adiabatic demagnetization".

(b) Show that, in an ideal paramagnet, the specific heat at constant field is related to the susceptibility by the equation

$$c_H = T\left(\frac{\partial s}{\partial T}\right)_H = \frac{H^2\,\chi}{T} \ .$$

Further assuming all the paramagnetic ions to have spin J, and assuming Curie's law to be valid, this gives

$$c_H = \tfrac{1}{3} n_{\rm p} k_{\rm B} J(J+1)\left(\frac{g\mu_{\rm B}H}{k_{\rm B}T}\right)^2 \ ,$$

where $n_{\rm p}$ is the density of paramagnetic ions. You are invited to compute the temperature T^* below which the specific heat due to lattice vibrations is smaller than the paramagnetic contribution. Recall the Debye result

$$c_V = \tfrac{12}{5}\pi^4\, n k_{\rm B}\left(\frac{T}{\Theta_{\rm D}}\right)^3 \ ,$$

where $n = 1/\Omega$ is the inverse of the unit cell volume (*i.e.* the density of unit cells) and $\Theta_{\rm D}$ is the Debye temperature. Compile a table of a few of your favorite insulating solids, and tabulate Θ_D and T^* when 1% paramagnetic impurities are present, assuming $J = \frac{5}{2}$.

[3] *Ferrimagnetism* – A *ferrimagnet* is a magnetic structure in which there are different types of spins present. Consider a sodium chloride structure in which the A sublattice spins have magnitude $S_{\rm A}$ and the B sublattice spins have magnitude $S_{\rm B}$ with $S_{\rm B} < S_{\rm A}$ (*e.g.* $S = 1$ for the A sublattice but $S = \frac{1}{2}$ for the B sublattice). The Hamiltonian is

$$\mathcal{H} = J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j + g_{\rm A} \mu_0 H \sum_{i \in {\rm A}} S_i^z + g_{\rm B} \mu_0 H \sum_{j \in {\rm B}} S_j^z$$

where $J > 0$, so the interactions are antiferromagnetic.

(a) Work out the mean field theory for this model. Assume that the spins on the A and B sublattices fluctuate about the mean values

$$\langle \boldsymbol{S}_{\rm A} \rangle = m_{\rm A}\, \hat{\boldsymbol{z}} \qquad , \qquad \langle \boldsymbol{S}_{\rm B} \rangle = m_{\rm B}\, \hat{\boldsymbol{z}}$$

and derive a set of coupled mean field equations of the form

$$\begin{aligned} m_{\rm A} &= F_{\rm A}(\beta g_{\rm A} \mu_0 H + \beta J z m_{\rm B}) \\ m_{\rm B} &= F_{\rm B}(\beta g_{\rm B} \mu_0 H + \beta J z m_{\rm A}) \end{aligned}$$

where z is the lattice coordination number ($z = 6$ for NaCl) and $F_{\rm A}(x)$ and $F_{\rm B}(x)$ are related to Brillouin functions. Show graphically that a solution exists, and fund the criterion for broken symmetry solutions to exist when $H = 0$, *i.e.* find $T_{\rm c}$. Then linearize, expanding for small $m_{\rm A}$, $m_{\rm B}$, and H, and solve for $m_{\rm A}(T)$ and $m_{\rm B}(T)$ and the susceptibility

$$\chi(T) = -\frac{1}{2} \frac{\partial}{\partial H} (g_{\rm A} \mu_0 m_{\rm A} + g_{\rm B} \mu_0 m_{\rm B})$$

in the region $T > T_{\rm c}$. Does your $T_{\rm c}$ depend on the sign of J? Why or why not?

(b) Work out the spin wave theory and compute the spin wave dispersion. (You should treat the NaCl structure as an FCC lattice with a two element basis.) Assume a classical ground state $\big| {\rm N} \big\rangle$ in which the spins are up on the A sublattice and down on the B sublattice, and choose

A Sublattice	B Sublattice
$S^+ = a^\dagger \, (2S_{\rm A} - a^\dagger a)^{1/2}$	$S^+ = -(2S_{\rm B} - b^\dagger b)^{1/2}\, b$
$S^- = (2S_{\rm A} - a^\dagger a)^{1/2}\, a$	$S^+ = -b^\dagger \, (2S_{\rm B} - b^\dagger b)^{1/2}$
$S^z = a^\dagger a - S_{\rm A}$	$S^z = S_{\rm B} - b^\dagger b$

How does the spin wave dispersion behave near $\boldsymbol{k} = 0$? Show that the spectrum crosses over from quadratic to linear when $|\boldsymbol{k} a| \approx |S_{\rm A} - S_{\rm B}| / \sqrt{S_{\rm A} S_{\rm B}}$.

[4] *Thinking about singlets* – Consider the antiferromagnetic Heisenberg model on a bipartite lattice:

$$\mathcal{H} = J \sum_{\langle ij \rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$$

where $J > 0$ and the sum is over the bonds of the lattice.

(a) Break up the lattice into a dimer covering. There are exponentially many such dimer coverings, *i.e.* the number grows as $e^{\alpha N}$ where N is the number of lattice sites. Think about tiling a chessboard with with dominoes. The analysis of this problem was performed by H. N. V. Temperley and M. E. Fisher, *Phil. Mag.* **6**, 1061 (1961). Denote one sublattice as A and the other as B. You are to develop a mean field theory of interacting dimers in the presence of a self-consistent staggered field

$$\langle \boldsymbol{S}_{\mathrm{A}} \rangle = -\langle \boldsymbol{S}_{\mathrm{B}} \rangle \equiv m\hat{\boldsymbol{z}} \ .$$

The mean field Hamiltonian then breks up into a sum over dimer Hamiltonians

$$\begin{aligned} \mathcal{H}_{\mathrm{dimer}} &= J\boldsymbol{S}_{\mathrm{A}} \cdot \boldsymbol{S}_{\mathrm{B}} + (z-1)J\,\langle \boldsymbol{S}_{\mathrm{B}} \rangle \cdot \boldsymbol{S}_{\mathrm{A}} + (z-1)J\,\langle \boldsymbol{S}_{\mathrm{A}} \rangle \cdot \boldsymbol{S}_{\mathrm{B}} \\ &= J\boldsymbol{S}_{\mathrm{A}} \cdot \boldsymbol{S}_{\mathrm{B}} - H_{\mathrm{s}}\,(S^z_{\mathrm{A}} - S^z_{\mathrm{B}}) \end{aligned}$$

where the effective staggered field is $H_{\mathrm{s}} = (z-1)Jm$, and z is the lattice coordination number. Find the eigenvalues of the dimer Hamiltonian when $S = \frac{1}{2}$.

(b) Define $x = 2h/J$. What is the self-consistent equation for x when $T = 0$? Under what conditions is there a nontrivial solution? What then is the self-consistent staggered magnetization? How does it compare with the result of spin-wave theory?

[5] *Let's all do the spin flop* – In real solids crystal field effects often lead to anisotropic spin-spin interactions. Consider the anisotropic Heisenberg antiferromagnet in a uniform magnetic field,

$$\mathcal{H} = J\sum_{\langle ij \rangle} (S^x_i\, S^x_j + S^y_i\, S^y_j + \Delta\, S^z_i\, S^z_j) + h\sum_i S^z_i$$

where the field is parallel to the direction of anisotropy. Assume $\delta \geq 0$ and a bipartite lattice.

(a) Think first about classical spins. In a small external field, show that if the anisotropy Δ is not too large that the lowest energy configuration has the spins on the two sublattices lying predominantly in the (x, y) plane and antiparallel, with a small parallel component along the direction of the field. This is called a canted, or 'spin-flop' structure. What is the angle θ_{c} by which the spins cant out of the (x, y) plane? What do I mean by not too large? (You may assume that the lowest energy configuration is a two sublattice structure, rather than something nasty like a four sublattice structure or an incommensurate one.)

(b) Now work out the quantum spin wave theory. To do this, you'll have to rotate the quantization axes of the spins to their classical directions. This means taking

$$\begin{aligned} S^x &\to \cos\theta\, S^x + \sin\theta\, S^z \\ S^y &\to S^y \\ S^z &\to -\sin\theta\, S^x + \cos\theta\, S^z \end{aligned}$$

with $\theta = \pm\theta_0$, depending on the sublattice in question. How is θ_0 related to $\theta_{\rm c}$ above? This may seem like a pain in the neck, but really it isn't so bad. Besides, you shouldn't complain so much. And stand up straight – you're slouching. And brush your teeth.

(c) Compute the spin wave dispersion and find under what conditions the theory is unstable.