PHYSICS 152B/232
Spring 2017
Homework Assignment #4 Solutions

[**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

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

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

Solution :

We have derived the expressions

$$\chi^{\text{dia}} = -\frac{Zne^2}{6mc^2}\,\langle r^2\rangle$$

and

$$\chi^{\text{para}} = \tfrac{1}{3}n\,(g_{\text{L}}\mu_{\text{B}})^2\,\frac{J(J+1)}{k_{\text{B}}T} \ ,$$

where

$$g_{\text{L}} = \tfrac{3}{2} + \frac{S(S+1)-L(L+1)}{2J(J+1)} \ ,$$

and where $\mu_{\text{B}} = e\hbar/2mc$ is the Bohr magneton. The ratio is thus

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

If we assume $\langle r^2\rangle = a_{\text{B}}^2$, so that $\hbar^2/m\langle r^2\rangle \simeq 27.2\,\text{eV}$, then with $T = 300\,\text{K}$ (and $k_{\text{B}}T \approx \frac{1}{40}\,\text{eV}$), $g_{\text{L}} = 2$, $J = 2$, and $Z \approx 30$, the ratio is $\chi^{\text{para}}/\chi^{\text{dia}} \approx -450$.

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

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

where $\gamma_i = g_i\mu_i/\hbar$ and $\boldsymbol{J}_i$ are the gyromagnetic factor and spin operator for the i^{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_{i} and field $H_{\text{i}}\,\hat{\boldsymbol{z}}$, and the field H_{i} is *adiabatically* lowered to a value H_{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 $J = \frac{5}{2}$.

Solution :

(a) The partition function s a product of single-particle partition functions, and is explicitly a function of the ratio H/T:

$$Z = \prod_i \sum_{m=-J_i}^{J_i} e^{-m\gamma_i H/k_{\rm B}T} = Z(H/T)\ .$$

Thus,

$$F = -k_{\rm B}T\,\ln Z = T\,\Phi(H/T)\ ,$$

where

$$\Phi(x) = -k_{\rm B}\sum_{i=1}^{N_{\rm p}} \ln\left[\frac{\sinh\big((J_i+\frac{1}{2})\gamma_i\,x/k_{\rm B}\big)}{\sinh\big(\gamma_i\,x/2k_{\rm B}\big)}\right]\ .$$

The entropy is

$$S = -\frac{\partial F}{\partial T} = -\Phi(H/T) + \frac{H}{T}\,\Phi'(H/T)\ ,$$

which is itself a function of H/T. Thus, constant S means constant H/T, and

$$\frac{H_{\rm f}}{H_{\rm i}} = \frac{T_{\rm f}}{T_{\rm i}} \qquad\Rightarrow\qquad T_{\rm f} = \frac{H_{\rm f}}{H_{\rm i}}\,T_{\rm i}\ .$$

(b) The heat capacity is

$$C_H = T\left(\frac{\partial S}{\partial T}\right)_H = -x\,\frac{\partial S}{\partial x} = -x^2\,\Phi''(x)\ ,$$

with $x = H/T$. The (isothermal) magnetic susceptibility is

$$\chi = -\left(\frac{\partial^2 F}{\partial H^2}\right)_T = -\frac{1}{T}\,\Phi''(x)\ .$$

Thus,

$$C_H = \frac{H^2}{T}\,\chi\ .$$

Next, write

$$C_H = \tfrac{1}{3} n_{\rm p}\, k_{\rm B}\, J(J+1)\left(\frac{g_{\rm L}\mu_{\rm B}H}{k_{\rm B}T}\right)^2$$
$$C_V = \tfrac{12}{5}\pi^4\, n\, k_{\rm B}\left(\frac{T}{\Theta_{\rm D}}\right)^3$$

and we set $C_H = C_V$ to find T^*. Defining $\Theta_H \equiv g_{\rm L}\mu_{\rm B}H/k_{\rm B}$, we obtain

$$T^* = \frac{1}{\pi}\left[\tfrac{5\pi}{36}\, J(J+1)\,\frac{n_{\rm p}}{n}\,\Theta_H^2\,\Theta_{\rm D}^3\right]^{1/5}\ .$$

Set $J \approx 1$, $g_{\rm L} \approx 2$, $n_{\rm p} = 0.01\,n$ and $\Theta_{\rm D} \approx 500\,{\rm K}$. If $H = 1\,{\rm kG}$, then $\Theta_H = 0.134\,{\rm K}$. For general H, find

$$T^* \simeq 3\,{\rm K}\cdot\big(H\,[{\rm kG}]\big)^{2/5}\ .$$

[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

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

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

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

$$m_{\rm A} = F_{\rm A}(\beta g_{\rm A}\mu_\circ H + \beta J z m_{\rm B})$$
$$m_{\rm B} = F_{\rm B}(\beta g_{\rm B}\mu_\circ H + \beta J z m_{\rm A})$$

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

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

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

Solution :

We apply the mean field *Ansatz* $\langle \boldsymbol{S}_i \rangle = \boldsymbol{m}_{\rm A,B}$ and obtain the mean field Hamiltonian

$$\mathcal{H}^{\rm MF} = -\tfrac{1}{2}NJz\boldsymbol{m}_{\rm A}\cdot\boldsymbol{m}_{\rm B} + \sum_{i\in{\rm A}}\big(g_{\rm A}\mu_\circ\boldsymbol{H} + zJ\boldsymbol{m}_{\rm B}\big)\cdot\boldsymbol{S}_i + \sum_{j\in{\rm B}}\big(g_{\rm B}\mu_\circ\boldsymbol{H} + zJ\boldsymbol{m}_{\rm A}\big)\cdot\boldsymbol{S}_j\ .$$

Assuming the sublattice magnetizations are collinear, this leads to two coupled mean field equations:

$$\begin{aligned} m_{\rm A}(x) &= F_{S_{\rm A}}\big(\beta g_{\rm A}\mu_\circ H + \beta Jzm_{\rm B}\big) \\ m_{\rm B}(x) &= F_{S_{\rm B}}\big(\beta g_{\rm B}\mu_\circ H + \beta Jzm_{\rm A}\big)\ , \end{aligned}$$

where

$$F_S(x) = -S\,B_S(Sx)\ ,$$

and $B_S(x)$ is the Brillouin function,

$$B_S(x) = \big(1+\tfrac{1}{2S}\big)\,{\rm ctnh}\,\big(1+\tfrac{1}{2S}\big)x - \tfrac{1}{2S}\,{\rm ctnh}\,\tfrac{x}{2S}\ .$$

The mean field equations may be solved graphically, as depicted in fig. 1.

Expanding $F_S(x) = -\frac{1}{3}S(S+1)x + \mathcal{O}(x^3)$ for small x, and defining the temperatures $k_{\rm B}T_{\rm A,B} \equiv \frac{1}{3}S_{\rm A,B}(S_{\rm A,B}+1)\,zJ$, we obtain the linear equations,

$$\begin{aligned} m_{\rm A} - \frac{T_A}{T}\,m_{\rm B} &= -\frac{g_{\rm A}\mu_\circ}{zJ}\,H \\ m_{\rm B} - \frac{T_B}{T}\,m_{\rm A} &= -\frac{g_{\rm B}\mu_\circ}{zJ}\,H\ , \end{aligned}$$

with solution

$$\begin{aligned} m_{\rm A} &= -\frac{g_{\rm A}T_{\rm A}T - g_{\rm B}T_{\rm A}T_{\rm B}}{T^2 - T_{\rm A}T_{\rm B}}\,\frac{\mu_\circ H}{zJ} \\ m_{\rm B} &= -\frac{g_{\rm B}T_{\rm B}T - g_{\rm A}T_{\rm A}T_{\rm B}}{T^2 - T_{\rm A}T_{\rm B}}\,\frac{\mu_\circ H}{zJ}\ . \end{aligned}$$

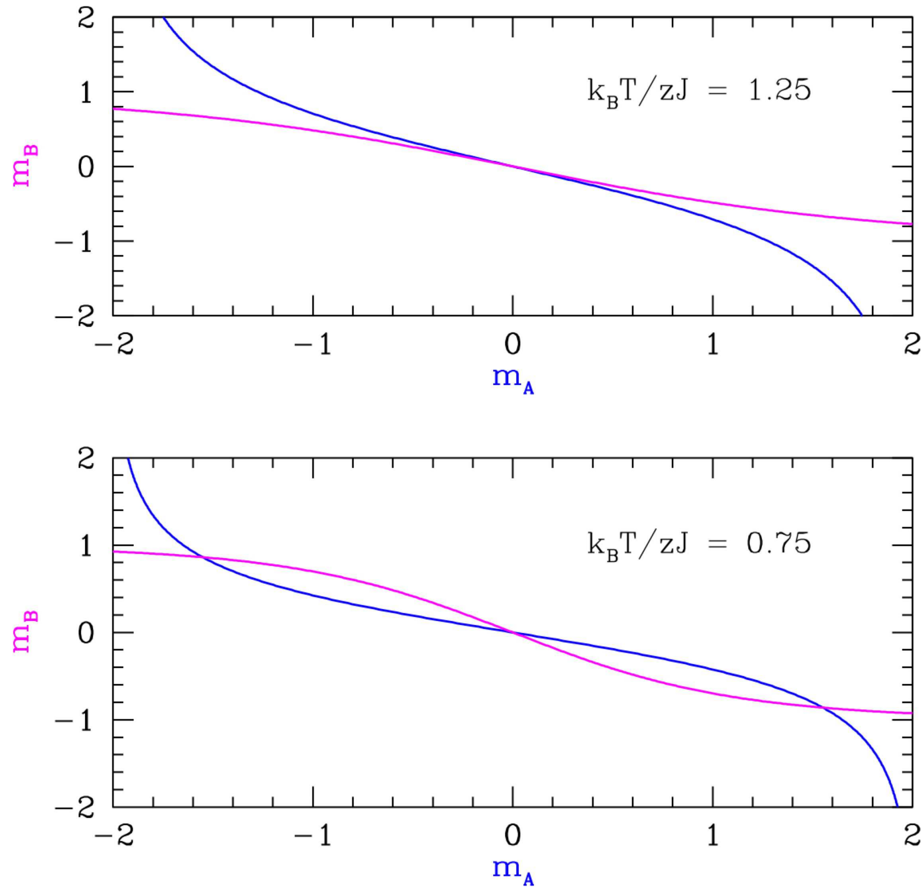

Figure 1: Graphical solution of of mean field equations with $S_A = 1$, $S_B = 2$, $g_A = g_B = 1$, $zJ = 1$, and $H = 0$. Top: $T > T_c$; bottom: $T < T_c$.

The susceptibility is

$$\begin{aligned} \chi = \frac{1}{N}\frac{\partial M}{\partial H} &= -\frac{1}{2}\frac{\partial}{\partial H}(g_A \mu_\circ m_A + g_B \mu_\circ m_B) \\ &= \frac{(g_A^2\, T_A + g_B^2\, T_B)T - 2g_A g_B\, T_A T_B}{T^2 - T_A T_B}\,\frac{\mu_0^2}{2zJ} \ , \end{aligned}$$

which diverges at

$$T_c = \sqrt{T_A T_B} = \sqrt{S_A S_B (S_A + 1)(S_B + 1)}\,\frac{z|J|}{3k_B} \ .$$

Note that T_c does not depend on the sign of J. Note also that the signs of m_A and m_B may vary. For example, let $g_A = g_B \equiv g$ and suppose $S_A > S_B$. Then $T_B < \sqrt{T_A T_B} < T_A$ and while $m_A < 0$ for all $T > T_c$, the B sublattice moment changes sign from negative to positive at a temperature $T_B > T_c$. Finally, note that at high temperatures the susceptibility follows a Curie $\chi \propto T^{-1}$ behavior.

[**4**] *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,

$$\mathcal{H} = J \sum_{\langle ij \rangle} (S_i^x\, S_j^x + S_i^y\, S_j^y + \Delta\, S_i^z\, S_j^z) + h \sum_i S_i^z$$

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

Consider the case of 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.)

Solution :

We start by assuming a two-sublattice structure in which the spins lie in the $x - z$ plane. (Any two-sublattice structure is necessarily coplanar.) Let the A sublattice spins point in the direction $(\theta = \theta_A, \phi = 0)$ and let the B sublattice spins point in the direction $(\theta = \theta_B, \phi = \pi)$. The classical energy per bond is then

$$\varepsilon(\theta_A, \theta_B) = -JS^2 \sin\theta_A \sin\theta_B + JS^2 \Delta \cos\theta_A \cos\theta_B - \frac{hS}{z}\big(\cos\theta_A + \cos\theta_B\big) \ .$$

Note that in computing the energy per bond, we must account for the fact that for each site there are $\frac{1}{2}z$ bonds, where z is the coordination number. The total number of bonds is thus $N_{\text{bonds}} = \frac{1}{2}Nz$, where N is the number of sites. Note also the competition between Δ and h. Large Δ makes the spins antialign along $\hat{\boldsymbol{z}}$, while large h prefers alignment along $\hat{\boldsymbol{z}}$.

Let us first assume $\theta_A = \theta_B = \theta_c$ and determine θ_c. Let $e(\theta_A, \theta_B) \equiv \varepsilon(\theta_A, \theta_B)/JS^2$:

$$\begin{aligned} e(\theta_c) &\equiv e(\theta_A = \theta_c, \theta_B = \theta_c) \\ &= -\sin^2\theta_c + \Delta\cos^2\theta_c - \frac{2h}{zSJ}\cos\theta_c \\ \frac{\partial e}{\partial \theta_c} &= \sin\theta_c \cdot \left\{2(1+\Delta)\cos\theta_c - \frac{2h}{zSJ}\right\} \ . \end{aligned}$$

Thus, the extrema of $e(\theta_c)$ occur at $\sin\theta_c = 0$ and at

$$\cos\theta_c = \frac{h}{zSJ(1+\Delta)} \ .$$

The latter solution is present only when $\Delta > \big|h/zSJ\big| - 1$. The energy of this state is

$$e = -\left\{1 + \frac{1}{1+\Delta}\left(\frac{h}{zSJ}\right)^2\right\}$$

per bond.

To assess stability, we'll need the second derivatives,

$$\left.\frac{\partial^2 e}{\partial\theta_{\rm A}^2}\right|_{\substack{\theta_{\rm A}=\theta_{\rm c}\\ \theta_{\rm B}=\theta_{\rm c}}} = \left.\frac{\partial^2 e}{\partial\theta_{\rm B}^2}\right|_{\substack{\theta_{\rm A}=\theta_{\rm c}\\ \theta_{\rm B}=\theta_{\rm c}}} = \sin^2\!\theta_{\rm c} - \Delta\cos^2\!\theta_{\rm c} + \frac{h}{zSJ}\,\cos\theta_{\rm c}$$

$$\left.\frac{\partial^2 e}{\partial\theta_{\rm A}\,\partial\theta_{\rm B}}\right|_{\substack{\theta_{\rm A}=\theta_{\rm c}\\ \theta_{\rm B}=\theta_{\rm c}}} = -\cos^2\!\theta_{\rm c} + \Delta\sin^2\!\theta_{\rm c}\ ,$$

from which we obtain the eigenvalues of the Hessian matrix,

$$\begin{aligned}\lambda_+ &= (1+\Delta)(1-2\cos^2\!\theta_{\rm c}) + \frac{h}{zSJ}\,\cos\theta_{\rm c}\\ &= (1+\Delta)\left\{1 - \left(\frac{h}{zSJ(1+\Delta)}\right)^2\right\}\\ \lambda_- &= (1-\Delta) + \frac{h}{zSJ}\,\cos\theta_{\rm c}\\ &= \frac{1}{1+\Delta}\left\{1-\Delta^2 + \left(\frac{h}{zSJ}\right)^2\right\}\ .\end{aligned}$$

Assuming $\Delta > 0$, we have that $\lambda_+ > 0$ requires

$$\Delta > \frac{|h|}{zSJ} - 1\ ,$$

which is equivalent to $\cos^2\!\theta_{\rm c} < 1$, and $\lambda_- > 0$ requires

$$\Delta < \sqrt{1 + \left(\frac{h}{zSJ}\right)^2}\ .$$

This is the meaning of "not too large."

The other extrema occur when $\sin\theta_{\rm c} = 0$, *i.e.* $\theta_{\rm c} = 0$ and $\theta_{\rm c} = \pi$. The eigenvalues of the Hessian at these points are:

$$\begin{aligned}\theta_{\rm c} = 0: &\qquad \lambda_+ = -(1+\Delta) + \frac{h}{zSJ}\\ &\qquad \lambda_- = 1 - \Delta + \frac{h}{zSJ}\\ \theta_{\rm c} = \pi &\qquad \lambda_+ = -(1+\Delta) - \frac{h}{zSJ}\\ &\qquad \lambda_- = 1 - \Delta - \frac{h}{zSJ}\ .\end{aligned}$$

Without loss of generality we may assume $h \geq 0$, in which case the $\theta_{\rm c} = \pi$ solution is always unstable. This is obvious, since the spins are anti-aligned with the field. For $\theta_{\rm c} = 0$, the solution is stable provided $\Delta < (h/zJS) - 1$. For general h, the stability condition is $\Delta < |h|/zJS - 1$.

The other possibility is that Δ is so large that neither of these solutions is stable, in which case we suspect $\theta_{\rm A} = 0$ and $\theta_{\rm B} = \pi$ or *vice versa*.

Thus, for $h < zJS(1+\Delta)$, the solution with $\theta_{\rm c} = \cos^{-1}\big(h/zJS(1+\Delta)\big)$ is stable. The Hessian matrix in this case is

$$\begin{pmatrix} \frac{\partial^2 e}{\partial\theta_{\rm A}^2} & \frac{\partial^2 e}{\partial\theta_{\rm A}\,\partial\theta_{\rm B}} \\ \\ \frac{\partial^2 e}{\partial\theta_{\rm B}\,\partial\theta_{\rm A}} & \frac{\partial^2 e}{\partial\theta_{\rm B}^2} \end{pmatrix}_{\substack{\theta_{\rm A}=0 \\ \theta_{\rm B}=\pi}} = \begin{pmatrix} \Delta + \frac{h}{zSJ} & 1 \\ \\ 1 & \Delta - \frac{h}{zSJ} \end{pmatrix}$$

whose eigenvalues are

$$\lambda_\pm = \Delta \pm \sqrt{1 + \left(\frac{h}{zSJ}\right)^2}\ .$$

Thus, this configuration is stable only if

$$\Delta > \sqrt{1 + \left(\frac{h}{zSJ}\right)^2}\ .$$