7. *Statistical Mechanics and Thermodynamics* (Fall 2004)

Some organic molecules have a triplet excited state at energy $k_B\Delta$ above a singlet ground state.

(a) Find an expression for the magnetic moment in a field B in terms of Δ, B, the temperature T, the Bohr magneton μ_B, and the gyromagnetic ratio g.

(b) Show that the susceptibility for $T \gg \Delta$ is given by $N(g\mu_B)^2/2k_BT$, where N is the total number of molecules in the system.

(c) With the help of a diagram of energy levels versus field and a rough sketch of entropy versus field, explain how this system might be cooled by adiabatic magnetization (*not demagnetization*).

a. $\vec{\mu} = g\mu_B \vec{s}$ where $\hbar\vec{s}$ is the spin angular momentum

The singlet state has $|\vec{s}| = 0$ and the triplet state has $|\vec{s}| = 1$.

But we want to find $\langle \mu_z \rangle$ where $\hat{z}$ is the direction of the applied magnetic field. So $\mu_z = g\mu_B s_z$

$$(\mu_S)_z = 0 \qquad (\mu_T^1)_z = g\mu_B \qquad (\mu_T^0)_z = 0 \qquad (\mu_T^{-1})_z = -g\mu_B$$

The energy of a magnetic moment in a field is $U = -\vec{\mu}\cdot\vec{B} = -\mu_z B$

$$\epsilon_S = 0 \qquad \epsilon_T^1 = K\Delta - g\mu_B B \qquad \epsilon_T^0 = K\Delta \qquad \epsilon_T^{-1} = K\Delta + g\mu_B B$$

$$\langle \mu_z \rangle = \frac{(\mu_S)_z e^{-\beta\epsilon_S} + (\mu_T^1)_z e^{-\beta\epsilon_T^1} + (\mu_T^0) e^{-\beta\epsilon_T^0} + (\mu_T^{-1}) e^{-\beta\epsilon_T^{-1}}}{e^{-\beta\epsilon_S} + e^{-\beta\epsilon_T^1} + e^{-\beta\epsilon_T^0} + e^{-\beta\epsilon_T^{-1}}}$$

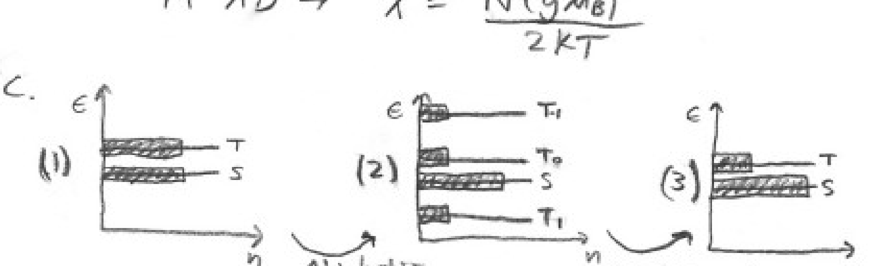
$$= g\mu_B \frac{e^{-\beta(K\Delta - g\mu_B B)} - e^{-\beta(K\Delta + g\mu_B B)}}{1 + e^{-\beta(K\Delta - g\mu_B B)} + e^{-\Delta/T} + e^{-\beta(K\Delta + g\mu_B B)}}$$

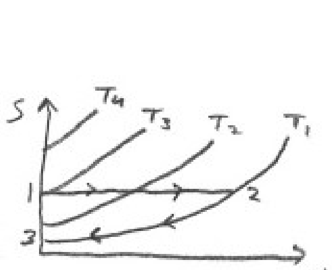
$$M = N\langle \mu_z \rangle = Ng\mu_B \frac{e^{\beta g\mu_B B} - e^{-\beta g\mu_B B}}{e^{\Delta/T} + e^{\beta g\mu_B B} + 1 + e^{-\beta g\mu_B B}}$$

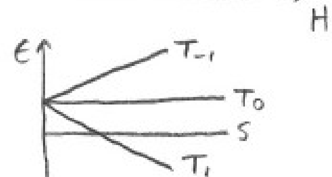
b. $T \gg \Delta \Rightarrow$ $$M \cong Ng\mu_B\left(\frac{1 + \beta g\mu_B B - 1 + \beta g\mu_B B}{1 + 1 + 1 + 1}\right) = \frac{N(g\mu_B)^2}{2KT} B$$

$$M = \chi B \Rightarrow \chi = \frac{N(g\mu_B)^2}{2KT}$$

c.







All the particles in the triplet state are split among the three levels when the field is applied adiabatically and settle down preferentially into the singlet state when the field is removed isothermally.