Physics 540 Fall 2005 practise problem – answer will be posted Wednesday Dec. 14.

This graph is from S. Arajs and R. V. Colvin, J. Appl. Phys. 32, S336 (1961). They measured the magnetic susceptibility χ of Gadolinium metal and plotted the reciprocal of χ versus temperature. Gd has 7 f electrons (half-filled f shell, spins all parallel by Hund's rule) and 3 valence electrons with atomic s or p character. These 3 are not very important for the magnetization, which is why the captions are comparing data with "noninteracting Gd^{3+} ions. You might imagine an Ising model for Gd spin-spin interactions, $H=-J\sum \mu_{iz}\mu_{jz}$, where the sum goes over each nearest neighbor pair once. Each Gd atom has 12 nearest neighbors. The volume per Gd atom is 33 cubic Angstroms and the moment per Gd in the simplest picture is 7 Bohr magnetons. The mass density of Gd is ρ=7.89 g/cm^3.

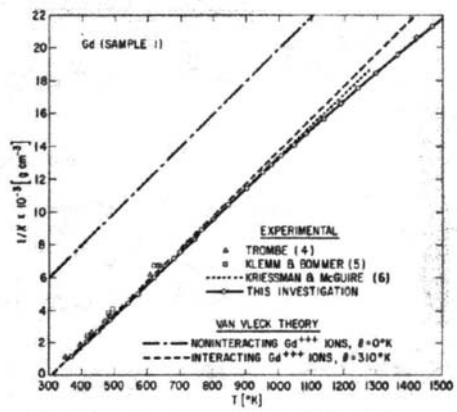

FIG. 1. Inverse paramagnetic susceptibility of Gd as a function of temperature.

(a) What is the magnetic part of the partition function for a single Gd atom with S=7/2?

(b) What is the formula for the susceptibility of non-interacting spins of density n with S=7/2 and $\mu=7\mu_B$? Does this agree with the number given on the graph above (dot-dash curve)? The experimental χ in cm^3/g is the actual χ divided by the mass density ρ.

(c) Estimate the exchange coupling J using a mean field approximation. What is J in eV?

$E_n = -\mu_z B = -s_z(\mu B/S)$ where $S=7/2$, $s_z = 7/2, 5/2, 3/2, \ldots, -7/2$ and $\mu = 7\mu_B$.

$Z = e^{(7/2)x} + e^{(5/2)x} + \ldots + e^{-(7/2)x}$ where $x = \mu B/SkT$

$= \sinh(4x)/\sinh(x/2)$

$F = -Nk_BT\ln Z$, $M = -\frac{1}{V}\frac{\partial F}{\partial B}$, $\chi = -\frac{1}{V}\frac{\partial^2 F}{\partial B^2}\Big|_{B=0}$

$F = -Nk_BT[\ln(\sinh 4x) - \ln(\sinh x/2)]$.

we need to keep the part of F quadratic in x

$F \approx -Nk_BT\ln 8 - \frac{63}{24}N(\mu B/SkT)^2$

$\chi = \frac{63}{12}\frac{N}{V}\frac{\mu^2}{S^2k_BT}$. Evaluate at 300 K

$= \frac{63}{12(7/2)^2}\left(\frac{1}{33\times10^{-8}\,\text{cm}^3}\right)\frac{[0.927\times10^{-20}\,\text{erg/Gauss}\times 7]^2}{(1.38\times10^{-16}\,\text{erg/K})(3\times10^2\,\text{K})}$

$= 13\times10^3$

From the graph $\rho/\chi^0_{300} = 6\times10^{-3}$ g/cm^3 $\Rightarrow \chi = 1.3\times10^3$

off by 10 – I don't know why.

(c) Estimate the exchange constant J.
actually I should have asked for an estimate of the exchange energy:

$$E_x \equiv -\frac{1}{2}\left[E(\uparrow\uparrow) - E(\uparrow\downarrow)\right]$$

$$E_{\uparrow\uparrow} = -J\mu^2, \quad E_{\uparrow\downarrow} = J\mu^2, \quad E_x = J\mu^2$$

The mean field argument is this

$$\mathcal{H} = -\sum_i \mu_{iz} B - J\sum_{\langle ij\rangle} \mu_{iz}\mu_{jz}$$

$$\mathcal{H}_{MF} = -\sum_i \mu_{iz}\left(B + zJ\langle\mu_z\rangle\right)$$

$$M = \chi_0\left(B + zJ\langle\mu_z\rangle\right) \quad \text{and} \quad M = \frac{N}{V}\langle\mu_z\rangle$$

$$\left[1 - \chi_0 Jz/(N/V)\right] M = \chi_0 B$$

$$\chi_{MF} = \frac{\chi_0 T}{T - \frac{\chi_0 T J z}{N/V}} = \frac{\chi_0 T}{T - T_c}$$

$$T_c = \frac{\chi_0 T J z}{N/V} = \frac{63}{3}\frac{\mu_B^2 J z}{k_B}$$

$$\therefore J\mu^2 = 49 J\mu_B^2 = E_x = \frac{49.3}{63}\frac{k_B T_c}{z}$$

From the graph, $1/\chi \to 0$ at $T = T_c = 300K$

$$E_x = \frac{21}{9}\frac{k_B T_c}{12} = \frac{7(.025\,eV)}{36} = \underline{\underline{0.005\,eV}}$$

But $d\chi/dT = d\chi_0/dT$ on the graph is smaller by 10 than my estimate which makes J 10 times larger

$$\underline{J \sim 50\,meV}$$