

Lecture 3

Assuming for \vec{M} & \vec{H} are parallel & free-Heisenberg spins

Ising spins - only 1 fixed direction (up/down)

$$(31.1) \quad M(H) = - \frac{1}{V} \frac{\partial E_0(H)}{\partial H}$$

$$(31.2) \quad M(H, T) = \frac{\sum_n M_n(H) e^{-E_n/k_B T}}{\sum_n e^{-E_n/k_B T}}, \quad \text{for finite temperature}$$

$$(31.4) \quad M = - \frac{1}{V} \frac{\partial F}{\partial H}, \quad F \text{ is magnetic Helmholtz Free energy.}$$

$$(31.6) \quad \chi = \frac{\partial M}{\partial H} = - \frac{1}{V} \frac{\partial^2 F}{\partial H^2}$$

Interaction energy with each electron spin $s^i = \frac{1}{2} \sigma_i$:

$$\Delta H = g_0 \mu_B H S_z \quad (S_z = \sum_i s_z^i)$$

$$g_0 = 2 \left[1 + \frac{\alpha}{2\pi} + O(\alpha^2) + \dots \right], \quad \alpha = \frac{e^2}{4c} \approx \frac{1}{137}$$

$$= 2.0023 \approx 2$$

(31.15)

$$T = \frac{1}{2m} \sum_i \left[\vec{p}_i + \frac{e}{c} \vec{A}(\vec{r}_i) \right]^2 = \frac{1}{2m} \sum_i \left(p_i - \frac{e}{2c} \vec{r}_i \times \vec{H} \right)^2$$

$$= \frac{1}{2m} \sum_i \left(\vec{p}_i^2 - \frac{e}{c} \vec{p}_i \cdot (\vec{r}_i \times \vec{H}) + \frac{e^2}{4c^2} (\vec{r}_i \times \vec{H})^2 \right)$$

$$= \frac{1}{2m} \sum_i p_i^2 - \sum_i \frac{e}{2mc} \vec{p}_i \cdot (\vec{r}_i \times \vec{H}) + \sum_i \frac{e^2}{8mc^2} (\vec{r}_i \times \vec{H})^2$$

$$= T_0 + \sum_i \frac{e}{2mc} (\vec{r}_i \times \vec{p}_i) \cdot \vec{H} + \sum_i \frac{e^2}{8mc^2} H^2 (x_i^2 + y_i^2)$$

(31.16)

$$T = T_0 + \mu_B \vec{L} \cdot \vec{H} + \frac{e^2}{8mc^2} H^2 \sum_i (x_i^2 + y_i^2)$$

$$\vec{r}_i \times \vec{H} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & 0 \\ 0 & 0 & H \end{vmatrix}$$

$$\hbar \vec{L} = \sum_i \vec{r}_i \times \vec{p}_i$$

Second-order perturbation theory:

$$(31.19) \quad E_n \rightarrow E_n + \Delta E_n; \quad \Delta E_n = \langle n | \Delta \hat{H} | n \rangle + \sum_{n' \neq n} \frac{|\langle n | \Delta \hat{H} | n' \rangle|^2}{E_n - E_{n'}}$$

$$(31.20) \quad \Delta E_n = \mu_B \vec{H} \cdot \langle n | \vec{L} + g_0 \vec{S} | n \rangle + \sum_{n' \neq n} \frac{|\langle n | \mu_B \vec{H} \cdot (\vec{L} + g_0 \vec{S}) | n' \rangle|^2}{|E_n - E_{n'}|} + \frac{e^2}{8mc^2} H^2 \langle n | \sum_i (x_i^2 + y_i^2) | n \rangle$$

$\Delta E_n^{(1)} \rightarrow$ local moment / Curie term / Langevin

$\Delta E_n^{(2)} \rightarrow$ Van Vleck mixing of different E states

$\Delta E_n^{(3)} \rightarrow$ Lenz's law / Larmor / Langevin diamagnetism

$$\Delta E_n^{(1)} = \mu_B \vec{H} \cdot \langle n | \vec{L} + g_0 \vec{S} | n \rangle = O(\mu_B H) \sim \frac{\hbar e H}{mc} \sim \hbar \omega_c$$

1 (in the order of unity)

$$\Delta E_n^{(3)} \approx \frac{e^2}{mc^2} H^2 a_0^2 = \left(\frac{eH}{mc} \right)^2 \frac{\hbar^2}{\hbar^2} m a_0^2 \left\{ \begin{array}{l} \frac{a_0}{\hbar^2 / m a_0} = \frac{a_0}{e^2} \\ \hbar^2 / m a_0 \end{array} \right.$$

$$= (\hbar \omega_c) \left(\frac{\hbar \omega_c}{e^2 / a_0} \right) \ll k_B T$$

e^2/a_0 is in the order of 27 eV (13.6 eV $\times 2$)

$$\Delta E_n^{(2)} \sim \frac{\hbar \omega_c}{\Delta}$$

$\Delta = \min |E_n - E_{n'}|$ is typically about 1 eV,

Δ will be large enough to make $\Delta E_n^{(2)}$ small.

CaPdCb

HW: From the data, 1. predict $\chi = \chi_0 + \frac{C}{T - \theta}$, where C is Curie constant, θ is Curie-Weiss factor

2. get the peff 3. $\chi_{\text{mol}}^{\text{Larmor}}$