8.512 Recitation 8

- Pset 4 due Monday 04/04

Today: 1) Langevin Paramagnetism
2) Curie-Weiss theory
3) Stoner Magnetism
4) Exchange Interaction

1) Atom in external magnetic field $\vec{B} = B\hat{z}$

$$H = -\mu_B g S_z B \qquad (S \to J \text{ on pset})$$

$$S_z = -S, \dots, S$$

$$M = \frac{\sum_{-S}^{S} \mu_B g S_z e^{\beta \mu_B g S_z B}}{\sum_{-S}^{S} e^{\beta \mu_B g S_z B}} = \mu_B L_S(x)$$

where $x = \beta \mu_B g S B$

$$L_S(x) = gS\left[\frac{2S+1}{2S}\coth\left(\frac{2S+1}{2S}x\right) - \frac{1}{2S}\coth\left(\frac{x}{2S}\right)\right]$$

Ex: $S = \frac{1}{2}$ $\Rightarrow L_{\frac{1}{2}}(x) = \frac{1}{2}g\left[2\coth(2x) - \coth(x)\right] = \frac{1}{2}g\tanh(x)$

$$M = \frac{1}{2}\mu_B g \tanh(x)$$

$$\chi = \frac{dM}{dB} = \frac{1}{4}(\mu_B g)^2 \beta \cdot \frac{1}{\cosh^2\left(\frac{1}{2}\beta\mu_B g B\right)}$$

At low temeratures $x \ll 1$ $\Rightarrow$ $\chi \approx \frac{(\mu_B g)^2}{4 k_B T} \sim \frac{1}{T}$

More generally $\chi \approx (\mu_B g)^2 \cdot \frac{S(S+1)}{} \sim \frac{1}{}$

More generally $\chi \approx \frac{(\mu_B g)^2}{k_B T} \cdot \frac{S(S+1)}{3} \sim \frac{1}{T}$

Ex: Classical Langevin limit $S \to \infty$

$$\sum S_z \to \int_{-\infty}^{\infty} dS_z$$

2) Weiss mean-field (molecular) theory ($e^- - e^-$ interaction)

$$H = -\frac{1}{2} \sum_{ij} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$$H \approx -\sum_i \vec{S}_i \cdot \sum_j J_{ij} \langle \vec{S}_j \rangle + \underbrace{\frac{1}{2} \sum_{ij} J_{ij} \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle}_{\text{const.}}$$

$\Rightarrow$ Effective magnetic field due to other electrons

$$\vec{B}_i = \frac{1}{g\mu_B} \sum_j J_{ij} \langle \vec{S}_j \rangle$$

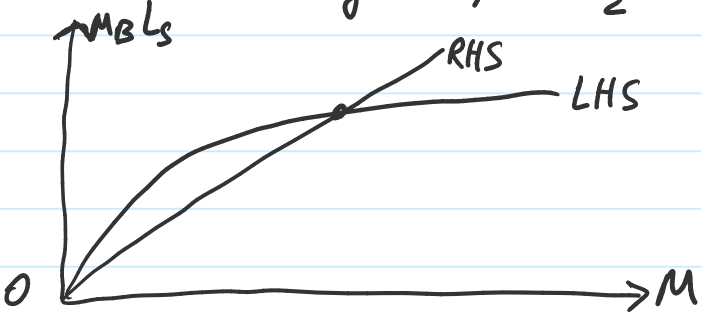
Let $J_{ij} = J$ uniform ferromagnet, $\vec{M} = \mu_B g \sum_j \langle \vec{S}_j \rangle$

$$\vec{B}_{int} = \boxed{\frac{J}{(\mu_B g)^2}} \vec{M} \qquad \equiv \lambda$$

- M solves the self-consistency eq.

$$M = \mu_B L_S(\beta \mu_B g S B_{int})$$

$g \approx 2$, $S = \frac{1}{2}$ on pset



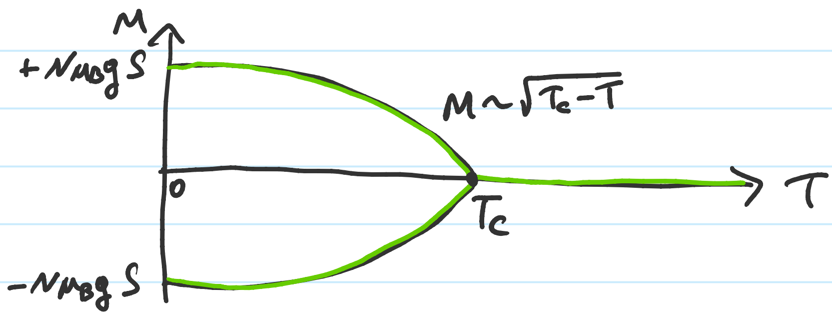
$M = 0$ always a solution

- Another solution $M \neq 0$ exists if

$$\mu_B \frac{d L_S(\beta \mu_B B_{int})}{dM}\bigg|_{M=0} > 1$$

- This determines the critical Curie temperature:

$$\boxed{T_c = \frac{S(S+1)}{3 k_B} (\mu_B g)^2 \lambda} \longrightarrow \frac{J}{4 k_B}$$



- For $T > T_c$ we have $M = N \cdot \frac{(g \mu_B)^2 B}{k_B (T - T_c)} \cdot \frac{S(S+1)}{3}$

$$\Rightarrow \chi = \frac{S(S+1)}{3} \cdot \frac{N (g \mu_B)^2}{k_B (T - T_c)} \sim \frac{1}{T - T_c}$$

- For AF we look at A and B sublattices

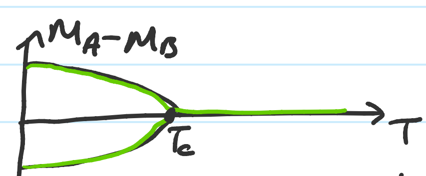
$$B^{int}_{A,B} = -\lambda M_{B,A}$$

Symmetry requires $M_A = -M_B$

$$\Rightarrow M = M_A + M_B = 0$$

Staggered magnetisation $M_A - M_B$ can be non-zero

T_c is the same as for FM!



- Note: depending on notation, T_c can be negative and one defines a Néel temperature $T_N = |T_c|$

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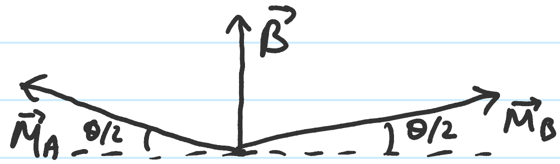
- For AF, suppose $T=0$ and we turn on small $\vec{B}$

Case 1: $\vec{B} \perp$ to axis of the spins



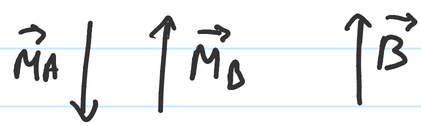
Energy $E = -\vec{B}_{int} \cdot \vec{M}_B - \vec{B} \cdot \vec{M} = \lambda \vec{M}_A \cdot \vec{M}_B - \vec{B} \cdot (\vec{M}_A + \vec{M}_B)$

$$= -\lambda |M_A|^2 \cos\theta - B|M_A| \sin\theta$$

$$\frac{\partial E}{\partial \theta} = 0 \quad \Rightarrow \quad \tan\theta \approx \theta = \frac{B}{\lambda |M_A|}$$ equilibrium angle

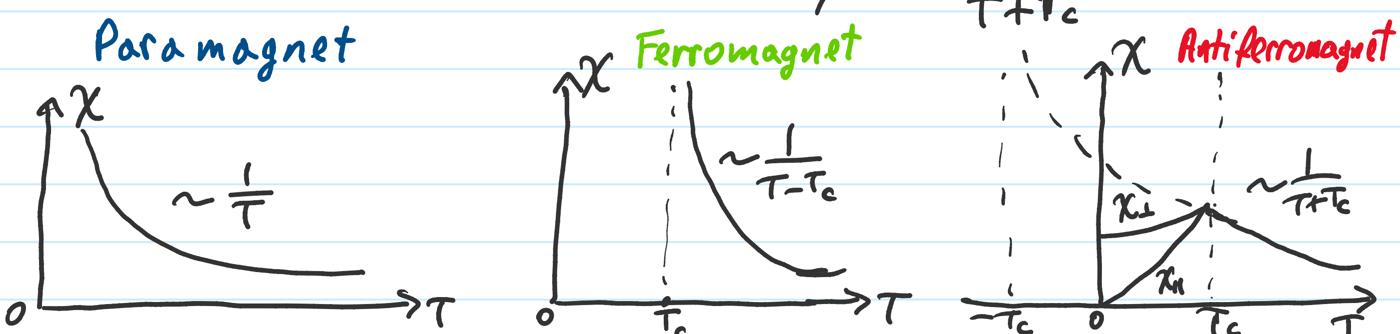
$$\chi_\perp = \frac{|M_A| \sin\theta}{B} \approx \frac{|M_A|\theta}{B} = \frac{1}{\lambda}$$

Case 2: $\vec{B} \parallel$ to axis of the spins



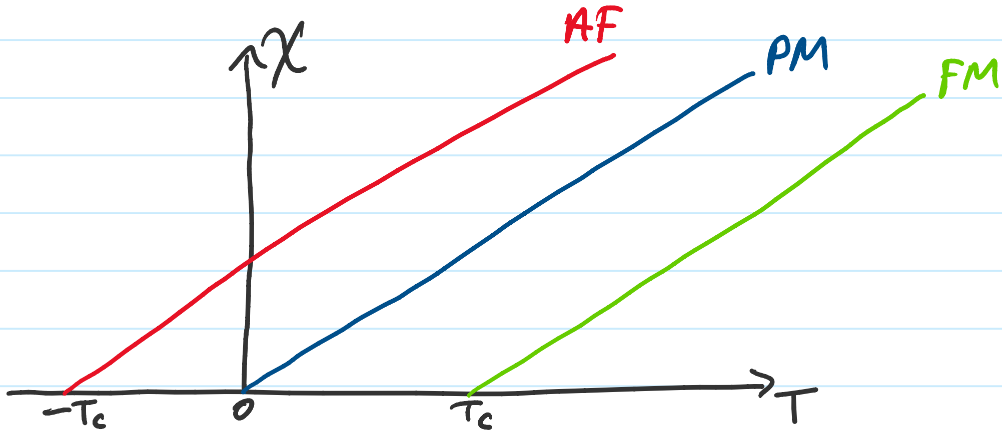
Magnetic energy is not changed if the spins make equal angles w/ the field $\Rightarrow \chi_\parallel = 0$

- For $T > T_c$ one can show $\chi \sim \frac{1}{T+T_c}$



Curie's law

Curie-Weiss law ($T > T_c$)



3) Itinerant magnetism is described by the Hubbard model

$$H = -t \sum_{ij\sigma} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$

Competition between kinetic term and interaction

- Stoner mean-field approximation:

$$U n_{i\uparrow} n_{i\downarrow} = \frac{U}{4}(n_{i\uparrow}+n_{i\downarrow})^2 - \frac{U}{4}(n_{i\uparrow}-n_{i\downarrow})^2$$

$$\approx \frac{U}{4}\langle n_{i\uparrow}+n_{i\downarrow}\rangle^2 - \frac{U}{4}\langle n_{i\uparrow}-n_{i\downarrow}\rangle^2$$

- Total # of fermions $N = \sum_i \langle n_{i\uparrow} + n_{i\downarrow}\rangle$
(local) magnetisation $M = \mu_B \langle n_{i\uparrow} - n_{i\downarrow}\rangle$

$$\Rightarrow \quad U n_{i\uparrow} n_{i\downarrow} \approx U(M=0) - \frac{U}{4}\left(\frac{M}{\mu_B}\right)^2$$

- Consider a system w/ the same # of ↑ and ↓ electrons
Flip a few spins so their Fermi energies are different

$$E_{F\uparrow} = E_F + \delta E/2 \qquad \delta E \ll E_F$$
$$E_{F\downarrow} = E_F - \delta E/2$$

$$E_{F\downarrow} = E_F - \delta E/2$$

$$n_{\uparrow,\downarrow} = \int_0^{E_F \pm \delta E/2} dE \, \frac{g(E)}{2}$$ half density for each type

$$M = \mu_B(n_\uparrow - n_\downarrow) = \delta E \cdot \frac{g(E_F)}{2}\mu_B$$

- Kinetic energy increases

$$K = \int_0^{E_F+\frac{\delta E}{2}} dE \cdot E \frac{g(E)}{2} + \int_0^{E_F-\frac{\delta E}{2}} dE \cdot E \cdot \frac{g(E)}{2} \simeq K(M=0) + \frac{g(E_F)}{2}\left(\frac{\delta E}{2}\right)^2$$

$$= K(M=0) + \frac{g(E_F)}{2}\left(\frac{M}{\mu_B \, g(E_F)}\right)^2$$

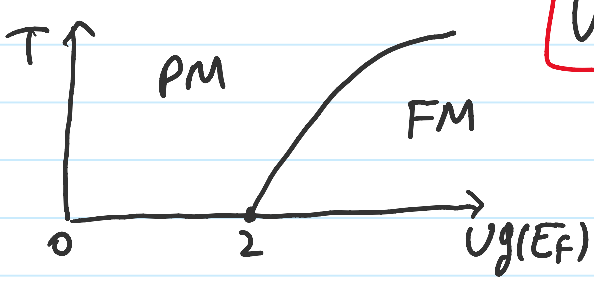
- Potential energy decreases

$$U = U(M=0) - \frac{U}{4}\left(\frac{M}{\mu_B}\right)^2$$

- Total energy $\quad E = E(M=0) + \left(\frac{M}{\mu_B}\right)^2\left(\frac{1}{2g(E_F)} - \frac{U}{4}\right)$

$\Rightarrow$ The energy is lowered by increasing M from zero if

$$\boxed{Ug(E_F) > 2}$$ Stoner criterion



4) Exchange interaction between 2 sites $(k=1,2)$

$$H = t\left(c^\dagger_{1,\alpha} c_{2,\alpha} + c^\dagger_{2,\alpha} c_{1,\alpha}\right) - \frac{1}{2}J\sum_{k=1,2} \vec{S}_k \cdot c^\dagger_{k,\alpha} \vec{\sigma}_{\alpha\beta} c_{k,\beta}$$

- $\vec{S}_k$ is a classical spin vector w/ magnitude $S \gg 1$
- $\vec{\sigma}$ is a vector of 2x2 Pauli matrices

$$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$$

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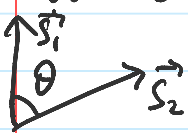
- α and β are spin indices $\uparrow$ or $\downarrow$
- sum over α and β is implicit
- there is only one electron $\sum_{k\alpha} c^\dagger_{k\alpha} c_{k\alpha} = 1$
- $J \gg t$

- WLOG take $\vec{S}_1 = S\hat{z} = (0,0,S)$
- Then $\vec{S}_2 = S(\sin\theta\cos\varphi,\ \sin\theta\sin\varphi,\ \cos\theta)$

WLOG place $\vec{S}_1$ and $\vec{S}_2$ in the same plane



$\varphi = 0 \implies \vec{S}_2 = (S\sin\theta,\ 0,\ S\cos\theta)$

$$\Rightarrow H = t\left(c^\dagger_{1\uparrow}c_{2\uparrow} + c^\dagger_{2\uparrow}c_{1\uparrow} + c^\dagger_{1\downarrow}c_{2\downarrow} + c^\dagger_{2\downarrow}c_{1\downarrow}\right) -$$

$$- \frac{JS}{2}\Big(c^\dagger_{1\uparrow}c_{1\uparrow} - c^\dagger_{1\downarrow}c_{1\downarrow} + \sin\theta\left(c^\dagger_{2\downarrow}c_{2\uparrow} + c^\dagger_{2\uparrow}c_{2\downarrow}\right) + \cos\theta\left(c^\dagger_{2\uparrow}c_{2\uparrow} - c^\dagger_{2\downarrow}c_{2\downarrow}\right)\Big)$$

- Only one electron $\Rightarrow$ reduced basis $\{\uparrow 0, \downarrow 0, 0\uparrow, 0\downarrow\}$

H in this basis is

$$\begin{array}{c} \\ |\uparrow 0\rangle \\ |\downarrow 0\rangle \\ |0\uparrow\rangle \\ |0\downarrow\rangle \end{array}
\begin{array}{c} \begin{array}{cccc} |\uparrow 0\rangle & |\downarrow 0\rangle & |0\uparrow\rangle & |0\uparrow\rangle \end{array} \\
\begin{pmatrix} -\frac{JS}{2} & 0 & t & 0 \\ 0 & \frac{JS}{2} & 0 & t \\ t & 0 & -\frac{JS}{2}\cos\theta & -\frac{JS}{2}\sin\theta \\ 0 & t & -\frac{JS}{2}\sin\theta & \frac{JS}{2}\cos\theta \end{pmatrix} \end{array}$$

Diagonalize and find GS:

$$E_0 = -\frac{1}{2}\sqrt{4JSt\cos\left(\frac{\theta}{2}\right) + J^2S^2 + 4t^2}$$

$$\approx -\frac{1}{2}JS\sqrt{1 + \frac{4t}{JS}\cos\left(\frac{\theta}{2}\right)} \approx -\frac{1}{2}JS\left(1 + \frac{2t}{JS}\cos\left(\frac{\theta}{2}\right)\right)$$

$$\vec{S}_1 \cdot \vec{S}_2 = S^2 \cos\theta = S^2\left(2\cos^2\left(\frac{\theta}{2}\right) - 1\right)$$

$$\Rightarrow \cos\left(\frac{\theta}{2}\right) \approx \frac{1}{\sqrt{2}}\left(1 + \frac{\vec{S}_1 \cdot \vec{S}_2}{2S^2}\right)$$

$$E_0 \approx \text{const} - \frac{t}{2\sqrt{2}S^2}\left(\vec{S}_1 \cdot \vec{S}_2\right) \Rightarrow \text{FM if } t > 0\,!$$