MAGNETISM

magnetic material : M^{n+} transition metal ion

$$\vec{J} = \vec{L} + \vec{S} \qquad M: \; Cu, \; Zn, \; Mn, \; Fe, \ldots$$

$\vec{B} = B\vec{e}_z$

$$\vec{m} = g\mu_B \vec{J} \longrightarrow \tilde{g}\,\mu_B \vec{S} \qquad \tilde{g} = -2$$

$$\vec{J} = \vec{S} \qquad \vec{L} = 0$$

independent magnetic moments @ sufficiently high T

$$|\vec{m}| = \tilde{g}\underbrace{\sqrt{S(S+1)}}_{\sqrt{|\vec{S}|^2}}$$

How does measure $|\vec{m}|$?

Thermodynamics of paramagnetic ions

$$\hat{\mathcal{H}} = -\vec{B}\cdot\vec{m}$$

$$= -g\mu_B B J^z \qquad J^z = S^z$$

$$J^z = -J, \ldots, J$$

$$(-S, \ldots, S)$$

$$Z = \sum_{J^z=-J}^{J} e^{\beta g \mu_B B J^z} \qquad \beta = \frac{1}{k_B T}$$

$$= \ldots = \frac{\sinh\left(\beta g \mu \frac{B}{2}(2J+1)\right)}{\sinh\left(\beta g \mu B/2\right)}$$

$$\langle m \rangle = \langle \vec{m} \cdot \vec{e}_z \rangle$$

$$= -\frac{\partial}{\partial B}\left(-k_B T \log Z\right) = k_B T \frac{\partial}{\partial B}\left(\log Z\right)$$

($-k_B T \log Z \to F$)

$$= k_B T \, \frac{1}{Z} \frac{\partial Z}{\partial B}$$

$$= \ldots = g\mu J \; B_J(y) \qquad y = \beta g \mu B J$$

B_J ↓ Brillouin function

$$B_J(y) = \frac{2J+1}{2J} \coth\left(y \, \frac{2J+1}{J}\right) - \frac{1}{2J} \coth\left(\frac{y}{2J}\right)$$

↓

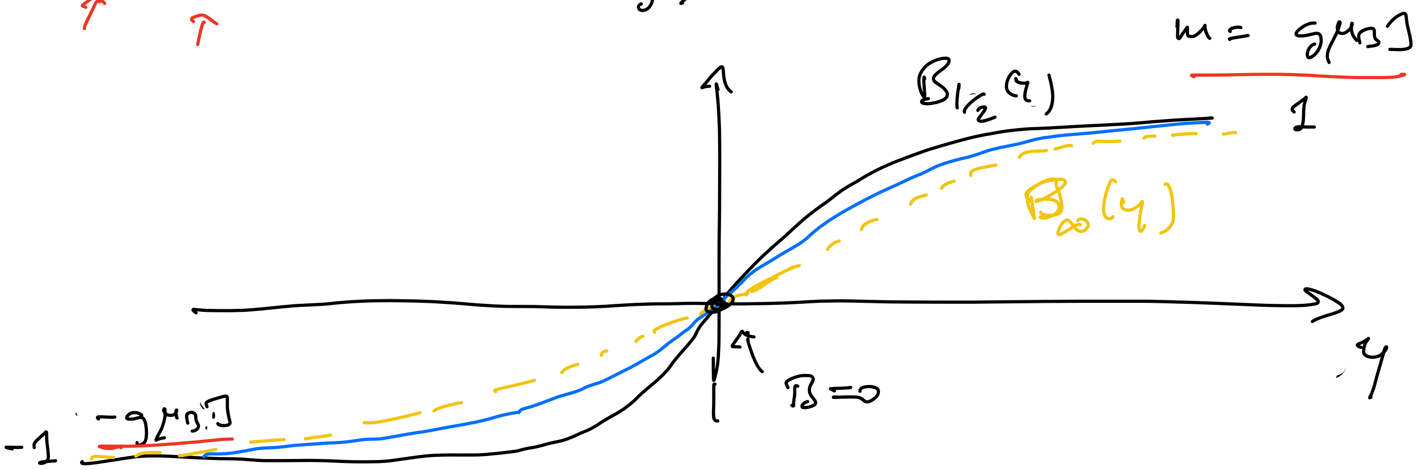
$$J = \frac{1}{2}, \ldots, \infty$$

$$\begin{cases} B_{1/2}(y) = \tanh(y) \\ B_\infty(y) = \coth(y) - \frac{1}{y} = \mathcal{L}(y) \end{cases}$$

Langevin function

$$\left[\frac{\hat{J}^x}{J}, \frac{\hat{J}^y}{J}\right] = i\hbar \frac{\hat{J}^z}{J^2} \underset{J \to \infty}{\Longrightarrow} 0$$

classical limit



$$B_J(y) \underset{y\to 0}{\to} \frac{1}{3}\frac{J+1}{J}\, y \left(-\; A y^3\right) + o(y^5)$$

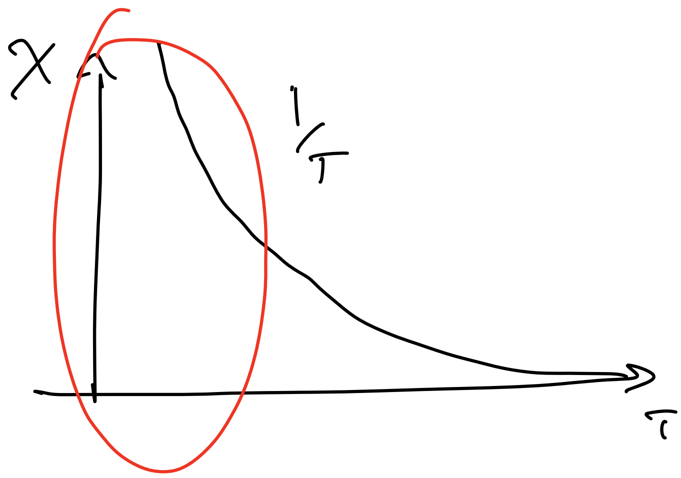
$$A = \frac{(2J+1)^4 - 1}{360\, J^3}$$

$$m(B) \underset{B\to 0}{\approx} \frac{1}{3}\frac{J+1}{J}\,(g\mu B J)\; g\mu J + \cdots$$

$$= (g\mu_B)^2 \frac{J(J+1)}{3k_BT}\, B + \cdots$$

$$\chi = \frac{\partial m}{\partial B} = \frac{(g\mu_B)^2 J(J+1)}{3k_BT} = \frac{\mu_B^2 \left(g\sqrt{J(J+1)}\right)^2}{3k_BT}$$

where $\mu_B^2 \left(g\sqrt{J(J+1)}\right)^2 = \mu_{eff}^2$



$$\chi \underset{B\to 0}{\simeq} \frac{m}{B}$$

Curie law of paramagnetism

$\frac{3k_B}{\mu_{eff}^2}$ ↗

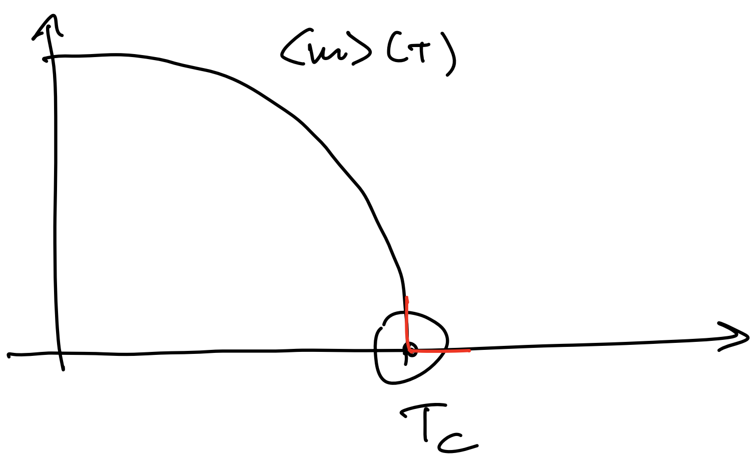
$T \to \infty$

Interactions among magnetic moments :

magnetic transition / ordering

phenomenology :

$\langle m \rangle_B \xrightarrow[B\to 0]{} \text{const}$ spontaneous magnetization (persistent)



$m(T) \simeq |T_c - T|^\beta$

different forms of persistent magnetization

$\langle m \rangle = g\mu_B \sum_i \langle \epsilon_i \, J_i \rangle$

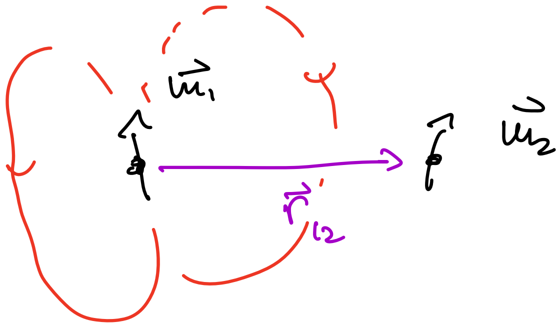
$\epsilon_i = \begin{cases} 1 & \text{everywhere} \\ & \text{ferromagnetism} \\ (-1)^i & \\ & \text{antiferromagnetism} \end{cases}$

ferromagnetism: ↑↑↑ ... ↑

antiferromagnetism: ↑↓↑↓↑↓

(helimagnetism ↑ ↗ → ↘ ↓ ... ← ↖)

What is the origin of magnetic ordering?



$$\frac{E_{dip-dip}}{k_B} = \frac{1}{k_B}\frac{\mu_0}{4\pi}\left(\frac{\vec{m}_1\cdot\vec{m}_2}{r_{12}^3} - 3\frac{(\vec{m}_1\cdot\vec{r}_{12})(\vec{m}_2\cdot\vec{r}_{12})}{r_{12}^5}\right)$$

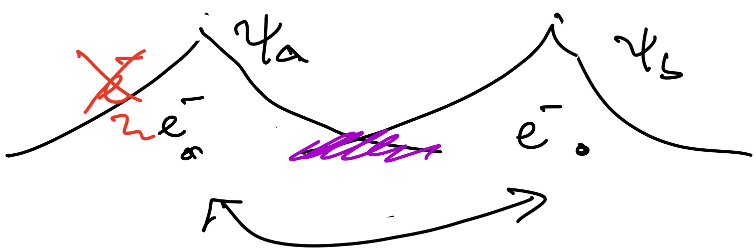
$$\simeq 1\ \text{K}$$

$r_{12} = 1\ \text{Å}$

$|\vec{m}_1|, |\vec{m}_2| \simeq 1\mu_B$

Electron exchange : → direct exchange (↻)
→ double exchange → ferromagnetism
→ super exchange → antiferromagnetism
(...)

Direct exchange



Two states

Singlet state

$$\psi_s(\vec{r}_1, \vec{r}_2)\chi_s = \overbrace{[\psi_a(\vec{r}_1)\,\psi_b(\vec{r}_2) + \psi_b(1)\,\psi_a(2)]}^{\text{bonding}}\ \frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}$$

triplet state

$$\psi_T(\vec{r}_1, \vec{r}_2)\,\underset{\text{spin state}}{\chi_T} = \overbrace{[\psi_a(1)\,\psi_b(2) - \psi_b(1)\,\psi_a(2)]}^{\text{anti bonding}}$$

$$\begin{cases} |\uparrow\uparrow\rangle \\ (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2} \\ |\downarrow\downarrow\rangle \end{cases}$$

Coulomb interaction

$$+\frac{e^2}{4\pi\epsilon_0 |\vec{r}_1 - \vec{r}_2|}$$

$$E_s = \frac{1}{2}\int d^3r_1\, d^3r_2 \Big(|\psi_a(1)|^2 |\psi_b(2)|^2 \frac{e^2}{4\pi\epsilon_0 r_{12}} \quad \rightarrow \text{Hartree}$$

$$+ \psi_a(1)\,\psi_b(2)\,\psi_a(2)\,\psi_b(1)\frac{e^2}{4\pi\epsilon_0 r_{12}} \Big)$$

overlap integral between orbitals

Fock (exchange)

$$= \frac{1}{2}(E_H + E_F)$$

$$E_T = \frac{1}{2}(E_H - E_F)$$

$E_S - E_T = E_F = \underline{\underline{\mathcal{J}}} > 0$ exchange energy

$$\frac{1}{2}\left(\vec{S}^2 - \underbrace{S_1^2 - S_2^2}_{-3/2}\right) \Rightarrow \underline{\text{ferromagnetism}}$$

$$\boxed{H_{eff} = -\mathcal{J}\,\underline{\vec{S}_1 \cdot \vec{S}_2}} \quad (+\ \text{const.}) \quad \begin{cases} \frac{3}{4}\mathcal{J} & \text{singlet} \\ -\frac{1}{4}\mathcal{J} & \text{triplet} \end{cases}$$

for the electronic spins

Heisenberg interaction

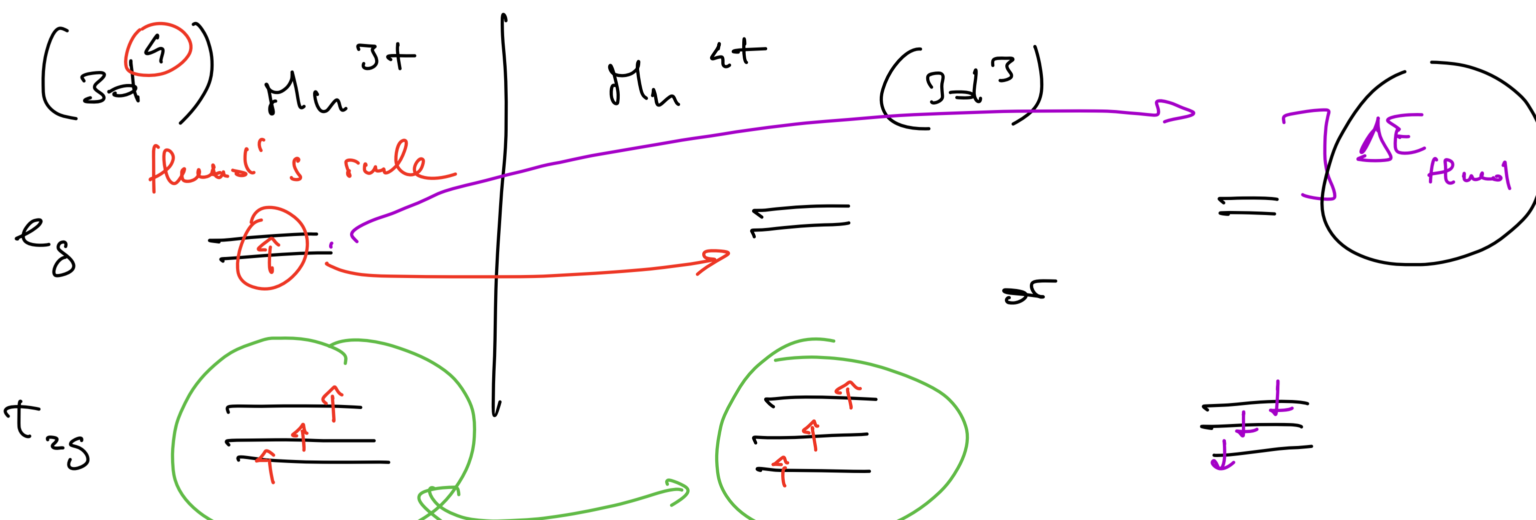
⇒ Hund's rule
(ferromagnetism)

Double exchange

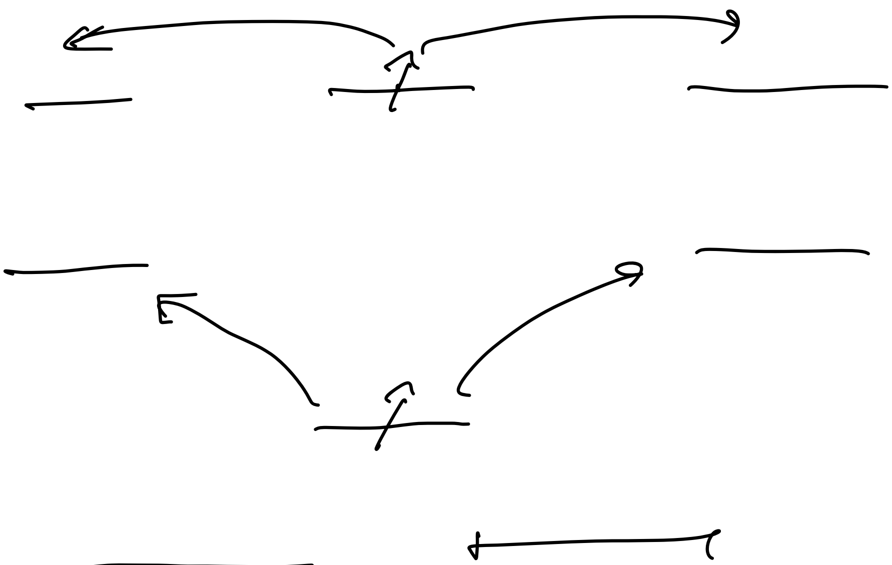
Ex. : $LaMnO_3$ $\quad (La_{1-x}Sr_xMnO_3)$

$x = (0, 1)$

Mn : double valency



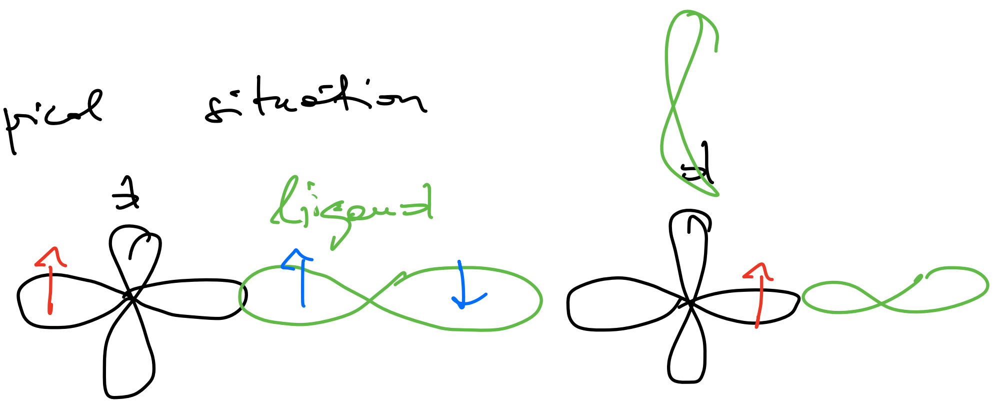
electron's delocalization + Hund's rule



$$\frac{(\Delta p)^2}{2m} \gtrsim \frac{\hbar^2}{2m(\Delta x)^2}$$

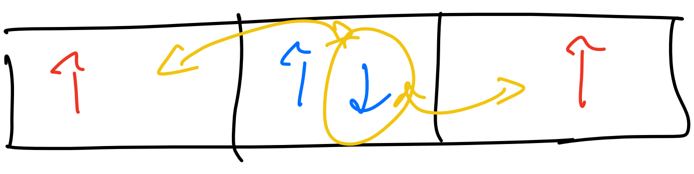
Super-exchange → antiferromagnetism

typical situation

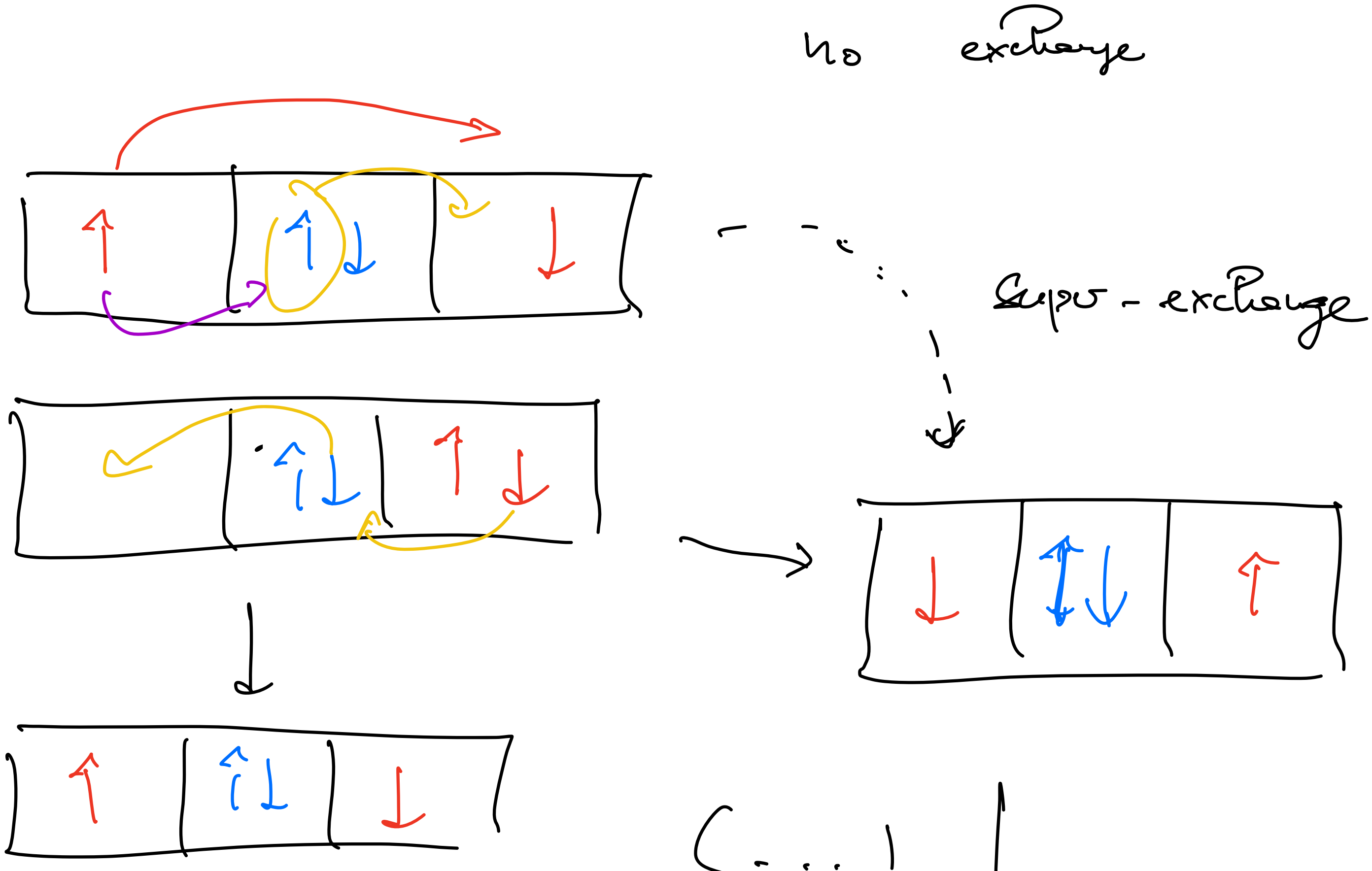


M^{2+} O^{2-} M^{2+}

(Cu^{2+}) (Cu^{2+})



electrons on M^{2+} are "pinned" by Pauli



$$(\ldots)$$

$$H_{eff} = (+)\, J\, \vec{S}_1 \cdot \vec{S}_2 + \text{const.}$$

Heisenberg antiferromagnetic model

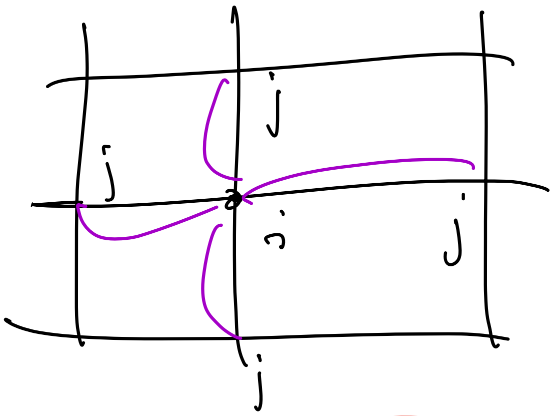
$$\left(S_1^z \; S_2^z \right)$$

Interactions : mean-field approximation

$$\hat{H} = \pm J \sum_{\langle i,j \rangle} \hat{\vec{S}}_i \cdot \hat{\vec{S}}_j$$

$\langle i,j \rangle$: nearest-neighboring sites

rotationally symmetric



spontaneous symmetry breaking (SSB)

Ferromagnetism

$$\hat{H} = - J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$\langle \vec{m} \rangle_{B=0} \neq 0$$

$$\langle \vec{S}_i \rangle_T \neq 0$$

(SSB)

"physical states" can have less symmetry than the Hamiltonian

$$\vec{S}_i = \langle \vec{S}_i \rangle_T + \delta \vec{S}_i$$

$|\delta \vec{S}_i| \ll |\langle \vec{S}_i \rangle|$

small fluctuations

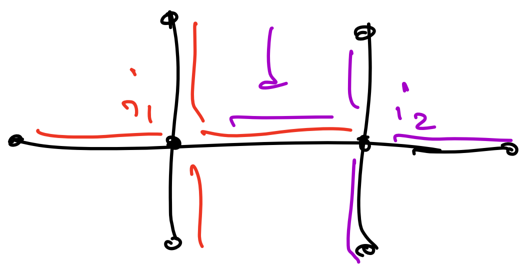
$$\vec{S}_i \cdot \vec{S}_j = \left(\langle \vec{S}_i \rangle + \delta\vec{S}_i\right) \cdot \left(\langle \vec{S}_j \rangle + \delta\vec{S}_j\right)$$

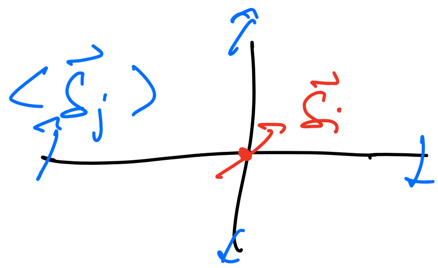
$$= \vec{S}_i \cdot \langle \vec{S}_j \rangle + \langle \vec{S}_i \rangle \cdot \vec{S}_j - \langle \vec{S}_i \rangle \cdot \langle \vec{S}_j \rangle + \delta\vec{S}_i \cdot \delta\vec{S}_j$$

mean-field approx. : $\vec{S}_i$ only interacts with $\langle \vec{S}_i \rangle$

$$\mathcal{H} = -\frac{J}{2} \sum_i \left(\sum_{j \text{ n.n. } i} \vec{S}_j \right) \cdot \vec{S}_i - g\mu_B \sum_i \vec{B} \cdot \vec{S}_i$$

n.n. = nearest neighbor





$$\mathcal{H}_{MF} \simeq -\frac{J}{2} \sum_i \left[\left(\sum_{j \text{ n.n. } i} \langle \vec{S}_j \rangle \right) \cdot \vec{S}_i + \left(\sum_{j \text{ n.n. } i} \vec{S}_j \right) \cdot \langle \vec{S}_i \rangle \right] - g\mu_B \sum_i \vec{B} \cdot \vec{S}_i$$

$$= -g\mu_B \sum_i \vec{B}_{eff}^{(i)} \cdot \vec{S}_i$$

(Weiss molecular field)

mean field

$$\vec{B}_{eff}^{(i)} = \vec{B} + \frac{J \sum_{j \text{ n.n. } i} \langle \vec{S}_j \rangle}{g\mu_B}$$

Ferromagnetism

$$\langle \vec{S}_i \rangle = \sigma \, \vec{e}_z \qquad \vec{B} = B \vec{e}_z$$

$$\vec{B}_{eff} = \left(B + \frac{J \sigma z}{g \mu_B} \right) \vec{e}_z \qquad \sum_{j \, n.n. \, i} \langle \vec{S}_j \rangle = z \sigma \vec{e}_z$$

z = coordination number
= # of nearest neighbors

$$\mathcal{H}_{eff} = - g \mu_B \sum_i B_{eff} \, S_i^z$$

$$\frac{\langle m \rangle}{g \mu_B} = g \mu_B \, \sigma$$

$$= g \mu_B S \, B_S \left(\beta g \mu_B \left(B + \frac{J \sigma z}{g \mu_B} \right) S \right)$$

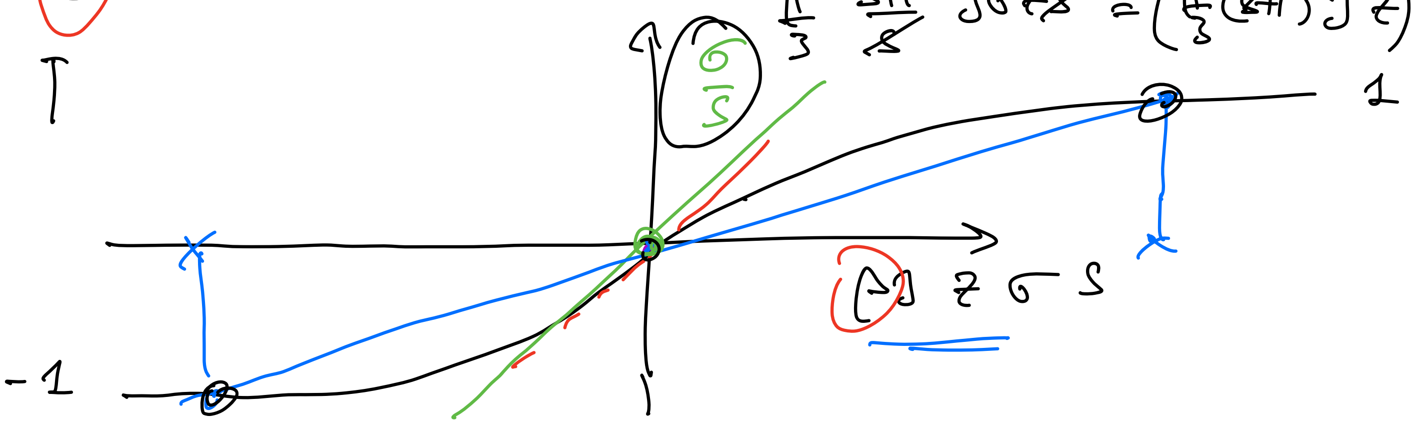
$B = 0$

$$\langle m \rangle = g \mu_B \sigma \neq 0$$

$$\frac{\sigma}{S} = B_S (\beta J \sigma z S)$$

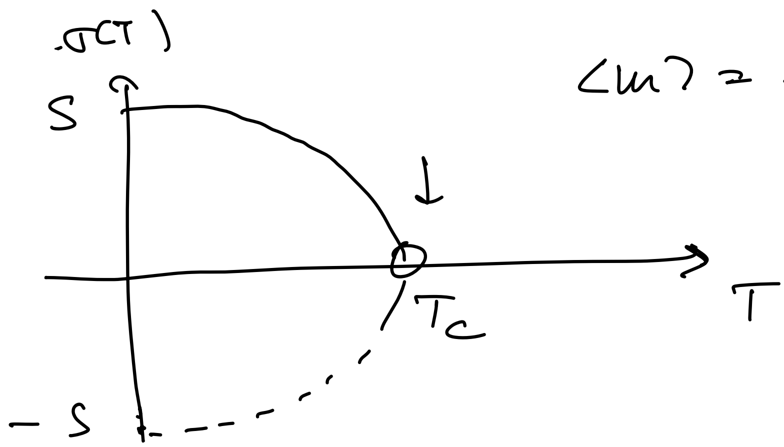
$$\frac{\beta}{3} \frac{S+1}{S} J \sigma z S = \left(\frac{\beta}{3} (S+1) J z \right) \sigma$$

T



$$\frac{\sigma}{S} \le \frac{\beta}{3}(S+1) J z \sigma$$

$$k_B T \le k_B T_c = \frac{J z S (S+1)}{3} \qquad \sigma \neq 0$$



$$\langle m \rangle = g \mu_B \sigma$$

$$T \lesssim T_c$$

$$T \to T_c \qquad \sigma \to 0$$

$$\frac{\sigma}{S} = B_S(\beta J \sigma z S) \underset{\sigma \to 0}{\simeq} \frac{1}{S}\left(\frac{1}{3}\frac{(S+1)S}{S}\beta J \sigma z S\right) - \frac{1}{S}(\tilde{A}S)\sigma^3 + O(\sigma^5)$$

$$\sigma \neq 0 \qquad \sigma^2 = -\frac{1}{\tilde{A} S}\left(1 - \frac{T_c}{T}\right) = \frac{1}{\tilde{A} S}\left(\frac{T_c - T}{T}\right)$$

$$\sigma \overset{T \to T_c}{\sim} (T_c - T)^{\frac{1}{2}} \quad \beta$$

$$\underline{\beta = \frac{1}{2}} \qquad \left(\neq \frac{1}{k_B T}\right)$$

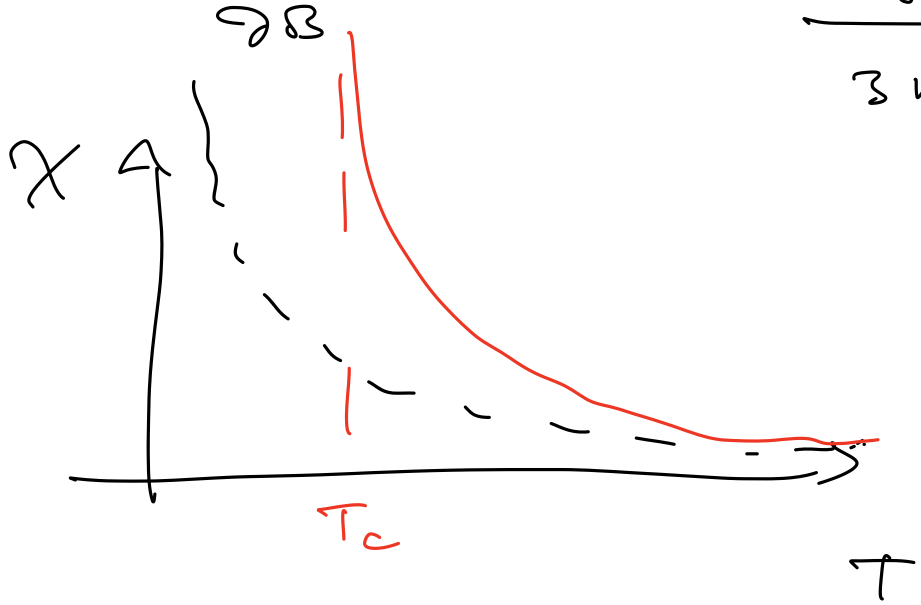
$\underline{\underline{B > 0}}$ $T \geq T_c$

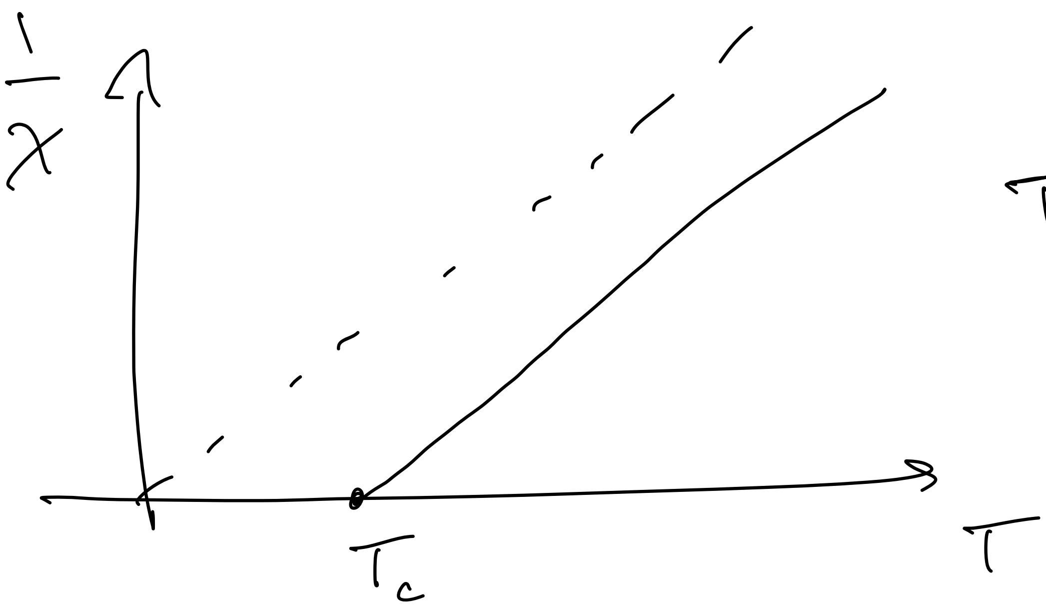
$g\mu_B \sigma = g\mu_B S \, B_S\left(\beta g\mu_B \left(B + \frac{J\sigma z}{g\mu_B}\right) S\right)$

m

$\underset{B \to 0}{\simeq}$ $\underline{(\text{expand})}$

$$\chi = \frac{\partial m}{\partial B} = \ldots = \frac{(g\mu_B)^2 S(S+1)}{3 k_B (T - T_c)}$$





T_c: Curie transition