MAGNETISM : interactions between magnetic moments

Ferromagnetism : double exchange (kinetic energy + Hund's rule)

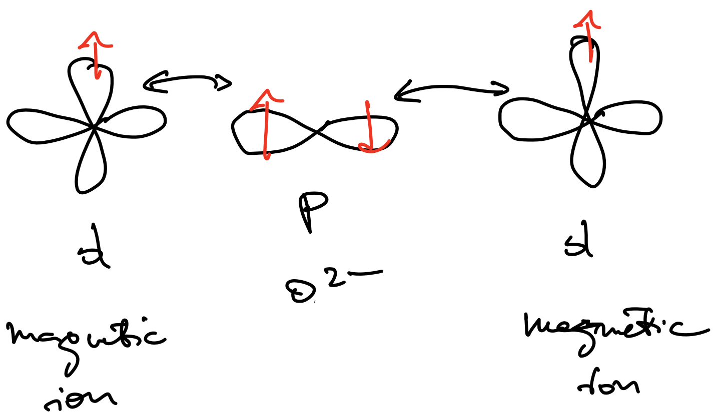
Fe_3O_4

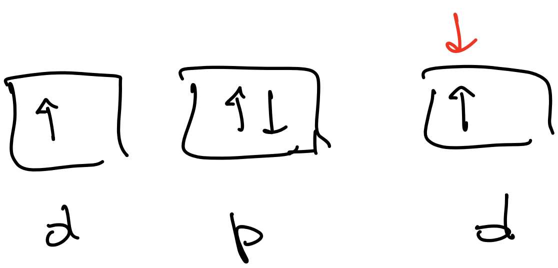
Antiferromagnetism : transition metal oxides

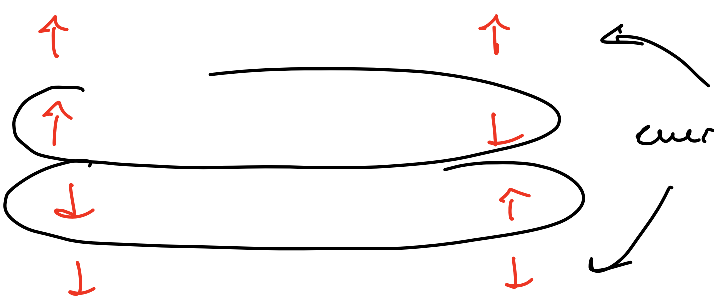
MnO , La_2CuO_4 , ...

magnetic ion

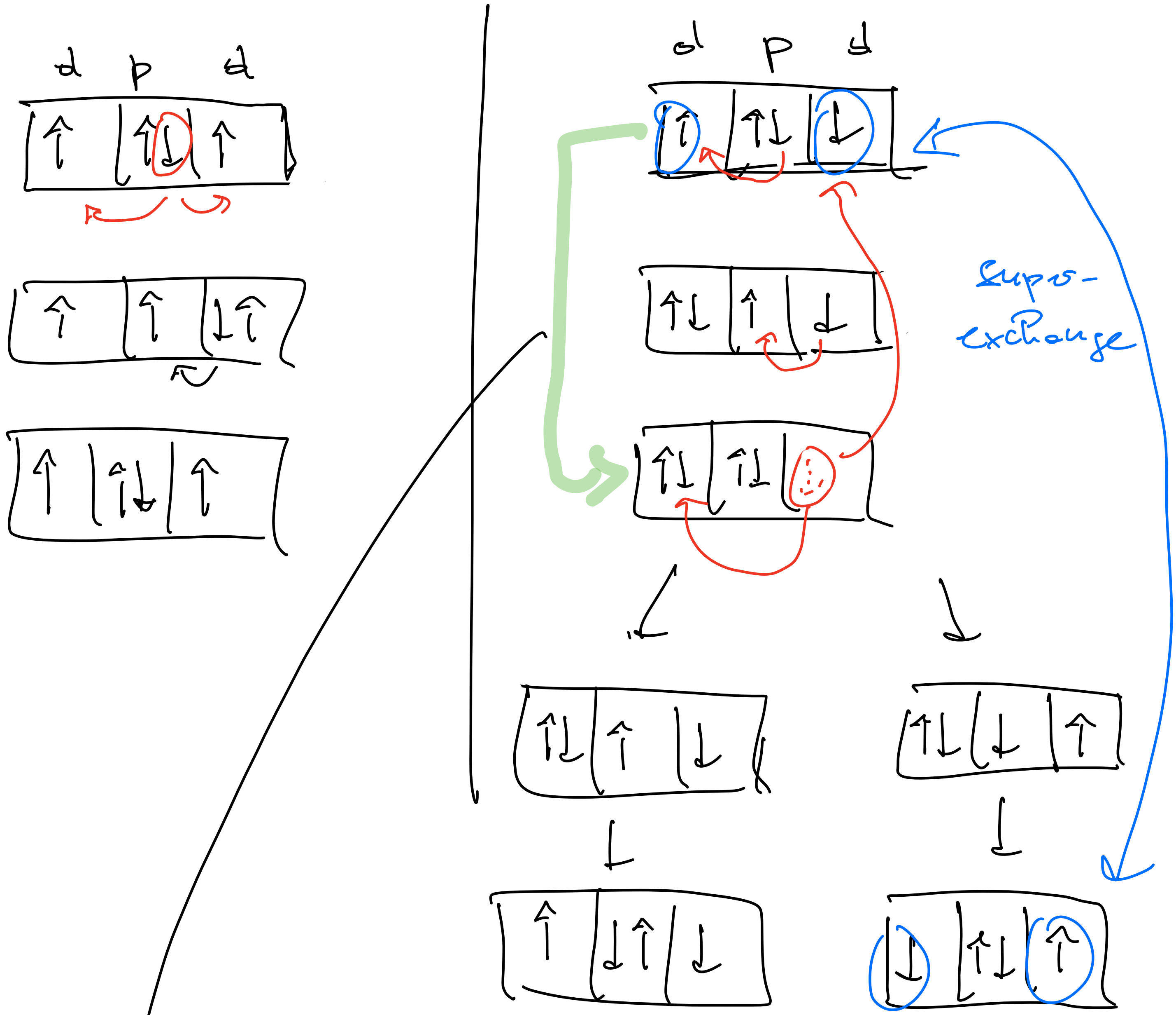
O^{2-}

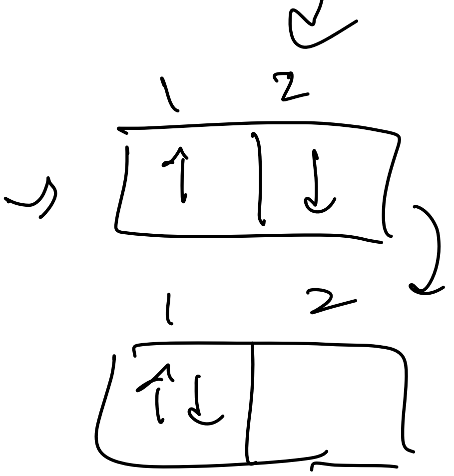






energetically favored





t hopping amplitude

energy cost $U =$

minimal model : Hubbard model [Mott insulator]

$$\mathcal{H} = \mathcal{H}_t + \mathcal{H}_U \qquad \{c_{i\sigma}^{(+)}, c_{j\sigma'}^{(+)}\} = 0$$

$$= -t \sum_{\sigma=\uparrow,\downarrow} \left(c^+_{1\sigma} c_{2\sigma} + c^+_{2\sigma} c_{1\sigma} \right)$$

↳ hopping

$$+ U \left(\underbrace{n_{1\uparrow}}_{c^+_{1\uparrow} c_{1\uparrow}} \underbrace{n_{1\downarrow}}_{c^+_{1\downarrow} c_{1\downarrow}} + n_{2\uparrow} n_{2\downarrow} \right)$$

↳ interaction term

perturbation to $\mathcal{H}_U$

unperturbed ground states of $\mathcal{H}_U$:

degenerate

↑	↓
↓	↑
↑	↑
↓	↓
d(1)	d(2)

$\rightarrow |\psi_{0,j}\rangle$

$j = 1, \dots, 4$

$$\langle \uparrow \downarrow | \mathcal{H}_t | \uparrow \downarrow \rangle \Rightarrow$$

2^{nd}-order degenerate perturbation theory

2^{nd}-order non-degenerate perturbation theory

$|\Psi_0\rangle$ unique unperturbed ground state

$$\Delta E_0^{(2)} = (-) \sum_{n \neq 0} \frac{|\langle \Psi_n | H_t | \Psi_0 \rangle|^2}{E_n - E_0}$$

$$= (-) \langle \Psi_0 | H_t \underbrace{\left(\sum_{n\neq 0} \frac{1}{E_n - E_0} \right)}_{Q \frac{1}{H_0 - E_0} Q} H_t | \Psi_0 \rangle$$

$$Q = \mathbb{1} - |\Psi_0\rangle\langle\Psi_0|$$

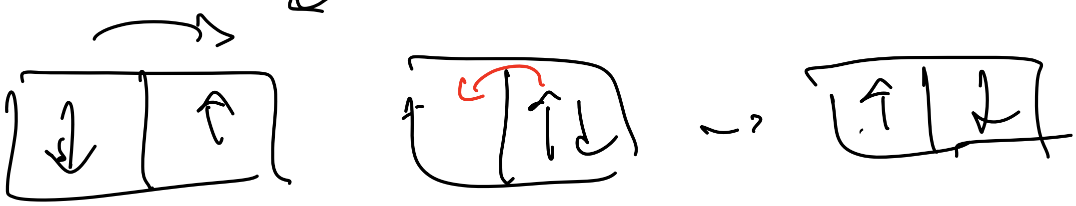
degenerate perturbation theory

$$H_{eff}^{(2)} = - P H_t Q \frac{1}{H_0 - \cancel{E_0}} Q H_t P$$

$$\sum_j |\Psi_{0,j}\rangle\langle\Psi_{0,j}|$$

$$= -\frac{t^2}{U} P \left(c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{1\downarrow} c_{2\downarrow} + h.c.\right)\left(c^\dagger_{1\uparrow} c_{2\uparrow} + c^\dagger_{1\downarrow} c_{2\downarrow} + c^\dagger_{2\uparrow} c_{1\uparrow} + c^\dagger_{2\downarrow} c_{1\downarrow}\right) P$$

$$c^\dagger_{1\uparrow} c_{2\uparrow} c^\dagger_{2\downarrow} c_{1\downarrow}$$



1 2

Spin operators made of fermions

(Abrikosov transformation)

$$S^z_{i} = \frac{1}{2}\left(c^\dagger_{1\uparrow} c_{1\uparrow} - c^\dagger_{1\downarrow} c_{\downarrow}\right)$$

(2) (2) (2) (2) (2)

$$\begin{cases} S_1^+ = c_{1\uparrow}^+ \, c_{1\downarrow} & S_1^- = c_{1\downarrow}^+ \, c_{1\uparrow} \\ (2) \quad (2) \quad (2) & (2) \quad (2) \quad (2) \end{cases}$$

$$n_1 = n_{1\uparrow} + n_{1\downarrow}$$

$$\mathcal{H}_{eff}^{(2)} = \underbrace{\frac{4t^2}{U}}_{-J} P \left[\vec{S}_1 \cdot \vec{S}_2 + \underbrace{\frac{1}{4} n_1 n_2 + \frac{N}{4}}_{\text{const}} \right] P$$

$$J = -\frac{4t^2}{U} < 0$$

$S = 1/2$

$$\mathcal{H} = \underbrace{-J \, \vec{S}_1 \cdot \vec{S}_2}_{\text{Heisenberg interaction}} + \text{const.}$$

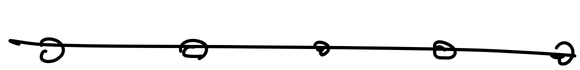
Heisenberg model for N spins

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

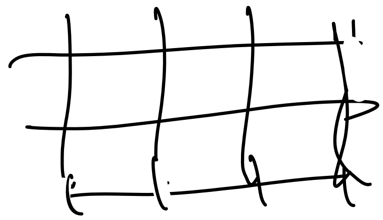
d

nearest neighbors on a lattice

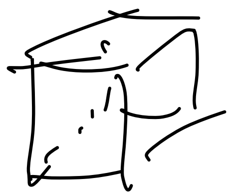
hypercubic lattice



$d=1$



$d=2$



$d=3$

→ emergence of magnetic long-range order

transition

Assumption of spontaneous symmetry breaking (SSB)

static net magnetic moment

$$\boxed{\langle \vec{S}_i \rangle \neq 0}$$

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$\hat{\vec{S}}_i = \langle \vec{S}_i \rangle + \delta \hat{\vec{S}}_i$$

$$\langle \delta \vec{S}_i \rangle = 0$$

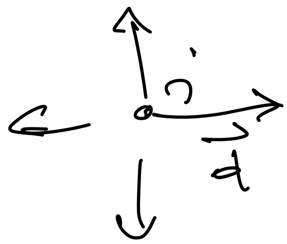
<u>Mean-field approximation</u>

$$\sqrt{\langle (\delta \hat{\vec{S}}_i)^2 \rangle} \ll |\langle \vec{S}_i \rangle|$$

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

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

$$\mathcal{H} = -\frac{J}{2} \sum_i \sum_{\vec{d}} \vec{S}_i \cdot \vec{S}_{i+\vec{d}}$$



$$\mathcal{H} \simeq -\frac{J}{\cancel{2}} \sum_i \sum_{\vec d} \left(\cancel{\langle \vec S_i \rangle \cdot \vec S_{i+d}} + \langle \vec S_{i+d} \rangle \cdot \vec S_i \right)$$

$$+ \text{const}$$

$$= -J \sum_i \Big(\underbrace{\sum_{\vec d} \langle \vec S_{i+d} \rangle}_{\frac{g\mu_B B_{\text{eff}}}{J}} \Big) \cdot \vec S_i + \text{const}$$

Ferromagnetism $(J>0)$

$\tilde m$

$$\langle \vec S_i \rangle = \text{uniform} = \frac{m}{g\mu_B} \vec e_z$$

$$\mathcal{H} \simeq -J \sum_i \Big(\underbrace{\sum_{\vec d} \tilde m}_{z\tilde m} \Big) S_i^z + C$$

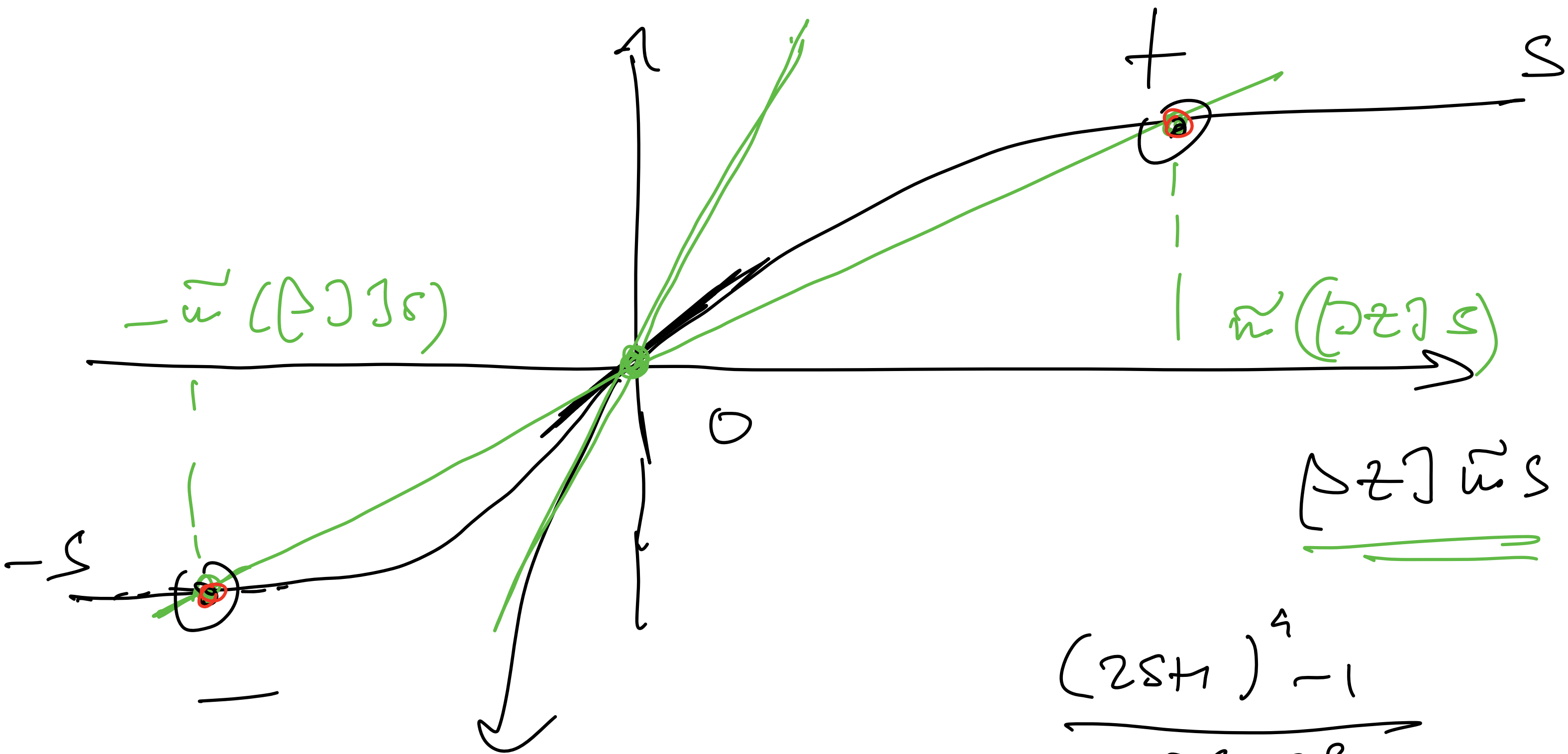
z = coordination number

$$= - \underbrace{J z \tilde{m}}_{g\mu_B B_{eff}(\tilde{m})} \sum_i S_i^z + C$$

$$\overset{\frac{1}{k_B T}}{\beta}\, g\mu_B B S$$

$$\langle S_i^z \rangle = \tilde{m} = S\, B_S(\beta J z \tilde{m} S)$$

$$\tilde{m}(T)$$



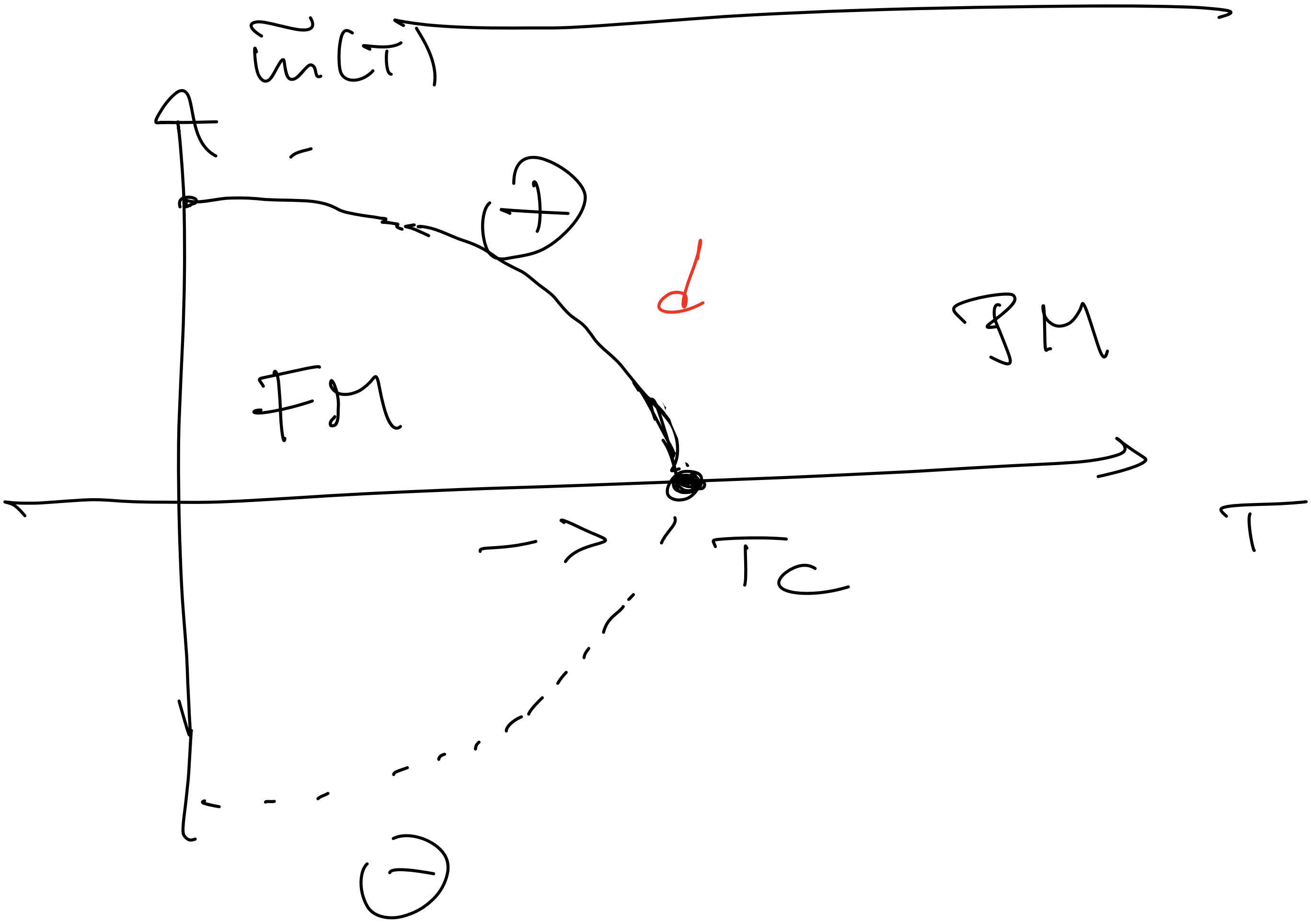
$$A = \frac{(2S+1)^4 - 1}{360 S^3}$$

$$B_S(y) \underset{y\simeq 0}{=} \frac{S+1}{3S}\, y - A y^3 + \dots$$

$$\frac{\cancel{\tilde{m}}}{\cancel{s}} < \frac{s+1}{3\cancel{s}}\Big(\underbrace{\beta}_{\frac{1}{k_B T}} J z\, \cancel{\tilde{m}}\, s\Big)$$

intersection at $\tilde{m} \neq 0$

$$k_B T < \frac{s(s+1)Jz}{3} = k_B T_c$$



Critical behavior

$T \to T_c^-$ $\quad\quad$ $\tilde{m} \to 0$

$T \sim T_c$

$$\frac{\tilde{m}}{S} = \frac{S+1}{3\cancel{S}}\left(\beta J z \tilde{m} \cancel{S}\right) - A\left(\beta J z \tilde{m} S\right)^3$$

$$\cancel{\tilde{m}} = \frac{S(S+1)\beta J z}{3}\cancel{\tilde{m}} - \underbrace{A(\beta J z S)^3}_{a^{-1}}\tilde{m}^{\cancel{3}\,2}$$

$$\frac{T_c}{T}$$

$$\tilde{m}^2 = a\left(\frac{T_c}{T} - 1\right)$$

$$\tilde{m} = \pm\sqrt{a\left(\frac{T_c - T}{T}\right)}$$

$$\sim (T_c - T)^{1/2} \to \beta$$

$T > T_c$ $\qquad \tilde{m} = 0$

unless I apply a field

$$\mathcal{H} \to \mathcal{H} - g\mu_B B \sum_i S_i^z$$

$$\frac{\tilde{m}}{S} = B_S\left(\beta \underbrace{\left(zJ\tilde{m} + g\mu_B B\right)}_{B_{\text{eff}}} S\right)$$

$$\underset{\substack{\tilde{m}\to 0\\ B\to 0}}{\simeq} \frac{(S+1)}{3S}\,\beta\left(zJ\tilde{m} + g\mu_B B\right) S$$

$$\frac{\partial \tilde{m}}{\partial B} = \chi = g\mu_B S\,\frac{(S+1)}{3\cancel{S}}\,\beta \left(zJ\frac{\chi}{g\mu_B} + g\mu_B\right)\cancel{S}$$

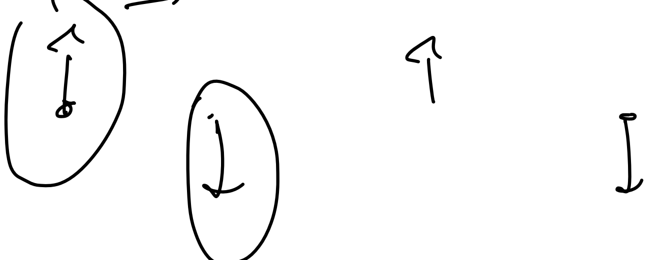
$$\chi = \frac{(g\mu_B)^2 \, S(S+1)}{3 k_B (T - T_c)}$$

Curie-Weiss

T_c FM

Antiferromagnetism

$\tilde{m}\,\vec{e}_z = \langle \vec{S}_i \rangle$



$J < 0$ $\rightarrow \langle \vec{S}_{i+1} \rangle = -\tilde{m}\,\vec{e}_z$

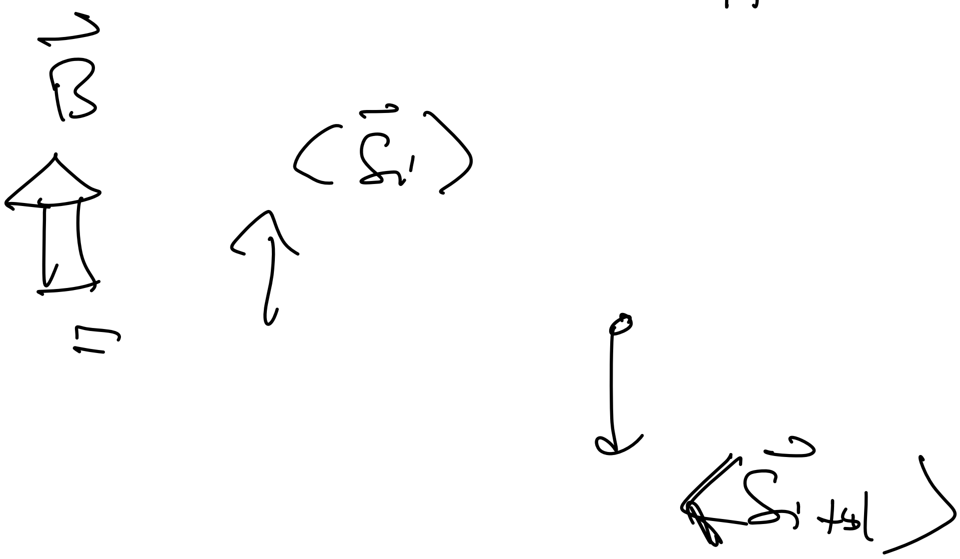
$$B_{eff} = J z (-\bar{m}) = |J| z \bar{m}$$

$$\frac{\bar{m}}{S} = B_S\left(\beta z |J| \bar{m} S\right)$$

$$\beta g \mu_B B_{eff} S$$

same critical behavior of the magnetization $\bar{m}$.

uniform field induces a magnetization on $\langle \vec{S}_{i+d} \rangle$ opposed to the spontaneous one



$T < T_c$

$T > T_c \rightarrow T_N \rightarrow$ Niel Temperature

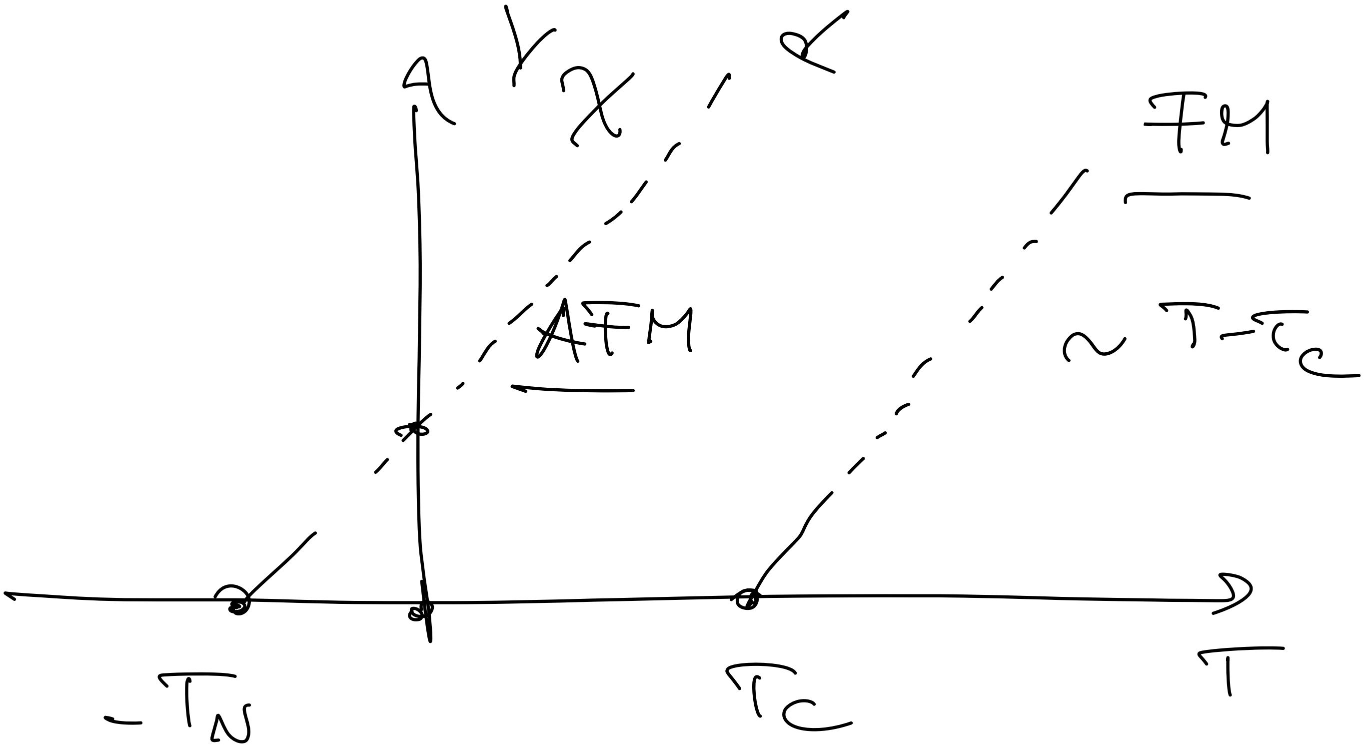
$\langle \tilde{S}_i \rangle \quad \langle \vec{S}_{tot} \rangle$

$$g \mu_B B_{tot} = g \mu_B B + J z \tilde{m}$$

$$= B - |J| z \tilde{m}$$

$$\frac{\tilde{m}}{S} = B_S (\beta g \mu_B B_{tot} S)$$

$$\chi = \frac{(g \mu_B)^2 S(S+1)}{k_B (T + T_N)}$$



$1/\chi$
α
AFM
FM
$\sim T - T_c$
$-T_N$
T_c
T