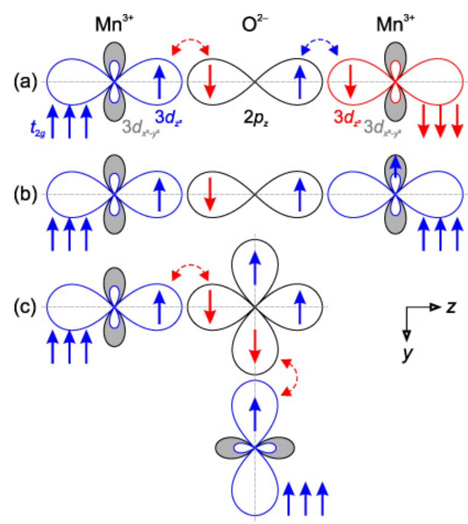
Exchange

- Last time we derived Heisenberg AF exchange from Hubbard model
  - AF sign can be understood as lowering of electron kinetic energy by zero point fluctuations, which are “blocked” for triplet states
  - SU(2) symmetry is due to neglect of SOC

Other exchanges

- Super-exchange: exchange due to electrons hopping through an intermediate orbital



usually antiferromagnetic

this can be ferromagnetic

With orbital degeneracy and complex structures, exchange can be pretty non-trivial

Exchange

- Typical exchange types

symmetric traceless

$$H_{ij} = J\vec{S}_i \cdot \vec{S}_j + \vec{D} \cdot \vec{S}_i \times \vec{S}_j + \vec{S}_i \underline{\underline{\Gamma}} \vec{S}_j$$

Dzyaloshinskii-Moriya (DM)

(symmetric) exchange anisotropy

- e.g. Ising $H_{ij} = JS_i^z S_j^z$
- XXZ $H_{ij} = J_x(S_i^x S_j^x + S_i^y S_j^y) + J_z S_i^z S_j^z$
- Fancier: biquadratic $H_{ij} = K(\vec{S}_i \cdot \vec{S}_j)^2$

Magnetic order

- In a crystal with a periodic lattice of spins, exchange interactions typically induce an *ordered* state at low temperature
- For example, the ferromagnetic Heisenberg model:

$$H = -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \qquad J > 0$$

- Wants every spin parallel to its neighbor, so they choose a global axis

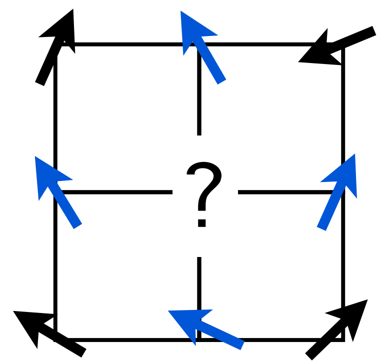
$$\langle \mathbf{S}_i \rangle = \mathbf{m}$$

Mean field theory

- When kT$\gtrsim$ J, spins will fluctuate thermally, and **m** will be reduced.
- We can study this with *mean field theory*

$$
\begin{aligned}
H &= -J \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \\
&\to -J \sum_{\langle ij \rangle} \left[\langle \mathbf{S}_i \rangle \cdot \mathbf{S}_j + \mathbf{S}_i \cdot \langle \mathbf{S}_j \rangle - \langle \mathbf{S}_i \rangle \cdot \langle \mathbf{S}_j \rangle \right] \\
&= -zJ \sum_i \mathbf{m} \cdot \mathbf{S}_i + \text{const.}
\end{aligned}
$$

Mean field theory



$$g\mu_B\mathbf{H}_{\text{eff}} = J\langle \nwarrow + \nearrow + \nwarrow + \nwarrow \rangle$$

- This reduces the problem to independent spins in an *effective* "exchange field"
- Note: this exchange field can be a thousand times larger than physical laboratory fields!

Mean field theory

- Define h = z J m (= g μ_B H_{eff})
- Then we know for a single spin

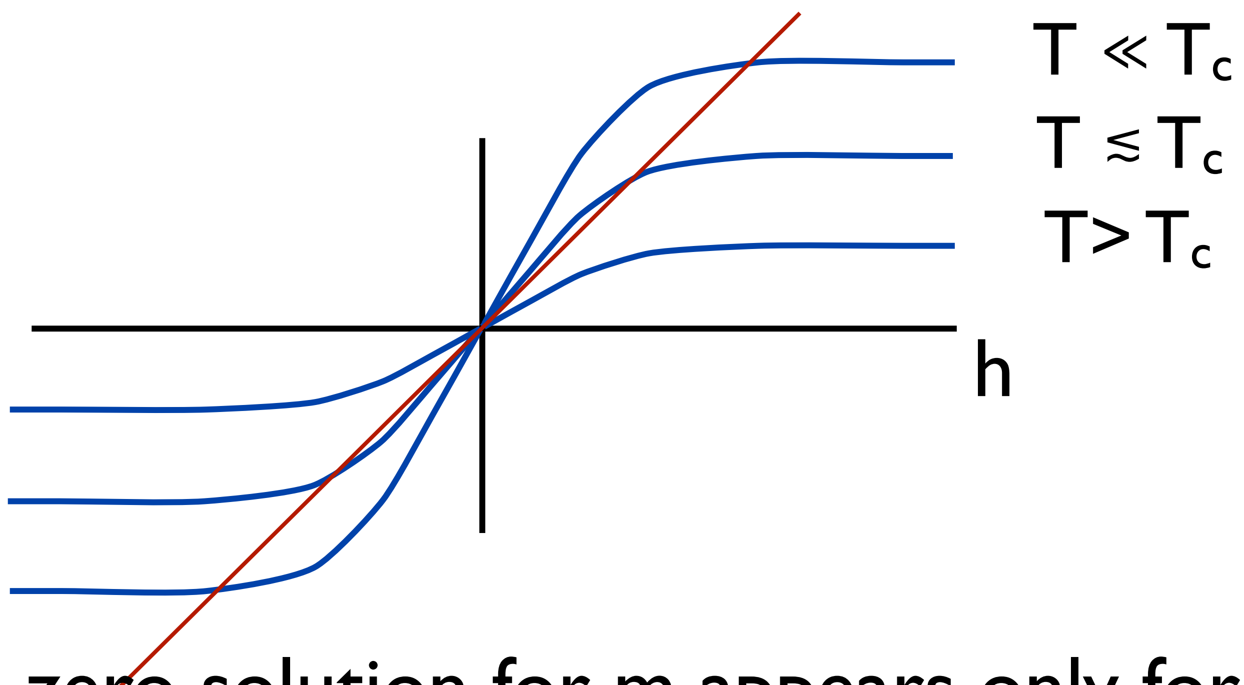
$$|\langle \mathbf{S}_i \rangle| = m = SB_S(\beta h S)$$

$$\Rightarrow \quad m = SB_S(\beta z J S m)$$

- For example for S=1/2

$$m = \frac{1}{2} \tanh\left[\frac{zJm}{2kT}\right]$$

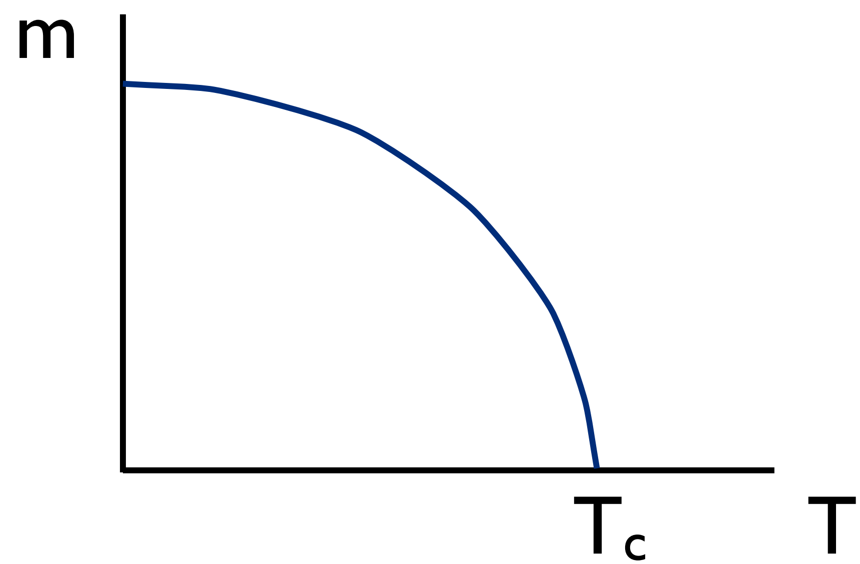
Mean field theory



- Non-zero solution for m appears only for $T<T_c$
- equality of slopes implies $kT_c = z\,J/4$ $\left(= \frac{zJS(S+1)}{3}\right)$

Mean field theory

- *Zero field* magnetization:



- T_c is called the "Curie point" or critical temperature

Susceptibility

- We may guess that the susceptibility gets large on approaching the Curie point, since the material almost forms a magnetization with no field at all.
- This is indeed true.
- Within MFT, just shift $h \to h + g\,\mu_B\,H$

Susceptibility

$$m = \frac{1}{2}\tanh\left[\frac{zJm + g\mu_B H}{2kT}\right] \approx \frac{zJm + g\mu_B H}{4kT}$$

$$M/N = g\mu_B m \approx \frac{g\mu_B}{1 - \frac{zJ}{4kT}} \frac{g\mu_B H}{4kT} = \frac{(g\mu_B)^2 H}{4kT - zJ}$$

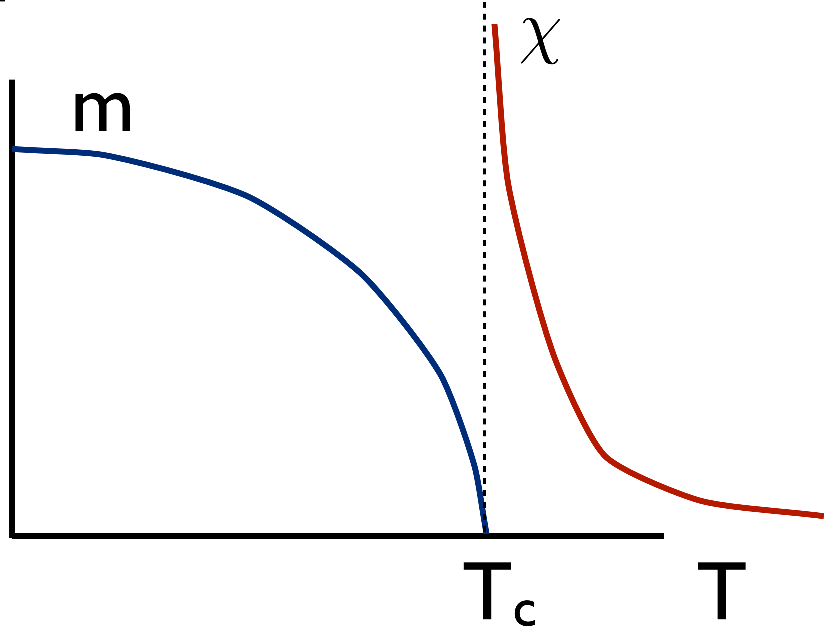
$$\chi = \frac{1}{N}\frac{\partial M}{\partial H} = \frac{A}{T - T_c}$$

"Curie-Weiss law"

Curie law is modified by shift of T by mean field T_c

Phase transition

- A lot happens at T_c



- Both m(T) and χ(T) are *non-analytic* at T_c
- This is actually a sign of a *phase transition*