

Physics 560A

Lecture 15

The Heisenberg model of

(anti)ferromagnetism

$$H = J \sum_{n.n.} \vec{S}_i \cdot \vec{S}_j$$

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

superexchange

↳ antiferromagnetism

$$J \sim -U < 0$$

exchange

↳ ferromagnetism

mean field theory (spin S) (2)

$$H_i = J \sum_{j=n.n.} \vec{S}_i \cdot \vec{S}_j - g\mu_B \vec{B} \cdot \vec{S}_i$$

$$\vec{B}_{\text{eff}} = \vec{B} - \frac{J}{g\mu_B} \sum_{j=n.n.} \langle \vec{S}_j \rangle$$

$$= \vec{B} - \frac{zJ}{g\mu_B} \langle \vec{S}_{n.n.} \rangle$$

Energy levels of atom i :

$$E_m = -g\mu_B B_{\text{eff}} m, \quad (\hbar = 1)$$

$$m = -S, -S+1, \dots, S$$

$$Z_i = \sum_{m=-S}^S e^{-\beta E_m}$$

$$Z_i = \sum_{m=-S}^S \left(e^{\beta g \mu_B B_{\text{eff}}} \right)^m \quad \boxed{3}$$

$$= \frac{\sinh \left[\left(S + \frac{1}{2} \right) \beta g \mu_B B_{\text{eff}} \right]}{\sinh \left(\frac{\beta g \mu_B B_{\text{eff}}}{2} \right)}$$

$$\langle S_{iz} \rangle = \hbar \langle m \rangle$$

$$\langle \mu_{iz} \rangle = g \mu_B \langle S_{iz} \rangle = \frac{1}{\beta} \frac{\partial \ln Z_i}{\partial B_{\text{eff}}}$$

$$= g \mu_B \left[\frac{\left(S + \frac{1}{2} \right) \cosh \left(S + \frac{1}{2} \right) \eta}{\sinh \left(S + \frac{1}{2} \right) \eta} - \frac{\frac{1}{2} \cosh \frac{\eta}{2}}{\sinh \frac{\eta}{2}} \right]$$

$$\eta = \beta g \mu_B B_{\text{eff}}$$

$$\text{or } \langle \mu_{iz} \rangle = g \mu_B S B_S(\eta)$$

$$B_S(\eta) \equiv \frac{1}{S} \left[\left(S + \frac{1}{2}\right) \coth \left(S + \frac{1}{2}\right) \eta - \frac{1}{2} \coth \left(\frac{\eta}{2}\right) \right] \quad (4)$$

$$\langle S_{iz} \rangle = S B_S(\eta)$$

$$\eta = \beta g \mu_B B_z - z \beta J \langle S_z \rangle_{n-n.}$$

By symmetry, we expect

$$\langle S_{iz} \rangle = \begin{cases} - \langle S_z \rangle_{n-n.} & \text{for } J > 0 \\ + \langle S_z \rangle_{n-n.} & \text{for } J < 0 \end{cases}$$

$$\text{So } \mu = \beta g \mu_B B + \beta z |J| \langle S_{iz} \rangle \quad (5)$$

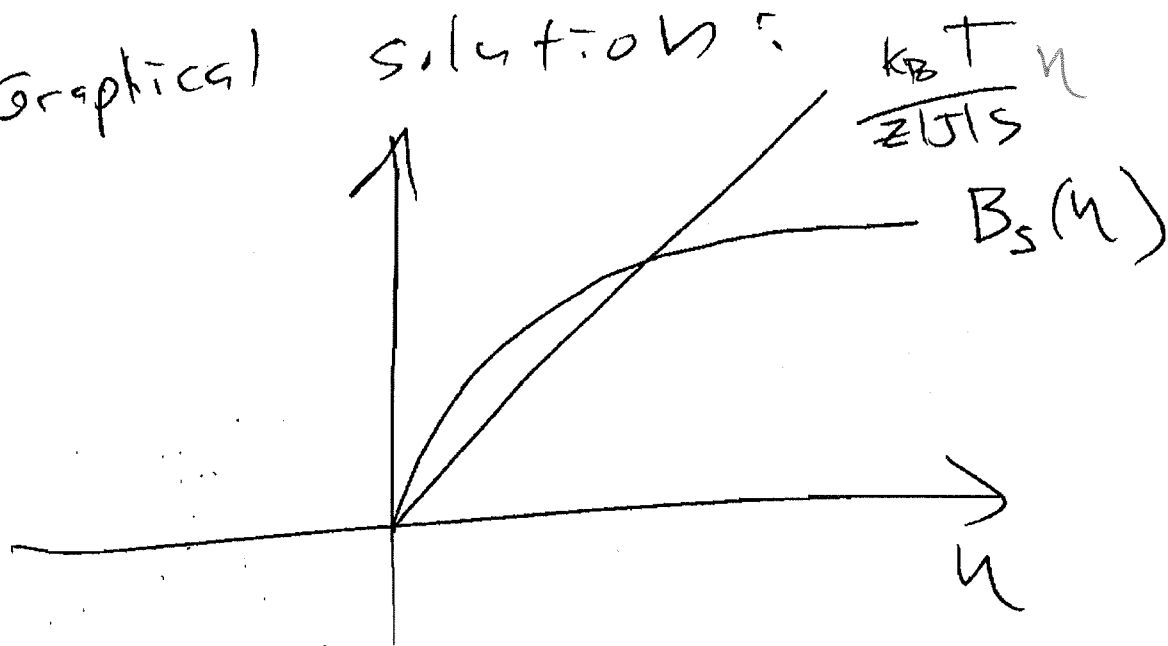
$$B_S(\mu) = \frac{k_B T}{z |J| S} \left(\mu - \frac{g \mu_B B}{k_B T} \right)$$

\Rightarrow must be solved self-consistently

For $B_{\text{ext}} = 0$, we have

$$B_S(\mu) = \frac{k_B T}{z |J| S} \mu$$

Graphical solution:



Solution w/ $\langle S_{iz} \rangle \neq 0$ exists if (6)

$$\left. \frac{dB_S}{d\mu} \right|_{\mu=0} > \frac{k_B T}{z |J| S}$$

For $\mu \ll 1$,

$$B_S(\mu) \approx \frac{1}{3}(S+1)\mu$$

$$\frac{1}{3}(S+1) > \frac{k_B T}{z |J| S}$$

or $T < T_c$, where

$$k_B T_c = \frac{z |J| S(S+1)}{3}$$

"Curie temperature"

Cases :

Antiferromagnet

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3D : MF OK

2D : AF exists
only at $T=0$

1D : AF does not
exist, even
at $T=0$

Ferrimagnet

3D : MF OK

2D : ?

1D : FM exists at $T=0$,
destroyed for $T > 0$