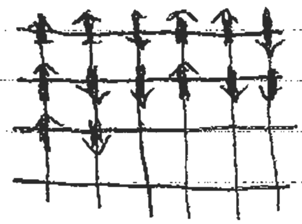
III. Ising model.

Phase Transition and Ginzburg-Landau theory

① Ising model:



s_i : +1 −1 +1 +1 −1

spin configuration $\{s_i\} = \{s_1\ s_2 \cdots\} = \{+1, -1, \cdots\}$

$$E(\{s_i\}) = -J \sum_{\langle ij \rangle} s_i s_j - h \sum_i s_i$$

Ground states: $(h=0)$

$J>0$ $\quad \uparrow\uparrow\uparrow\uparrow$ $\quad$ Ferromagnetic

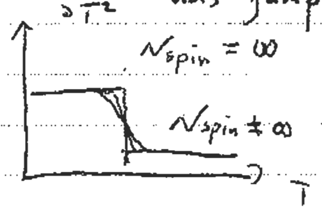
$J<0$ $\quad \uparrow\downarrow\uparrow\downarrow$ $\quad$ Antiferromagnetic

Finite temperature:

$$Z = \sum_{\{s_i\}} e^{-\beta E(\{s_i\})}$$

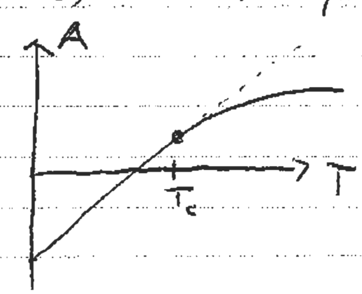
$$A = -k_B T \ln Z$$

$\frac{\partial^2 A}{\partial T^2}$ has jump



Phase transition

$(h=0)$ $\quad (2D,\ N_{spin} \to \infty)$



② Mean-field theory

$$\langle s_i\rangle s_j + s_i\langle s_j\rangle - \langle s_i\rangle\langle s_j\rangle$$
$$= \langle s_i\rangle\langle s_j\rangle \simeq \langle s_i s_j\rangle$$

$$E = -J\sum_{\langle ij\rangle} s_i s_j - h\sum_i s_i$$

↑ sum over different pairs

$$\simeq -J\sum_{\langle ij\rangle}\left(\langle s_i\rangle s_j + s_i\langle s_j\rangle - \langle s_i\rangle\langle s_j\rangle\right) - h\sum_i s_i$$

$\langle s_i\rangle = \langle s\rangle$ (do not depend on i)

$$= -zJ\sum_i\langle s\rangle s_i - h\sum s_i + J\langle s\rangle^2\,\frac{1}{2}zN_{spin}$$

$$= -(\overbrace{h + zJ\langle s\rangle}^{h_{eff}})\sum_i s_i + \frac{1}{2}zN_{spin}J\langle s\rangle^2$$

$= E_{mean}$ ← coordination number. $z=2$, $z=4$

$$Z = \sum_{\{s\}} e^{-\beta E} \simeq \sum_{\{s\}} e^{-\beta E_{mean}}$$

$$= \left(e^{-\beta h_{eff}} + e^{\beta h_{eff}}\right)^{N_{spin}} e^{-\frac{1}{2}\beta z N_{spin} J\langle s\rangle^2}$$

$$\boxed{A = \left[-k_BT\ln\left(e^{-\beta h_{eff}} + e^{\beta h_{eff}}\right) + \frac{1}{2}zJ\langle s\rangle^2\right]N_{spin} \qquad h_{eff} = zJ\langle s\rangle + h}$$

But what is $\langle s\rangle$

calculate $\langle s\rangle$ using $E_{mean} = -h_{eff}\sum_i s_i + \frac{z}{2}N_{spin}J\langle s\rangle^2$

Independent spin system within meanfield approximation

$$\langle s\rangle = \frac{e^{+\beta h_{eff}} - e^{-\beta h_{eff}}}{e^{\beta h_{eff}} + e^{-\beta h_{eff}}} = \tanh(\beta h_{eff})$$

$$\boxed{\langle S\rangle = \tanh\left[(h + zJ\langle s\rangle)\beta\right]}$$ self consistant equation

solve self consistant equation for $\langle s\rangle = f(T, h)$

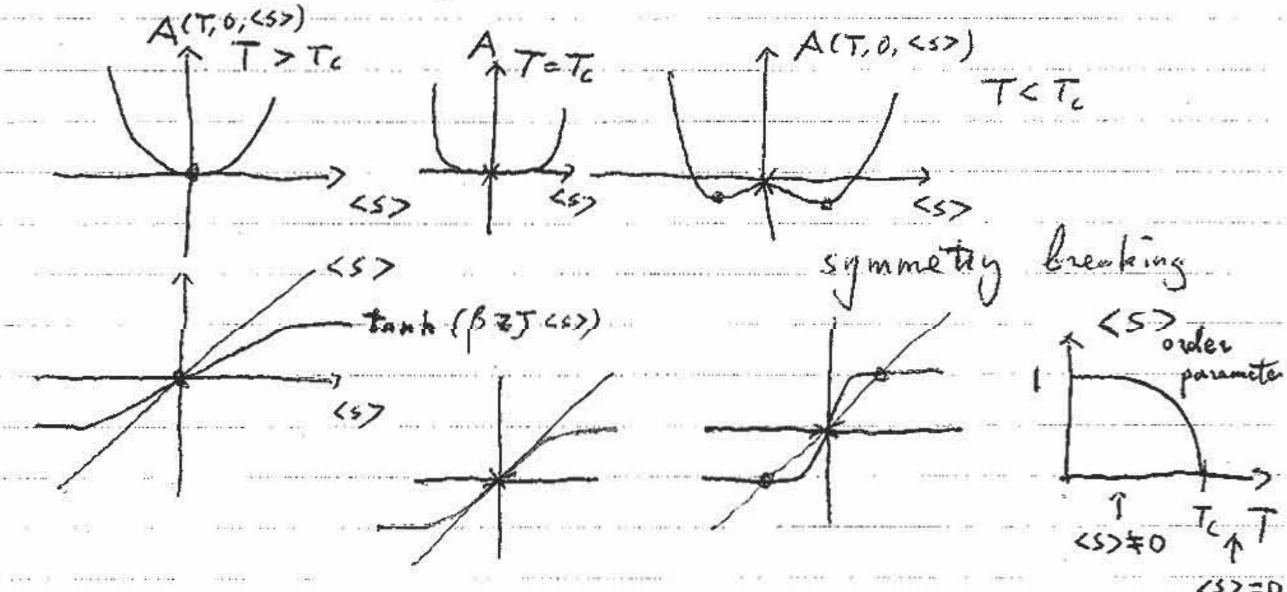
then $A(T, h, \langle s\rangle) \rightarrow A(T, h, f(T,h))$
meanfield free energy.

Second way: minimize $A(T, h, \langle s\rangle)$ resp. to $\langle s\rangle$

$$\frac{\partial A}{\partial\langle s\rangle} = -\frac{e^{\beta h_{eff}} - e^{-\beta h_{eff}}}{e^{\beta h_{eff}} - e^{-\beta h_{eff}}} zJ + zJ\langle s\rangle = 0$$

$$\Rightarrow \boxed{\langle s\rangle = \tanh(\beta h_{eff})}$$ same as the self consistent equation.

Phase transition: for $h = 0$



For small $\langle s\rangle$ $\tanh(\beta zJ\langle s\rangle) \simeq \beta zJ\langle s\rangle$

at T_c $\beta zJ = 1$ $\Rightarrow$ $\boxed{T_c = \frac{zJ}{k_B}}$

(3) Ginzburg - Landau Theory

Near the Transition, order parameter $\langle s \rangle$ is small

Expand $A(T, h=0, \langle s \rangle)$ $\quad A_0(T) = -k_B T \ln 2 \, N_{spin}$

$$\boxed{A = \frac{N_{spin}}{2} a \langle s \rangle^2 + \frac{N_{spin}}{4} b \langle s \rangle^4 + A_0(T)} \qquad \boxed{\begin{array}{l} \dfrac{\partial A}{\partial \langle s \rangle} = 0 \\ \ni a \langle s \rangle + b \langle s \rangle^3 = 0 \end{array}}$$

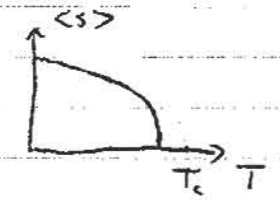
a, b function of T.

At Transition $\quad a(T_c) = 0 \qquad b(T_c) > 0$.

We may write $\quad a = a_0\left(\frac{T}{T_c} - 1\right) \qquad a_0 > 0$

$$\langle s \rangle = \begin{cases} 0, & T > T_c \\ \underline{\pm\sqrt{\frac{a_0}{b}}\sqrt{1 - \frac{T}{T_c}}}, & T < T_c \end{cases}$$

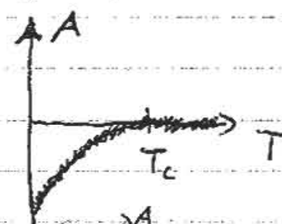
$\pm\sqrt{\frac{-a}{b}}$



Let $\quad t \equiv \left(1 - \frac{T}{T_c}\right)$

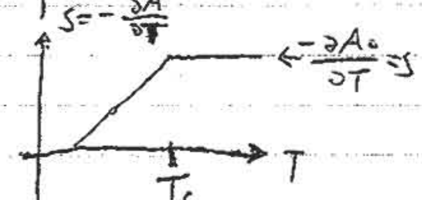
$\langle s \rangle \propto (t)^{\beta} \qquad \beta = 1/2 \quad$ (order parameter / magnetization)

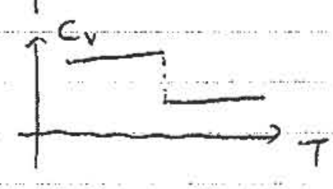
$$A = \begin{cases} A_0(T), & T > T_c \\ -\frac{N_{spin}}{4}\frac{a_0^2 t^2}{b} + A_0(T) & T < T_c \end{cases}$$



$$C_V = -\left(\frac{\partial^2 A}{\partial T^2}\right) T \propto |t|^{-\alpha} \qquad \alpha = 0$$

$$= T \frac{\partial S}{\partial T}$$





$h \neq 0$ case.

$$A = A_0(T) + \frac{N_{spin}}{2} a \langle s \rangle^2 + \frac{N_{spin}}{4} b \langle s \rangle^4 \overbrace{- N_{spin} \langle s \rangle h}^{-\sum_i s_i h}$$

Free energy as $A(T, N_{spin}, h) = A_{min}$

☆ $T > T_c$ $(a > 0)$ & small h.

$$A \simeq A_0 + \frac{N_{spin}}{2} a \langle s \rangle^2 - N_{spin} h \langle s \rangle \qquad \frac{\partial A}{\partial \langle s \rangle} = \cancel{N_{spin}} a \langle s \rangle - N_{spin} h = 0$$

$$\boxed{A_{min} = -\frac{1}{2} \frac{h^2}{a} N_{spin} + O(h^4)}$$

Magnetization

$$M = -\frac{\partial A(T, N_{spin}, h)}{\partial h} = -\frac{\partial A_{min}}{\partial h} = \sum_i s_i$$

$$= + \frac{N_{spin}}{a} h$$

magnetic susceptibility

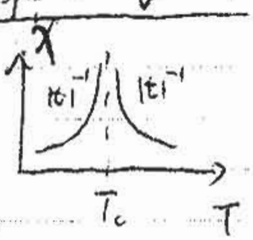
$$\chi = \frac{1}{V} \frac{\partial M}{\partial h} = + \frac{N_{spin}}{a V}$$

quick way to get χ:

$$A = \frac{1}{2} N_{spin} a \langle s \rangle^2 - h N_{spin} \langle s \rangle$$

$$\frac{N_{spin}^2}{N_{spin} a} \frac{1}{V} = \chi$$

as $T \to T_c$ $\boxed{\chi \propto t^{-\gamma} \quad \gamma = 1}$



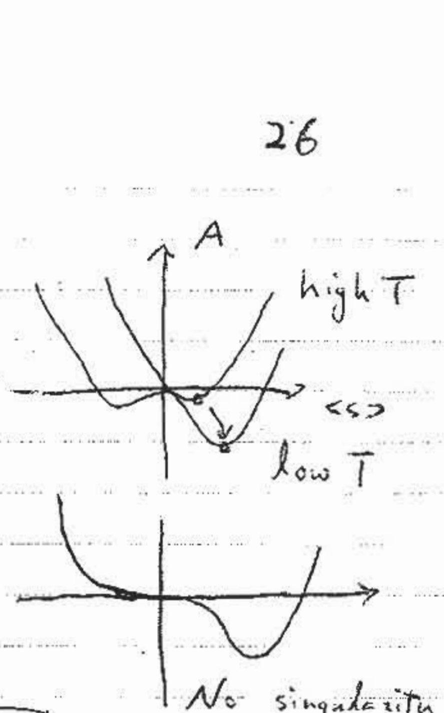
☆ $T < T_c$

$\langle s \rangle_{min} = \sqrt{\frac{-a}{b}}$ Let $\langle s \rangle = \langle s_{min} \rangle + \delta \langle s \rangle$

$$A = N_{spin} \frac{1}{2} \underbrace{\left(a + 3b \langle s \rangle_{min}^2 \right)}_{-2a} (\delta \langle s \rangle)^2 - N_{spin} h \, \delta \langle s \rangle$$

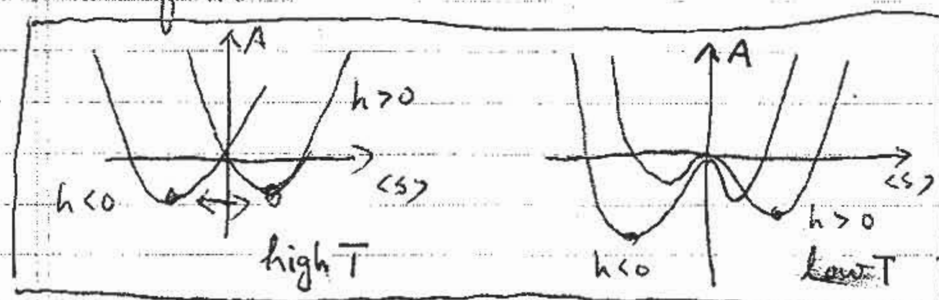
$$\chi = \frac{N_{spin}^2}{-2 a N_{spin} V} \propto |t|^{-\gamma} \quad \gamma = 1$$

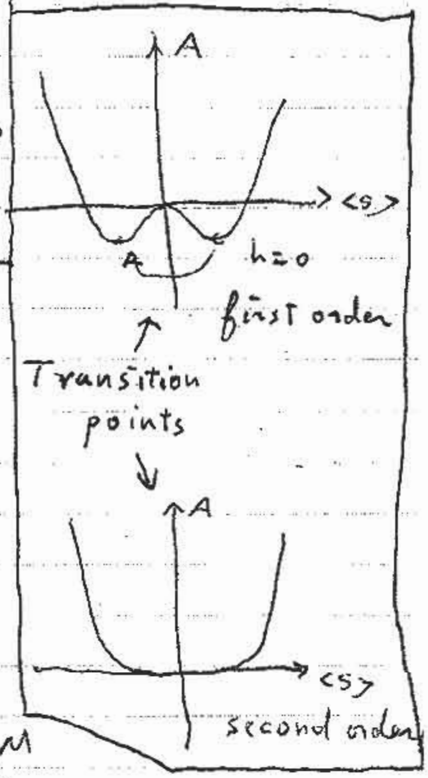
④ Phase diagram for $h \neq 0$

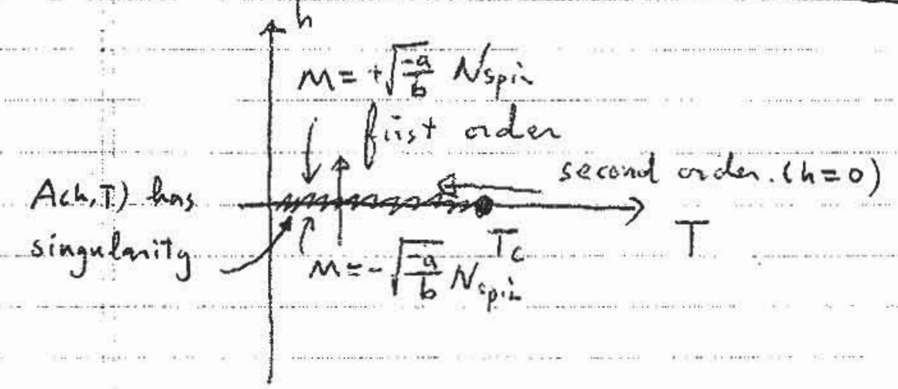


* if $h \neq 0$ & fixed, $A_{min}(T)$ is a smooth function of T. No phase transition.

* T fixed:

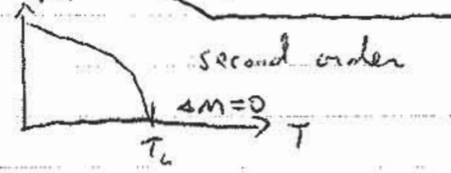






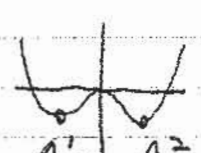
* Across first order transition

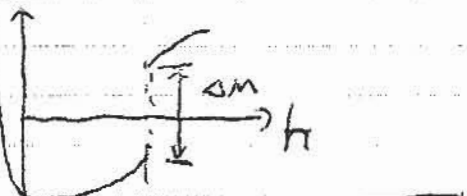
$$\Delta M = 2\sqrt{\frac{-a}{b}}$$



* Latent heat $= \Delta S\, T$

$$A^1_{min} = -\frac{N_{spin}}{2} a^2/b = A^2_{min}$$



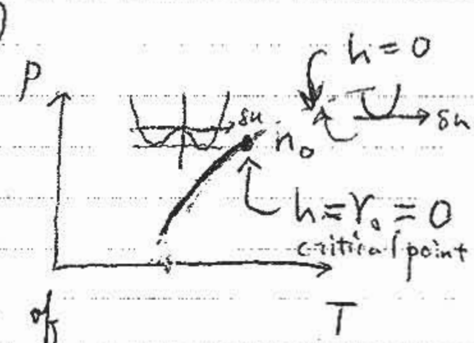


$$S_1 = -\frac{\partial A}{\partial T} = \frac{-N_{spin}}{2}\frac{\partial}{\partial T}\left(\frac{a^2}{b}\right) = S_2$$ (due to $\vec{S}_i \to -\vec{S}_i$ symmetry)

$\Delta S = 0$ Latent heat $= 0$ But in general $\Delta S \neq 0$

(5) Application of G-L theory

* Vapor-Water phase diagram



density $n = n_c(P,T) + \underbrace{\delta n}_{\text{play a role of order parameter}}$

Choose $n_c(P,T)$ to make:

$$\boxed{G(T,P;n) = h(T,P)\,\delta n + r_0(T,P)\,\delta n^2 + u_0\,\delta n^4}$$

(make δu^3 term disappear)

First order transition line is given by

$h = 0$ near the critical point

$\begin{cases} h(P_c,T_c)=0 \\ r_0(P_c,T_c)=0 \end{cases}$ gives $(P_c\ T_c)$ of the critical point

Near (P_c, T_c):

Critical point for water is the same as the critical point for Ising model. due to the same G-L theory

We see again the universality