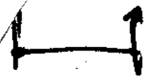
 dipole-dipole interaction

$\mu \sim \frac{\hbar e}{mc}$

$$V \sim \left(\frac{e\hbar}{mc}\right)^2 \frac{1}{r^3} = \frac{e^2\hbar^2c^2}{m^2c^4}\frac{1}{r^3}$$

$e^2 = 1.44$ MeV fm $\qquad \hbar c = 200$ MeV fm

$mc^2 = 0.5$ MeV.

$$V \sim \frac{1.44\times 4\times10^4}{0.25}\,\frac{\text{MeV fm}\ \cancel{\text{MeV}^2}\ \text{fm}^2}{\cancel{\text{MeV}^2}}\,\frac{1}{r^3}$$

$$\sim 20\times10^4\times10^6\ \text{eV}\times\frac{10^{-45}}{10^{-30}}\,\frac{\cancel{\text{m}^3}}{r^3(\text{Å})\ \cancel{\text{m}^3}}$$

$$\sim 2\times10^{41-45}\,\frac{\text{eV}}{(r(\text{Å}))^3} \sim 2\times10^{-4}\,\frac{\text{eV}}{(r(\text{Å}))^3}$$

if $r\sim 1$ Å $\rightarrow$ $V\sim 2\times10^{-4}$ eV

0.025 eV at least for magnetization at normal temp.

$T_{curie} \sim 700$°K $\rightarrow$ 0.05 eV >> 0.0002

Coulomb interaction much stronger.

exclusion pple. antisymmetric $\rightarrow$ symmetric in spin..

Simple model of paramagnetism.

$\uparrow \; \uparrow \; \nearrow$ magnets in magnetic field.

$$E = -\vec{\mu}\cdot\vec{B} = -\frac{e\hbar}{2mc} B_z \cdot \underset{\downarrow \pm 1}{\sigma}$$

$|\vec{\mu}| = \frac{e\hbar}{2mc}$; N, $\uparrow \downarrow$

$$Z = \sum_{\sigma_j = \pm} e^{+\beta \frac{e\hbar}{2mc} B_z \cdot \sum_j \sigma_j}$$

$$= \sum_{\sigma_j = \pm} \prod_j e^{\beta \frac{e\hbar}{2mc} B_z \sigma_j}$$

$$= \prod_j \left(e^{\beta \frac{e\hbar}{2mc} B_z} + e^{-\beta \frac{e\hbar}{2mc} B_z} \right)$$

$$= \left(2\,\mathrm{ch}\left(\beta \frac{e\hbar}{2mc} B_z\right) \right)^N$$

$$-\beta A = \ln Z = N \ln 2 + N \ln \mathrm{ch}\left(\beta \frac{e\hbar}{2mc} B_z\right)$$

$$A = -N k_B T \ln 2 - N k_B T \ln \mathrm{ch}\left(\beta \frac{e\hbar}{2mc} B_z\right)$$

$$dA = -S\,dT - \vec{M}\cdot d\vec{B}$$

$$Z = \sum e^{+\beta \vec{\mu}\cdot\vec{B}}$$

$$\frac{\partial \ln Z}{\partial B} = \beta \sum_i \vec{\mu} = \beta \vec{M}$$

$$-\beta \frac{\partial A}{\partial B} = \beta \vec{M} \quad \to \quad \frac{\partial A}{\partial B} = -M$$

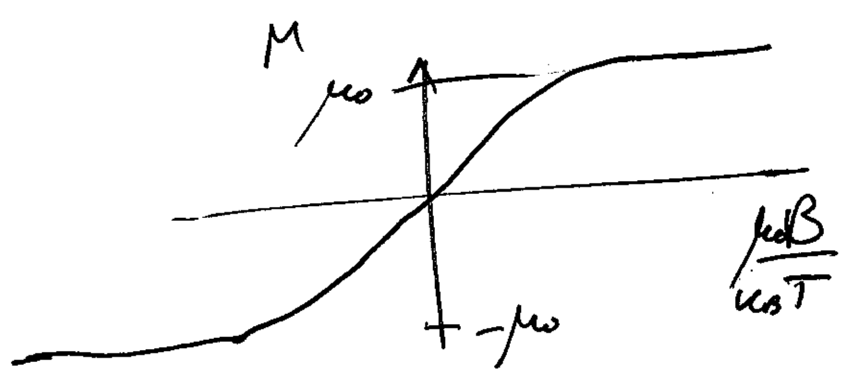
$$M = -\frac{\partial A}{\partial B} = N\cancel{k_BT}\,\frac{sh\left(\frac{\beta e\hbar}{2mc}B_z\right)}{ch\left(\frac{\beta e\hbar}{2mc}B_z\right)}\,\cancel{\beta}\frac{e\hbar}{2mc}$$

$$= N\mu_0\, Th(\beta\mu_0 B_z)$$

$$\boxed{\langle\mu\rangle = \frac{M}{N} = \mu_0\, Th(\beta\mu_0 B)}$$

$$B \to 0 \qquad \langle\mu\rangle = \mu_0\,\beta\mu_0 B = \frac{\mu_0 B}{k_BT}\mu_0$$

$$\chi = \frac{\partial\langle\mu\rangle}{\partial B} = \frac{\mu_0^2}{k_BT}$$



Ising model

$\uparrow\ \uparrow\ \downarrow\ \uparrow\ \downarrow\ \uparrow$.

$$E_f\{S_i\} = -\sum_{\langle ij\rangle} J s_i s_j - H \sum_j S_j$$

$\langle ij\rangle$ near neighbors

$$Z = \sum_{S_i = \pm 1} e^{-\beta E_f\{S_i\}}$$

(equivalent to lattice gas, binary alloy).

1-dimensional case

$$Z = \sum_{S_j=\pm 1} e^{+\beta J\sum_j S_j S_{j+1} + \beta H \sum_j S_j}$$

let's look at S_j

$$e^{\beta J S_{j-1}S_j + \beta J S_j S_{j+1} + \beta H S_j}$$

$$A_{S_{j-1}S_j}\ A_{S_j S_{j+1}}$$

$$e^{\beta J S_{j-1} S_j}\ e^{\beta J S_j S_{j+1}}$$

$$A_{S_{j-1}S_j} = e^{\beta J S_{j-1}S_j}$$

$$e^{\beta J S_{j-1}S_j + \frac{1}{2}\beta H S_{j-1} + \frac{1}{2}\beta H S_j}$$

$$\cdot\ e^{\beta J S_j S_{j+1} + \frac{1}{2}\beta H S_j + \frac{1}{2}\beta H S_{j+1}}$$

$$A_{s_{j-1}s_j} = e^{\beta J s_{j-1}s_j + \frac{1}{2}\beta H (s_{j-1}+s_j)}$$

$$Z = \sum_{s_j} A_{s_1 s_2} A_{s_2 s_3} \cdots A_{s_{j-1}s_j} A_{s_j s_{j+1}} \cdots$$

•) periodic chain $Z = \mathrm{Tr} A^L$

•) open chain $Z = \sum_{s_1, s_L = \pm 1} (A^L)_{s_1 s_L}$

$$A = \begin{array}{c|cc} & + & - \\ \hline + & e^{\beta J + \beta H} & e^{-\beta J} \\ - & e^{-\beta J} & e^{\beta J - \beta H} \end{array}$$

diagonalize A.

$$(e^{\beta J + H} - \lambda)(e^{\beta J - \beta H} - \lambda) - e^{-2\beta J} = 0$$

$$\lambda^2 - e^{\beta J} \lambda 2 \mathrm{ch} \beta H + e^{2\beta J} - e^{-2\beta J} = 0$$

$$\lambda^2 - 2\lambda e^{\beta J} \mathrm{ch} \beta H + 2 \mathrm{sh} 2\beta J = 0$$

$$\lambda = \frac{2e^{\beta J} ch\beta H \pm \sqrt{4e^{2\beta J} ch^2\beta H - 8 sh 2\beta J}}{2}$$

$$\lambda = e^{\beta J} ch\beta H \pm \sqrt{e^{2\beta J} ch^2\beta H - 2\, sh\, 2\beta J}$$

$$e^{2\beta J} ch^2\beta H - e^{2\beta J} + e^{-2\beta J}$$

$$e^{2\beta J} sh^2\beta H + e^{-2\beta J}$$

$$\lambda = e^{\beta J} \left(ch\beta H \pm \sqrt{sh^2\beta H + e^{-4\beta J}} \right)$$

$$Tr A^L = \lambda_+^L + \lambda_-^L$$

$$Z = e^{\beta J L} \left(ch\beta H + \sqrt{sh^2\beta H + e^{-4\beta J}} \right)^L$$

$$\ln Z = -\beta A = \beta J L + L \ln \left(ch\beta H + \sqrt{sh^2\beta H + e^{-4\beta J}} \right)$$

$H \to 0$

$$\ln Z = \beta J L + L \ln (1 + e^{-2\beta J})$$

$$M = \sum_j \langle s_j \rangle = \frac{1}{\beta} \frac{\partial \ln Z}{\partial H} = -\frac{\partial A}{\partial H}$$

$$dA = -S\,dT - M\,dH$$

$$A = -JL - k_B T L \ln\left(\mathrm{ch}\beta H + \sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}\right)$$

$$\frac{\partial A}{\partial H} = -k_B T L \frac{\beta\,\mathrm{sh}\beta H + \frac{\cancel{2}(\mathrm{sh}\beta H\,\mathrm{ch}\beta H)\beta}{\cancel{2}\sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}}}{\mathrm{ch}\beta H + \sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}}$$

$$= -L \frac{\mathrm{sh}\beta H + \mathrm{sh}\beta H\,\mathrm{ch}\beta H / \sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}}{\mathrm{ch}\beta H + \sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}}$$

$$= -L\,\mathrm{sh}\beta H \frac{\cancel{\mathrm{ch}\beta H + \sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}}}{\sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}\left(\cancel{\mathrm{ch}\beta H + \sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}}\right)}$$

$-\partial A/\partial H$

$$\boxed{M = +L \frac{\mathrm{sh}\beta H}{\sqrt{\mathrm{sh}^2\beta H + e^{-4\beta J}}}}$$

$H \to 0$

$$M = + L \beta H e^{2\beta J}$$

$$\chi = \frac{\partial M}{\partial H} = \beta L e^{2\beta J}$$

$$\boxed{\chi = \beta L e^{2\beta J}}$$

$$\uparrow\uparrow\uparrow \,\Big|\, \downarrow\downarrow\uparrow\uparrow$$

create domain wall

$$\left.\begin{array}{lll} \uparrow\uparrow & \to & E = -J \\ \uparrow\downarrow & \to & E = J \end{array}\right\} \Delta E = 2J$$

Can be put in N places. $\to$

$$\Delta A = 2J - T k_B \ln(N)$$

for any $T > 0$ domain walls are favored by A.

no phase transition.

Mean field approx. to Ising model

$$H = -\sum_{\langle ij\rangle} J s_i s_j - H \sum_j s_j$$

Consider a single spin.

assume $\langle s_i \rangle = s$ known

Approximation

$$\mathcal{H}_i = -\underbrace{2Jds}_{\text{field of neighboring spins}} s_j - H s_j$$

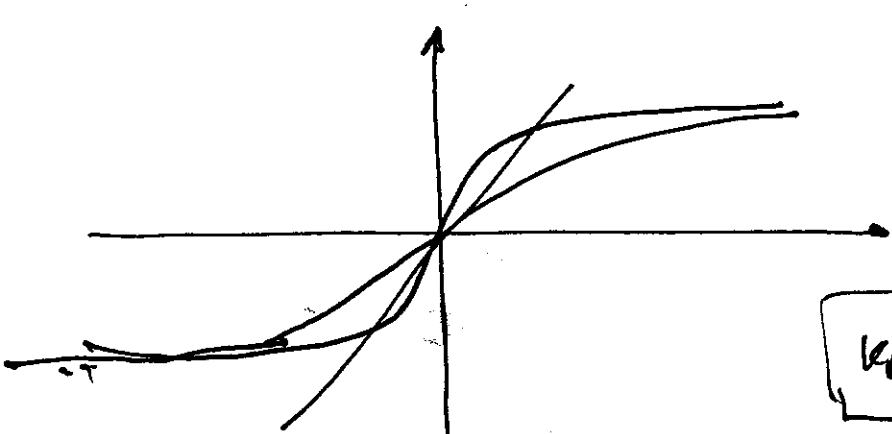
$$\mathcal{H}_i = -(H + 2Jd.s)\, s_j$$

$$\langle s \rangle = \mathrm{th}(\beta H + 2\beta J d s)$$

should be same!

H → 0

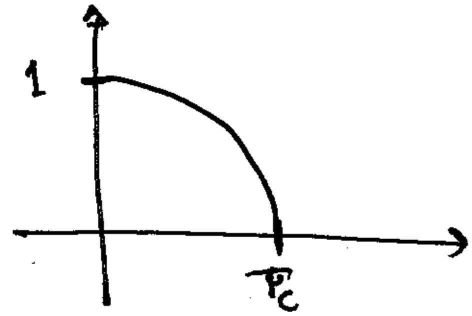
$$\langle s \rangle = \mathrm{th}\,(2\beta J d\, s)$$



if $2\beta J d > 1 \Rightarrow$ magnetization

$2\beta J d < 1 \Rightarrow s = 0$

$\boxed{k_B T < 2Jd}$ $\boxed{T_c = \frac{2J.d}{k_B}}$



$\beta \to \infty$ $\quad$ th $= 1$ $\quad$ $c(r) = 1$

$$\cancel{\langle s \rangle} = \quad s = \text{th}(2\beta J d s)$$

$s \to 0$ as $\beta \to \beta_c$.

$$y = \text{th}\, x \;;\; \frac{1}{\text{ch}^2 x} \;;\; -\frac{2}{\text{ch}^3 x}\,\text{sh}\, x \;;\; -2\left(\frac{\text{ch}^4 x - 3\,\text{ch}^2 x\,\text{sh}^2 x}{\text{ch}^6 x}\right)$$

$\frac{\text{sh}}{\text{ch}}$ $\quad$ $\frac{\text{ch}^2 - \text{sh}^2}{\text{ch}}$

$$1 \qquad 0 \qquad -2$$

(1) $\quad$ ''

$$\text{th}\, x \simeq x - \frac{2}{3!}x^3 = x - \frac{1}{3}x^3$$

$$s = 2\beta J d s - \frac{1}{3}(2\beta J d)^3 s^3$$

<u>$s \neq 0$</u> $\quad$ $\frac{1}{3}\underbrace{(\beta J d)^3}_{\substack{1 \\ T \sim T_c}} s^2 = \beta J d - 1$

$$= \frac{T_c}{T} - 1$$

$$s \simeq \left(3\,\frac{T_c - T}{T_c}\right)^{1/2}$$ critical exponent 1/2 in any dimension.

Variational improvement of mean field

$$B + \Delta B$$

B: external field

ΔB: mean field $= 2d\langle s\rangle$

$$E_{MF} = -(B+\Delta B)\sum_{j=1}^{N} S_j$$

$$Z = \sum_{S_j=\pm 1} e^{\beta(B+\Delta B)\sum_{j=1}^{N} S_j}$$

$$= \sum_{S_j=\pm 1} \prod_j e^{\beta(B+\Delta B)S_j}$$

$$= \left(2\,ch(\beta(B+\Delta B))\right)^N$$

$$-\beta A = N\ln 2 + N\ln ch(\beta(B+\Delta B))$$

$$A = -Nk_BT\ln 2 - Nk_BT\ln ch(\beta(B+\Delta B))$$

$\Delta B = 2d\langle s\rangle$ gives all thermodynamical quantities

$$Z = \sum_{\{S_j\}} e^{\beta \sum_{\langle ij\rangle} S_i S_j + \beta B \sum S_j}$$

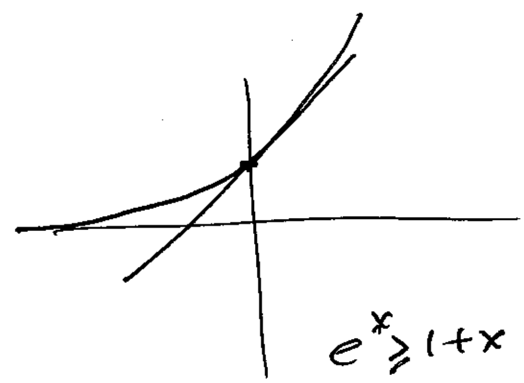
$$= \sum_{\{S_j\}} e^{\beta (B+\Delta B) \sum_j S_j + \underbrace{\beta \sum_{\langle ij\rangle} S_i S_j - \beta \Delta B \sum_j S_j}_{-\beta \Delta E}}$$

$$= \sum_{\{S_j\}} e^{\beta (B+\Delta B) \sum_j S_j - \beta \Delta E}$$

$$= \sum_{\{S_j\}} e^{-\beta E_{MF} - \beta \Delta E}$$

$$\Delta E = E - E_{MF}$$

$$Z = Z_{MF} \frac{\sum_{\{S_j\}} (e^{-\beta \Delta E}) e^{-\beta E_{MF}}}{Z_{MF}}$$



$$Z = Z_{MF} \langle e^{-\beta \Delta E} \rangle_{MF}$$

$$e^{x} \geq 1 + x$$

$$\langle e^{-\beta \Delta E} \rangle_{MF} = e^{-\beta \langle \Delta E \rangle_{MF}} \langle e^{-\beta (\Delta E - \langle \Delta E \rangle)} \rangle \geq$$

$$\geq e^{-\beta \langle \Delta E \rangle_{MF}} \left(1 - \cancel{\beta \langle \Delta E \rangle} + \cancel{\beta \langle \Delta E \rangle}\right)$$

$$Z \geq Z_{MF} \, e^{-\beta \langle \Delta E \rangle_{MF}}$$

$$\langle \Delta E \rangle_{MF} = - \left\langle \sum_{\langle ij \rangle} s_i s_j \right\rangle + \Delta B \sum_j \langle s_j \rangle$$

$$= -2N \langle s \rangle^2 + \Delta B \, N \langle s \rangle$$

$$Z \geq \left(2 \operatorname{ch}(\beta(B+\Delta B)) \right)^N e^{2\beta N \langle s \rangle^2 - \beta \Delta B N \langle s \rangle}$$

$$= \underset{Z_r}{e^{N \ln 2 + N \ln \operatorname{ch}(\beta(B+\Delta B)) + 2\beta N \langle s \rangle^2 - \beta \Delta B N \langle s \rangle}}$$

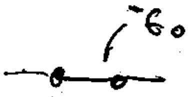
$$\cancel{\frac{\partial}{\partial \Delta B} \ln Z_r = \left(\beta N \langle s \rangle + 4\beta N \langle s \rangle - \beta N \langle s \rangle \right) = 0 \frac{\partial \langle s \rangle}{\partial B} = 0}$$

$$\cancel{\frac{\partial \ln Z}{\partial B} = \beta N \langle s \rangle}$$

$$\cancel{\beta N \langle s \rangle} + 4\beta N \langle s \rangle \frac{\partial \langle s \rangle}{\partial B} - \cancel{\beta N \langle s \rangle} - \Delta B \, \beta N \frac{\partial \langle s \rangle}{\partial B} = 0$$

$$4 \cancel{\beta} \cancel{N} \langle s \rangle = \cancel{\beta} \cancel{N} \Delta B \qquad \boxed{\Delta B = 4 \langle s \rangle}$$

~ to lattice gas



$$v(r) = \begin{cases} \infty & r=0 \\ -\epsilon_0 & r=1 \text{ (near neighbors)} \\ 0 & \text{otherwise.} \end{cases}$$

N: # of lattice sites

N_a: # of atoms $\qquad S_i = \pm 1 \qquad n_i = 1, 0$

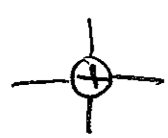
$$\Xi \; ? \; Z_{\text{Ising}}.$$

$$\Xi = \sum_{n_a = 0,1} e^{+\beta \epsilon_0 \sum_{\langle ij \rangle} (\text{occupied pairs}) + \beta\mu \sum_a n_a}$$

$$S_i S_j = \nearrow \begin{array}{ll} + + & \to + \\ + - & \to - \\ - + & \to - \\ - - & \to + \end{array}$$

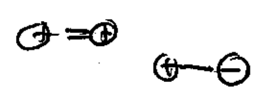
$$= \sum_{n_a = 0,1} e^{\beta \epsilon_0 N_{++} + \beta\mu N_+}$$

$$= \sum_{N_+ = 0}^{N} g(N)$$



1 line from each N_+

$4N_+$ lines.



$$4N_+ = 2N_{++} + N_{+-}$$

$$4N_- = 2N_{--} + N_{+-}$$

e

$$(N_+ - N_-) = 2(N_{++} - N_{--})$$

$$N_- = N - N_+$$

$$\overset{2}{\cancel{4}}(N_+ - N + N_+) = \cancel{2}N_{++} - \cancel{2}N_{--}$$

$$N_{--} = N_{++} - 4N_+ + 2N$$

$$Z_{Ising} = \sum_{S_i = \pm 1} e^{+\beta \sum_{\langle ij \rangle} S_i S_j + \beta B \sum S_j}$$

$$= \sum_{S_j = \pm 1} e^{\beta \underbrace{(N_{++} + N_{--} - N_{+-})}_{-E} + \beta B (N_+ - N_-)}$$

$$N_{++} + N_{--} + N_{+-} = 2N$$

$$N_{++} + N_{--} - N_{+-} = 2(N_{++} + N_{--}) - 2N$$

$$= 2N_{++} + 2N_{++} - 8N_+ + 4N - 2N$$

$$(-E) = 4N_{++} - 8N_+ + 2N$$

$$N_+ - N_- = 2N_+ - N$$

$$Z_{Ising} = \sum_{S_i = \pm 1} e^{\beta (4N_{++} - 8N_+ + 2N) + \beta B (2N_+ - N)}$$

$$\Xi = \sum_{S_i = \pm 1} e^{\beta \epsilon_0 N_{++} + \beta \mu N_+}$$

$$Z = \sum_{S_i = \pm 1} e^{4\beta N_{++} + (2\beta B - 8\beta) N_+ + N(2\beta - \beta B)}$$

$$\underline{\epsilon_0 = 4} \qquad \beta\mu = 2\beta B - 8\beta$$

$$\boxed{\mu = 2B - 8}$$

$$\Xi = e^{-\beta N (2 - B)} \cdot Z_{Ising}.$$

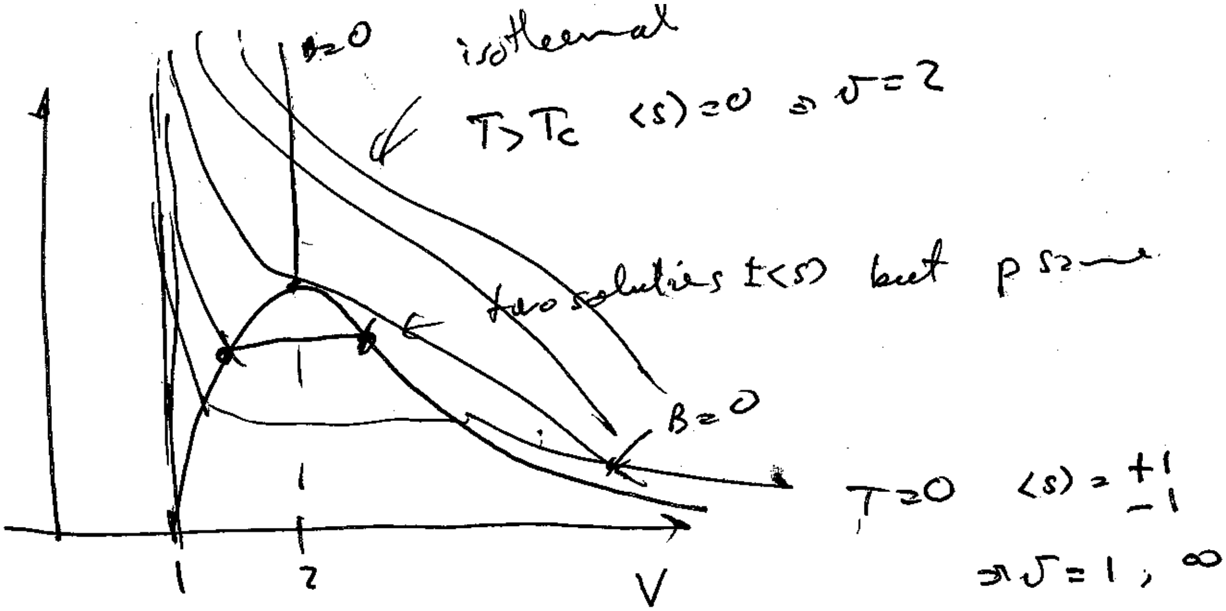
$$e^{\beta P V} = \Xi$$

$$\beta P V = -2\beta N + \beta B N - \beta A_{Ising}$$

$$\boxed{P = -2 + B - \frac{1}{N} A_{Ising}}$$

pressure.

$\underline{MF}$ $\quad P = -2 + B + k_B T \ln 2 + k_B T \ln ch \left(\beta (B + 2d\langle s \rangle)\right)$



<u>map</u>

Ising	lattice gas.
N_+	N_a
$4J$	ϵ_0
$e^{2\beta B - 8\beta J}$	$z = e^{\beta\mu}$
$-2J + B - \frac{1}{N} A_{Ising}$	Pressure.
$\frac{N_+}{N}$	$\frac{N}{V} = \frac{1}{v} = \rho$

We have to keep $\langle N_+ \rangle$ fixed by choosing $\underline{B}$.

$$\langle S \rangle = \frac{N_+ - N_-}{N} = \frac{2N_+ - N}{N} = 2\frac{N_+}{N} - 1 = \frac{2}{v} - 1 \Rightarrow v = \frac{2}{1+\langle s \rangle}$$

(B=0) $\quad p = -2J + k_B T \ln 2 + k_B T \ln ch(2\beta d \langle s \rangle)$