Ising-Paramagnet

N Spins

$$\boxed{\mathcal{H}(\{S_i\}) = -H\sum_i S_i}$$

H magnetic field (in energy units)

$S_i = \pm 1$

$\exp(-\beta\mathcal{H}) = ?$ $\quad -\beta\mathcal{H} = +\underbrace{\beta H}_{h}\sum_i S_i = h\sum_i S_i$

$$\exp(-\beta\mathcal{H}) = \exp(h S_1 + h S_2 + h S_3 + \ldots + h S_N) =$$

$$= \exp(h S_1)\exp(h S_2)\ldots\exp(h S_N)$$

$$Z = \sum_{\{S_i\}} \exp(-\beta \mathcal{H}) = \sum_{\{S_i\}} e^{hS_1} e^{hS_2} \dots e^{hS_N} =$$

$$= \sum_{S_1=-1,1} \sum_{S_2=-1,+1} \dots \sum_{S_N=-1,+1} e^{hS_1} \dots e^{hS_N} =$$

$$= \left(\sum_{S_1} e^{hS_1}\right)\left(\sum_{S_2} e^{hS_2}\right) \dots \left(\sum_{S_N} e^{hS_N}\right) =$$

$$= \left(\sum_{S} e^{hS}\right)^N = \left(e^{h} + e^{-h}\right)^N = \underline{\underline{\left(2\cosh \frac{H}{T}\right)^N}}$$

$$F = -T \ln Z = -NT \ln\left(2\cosh\frac{H}{T}\right) =$$

$$= -NT\ln 2 - NT\ln\cosh\frac{H}{T} = F$$

$$F(T,H) = F(T,-H)$$

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

$$S = -\frac{\partial F}{\partial T} = +N\ln 2 + N\ln\cosh\frac{H}{T}$$

$$+ NT\frac{1}{\cosh\frac{H}{T}}\sinh\frac{H}{T}\left(-\frac{H}{T^2}\right)$$

$$\frac{S}{N} = \ln 2 + \ln\cosh\frac{H}{T} - \frac{H}{T}\tanh\frac{H}{T}$$

$$S(T,H) = S(T,-H)$$

case 1 : $H = 0$ $\quad \underbrace{\mathcal{Z} = 0}$, $Z = \underline{\underline{2^N}} = \Omega_{tot}$

$\Rightarrow S = N \ln 2$

case 2 : $H \neq 0$; $T \to \infty$; $S \to N \ln 2$

assume $(H > 0)$. $T \to 0$ ($\beta \to \infty$):

$$\frac{1}{N} S = \ln\left(e^{\beta H} + e^{-\beta H}\right) - \beta H \frac{e^{\beta H} - e^{-\beta H}}{e^{\beta H} + e^{-\beta H}} =$$

$$= \ln\left\{e^{\beta H}\left(1 + e^{-2\beta H}\right)\right\} - \beta H \frac{e^{\beta H}\left(1 - e^{-2\beta H}\right)}{e^{\beta H}\left(1 + e^{-2\beta H}\right)} =$$

$$\cong \beta H + e^{-2\beta H} - \beta H\left(1 - 2e^{-2\beta H}\right) \longrightarrow 0$$

(only ONE configuration)

$$C_V = T\frac{\partial S}{\partial T} \Rightarrow \frac{C_V}{NT} = \frac{\partial}{\partial T}\left(\frac{S}{N}\right) =$$

$$= \frac{\partial}{\partial T}\left\{ \ln\cosh\frac{H}{T} - \frac{H}{T}\tanh\frac{H}{T} \right\} =$$

$$= \frac{1}{\cosh\frac{H}{T}}\sinh\frac{H}{T}\left(-\frac{H}{T^2}\right) + \frac{H}{T^2}\tanh\frac{H}{T}$$

$$- \frac{H}{T}\frac{1}{\cosh^2\frac{H}{T}}\left(-\frac{H}{T^2}\right) = \boxed{+\frac{H^2}{T^3}\frac{1}{\cosh^2\frac{H}{T}} = \frac{C_V}{NT}}$$

$$\frac{C_v}{N} = \frac{H^2}{T^2} \frac{1}{\cosh^2 \frac{H}{T}}$$

$H = 0 \Rightarrow C_v = 0$

$\underline{H > 0 \,;}$

(i) $T \to \infty \Rightarrow \frac{C_v}{N} \simeq \frac{H^2}{T^2}$

$$\frac{C_v}{N} = \frac{1}{T^2} \left\{ \underbrace{\langle \mathcal{H}^2 \rangle - \langle \mathcal{H} \rangle^2}_{\text{saturates for } T \to \infty} \right\}$$

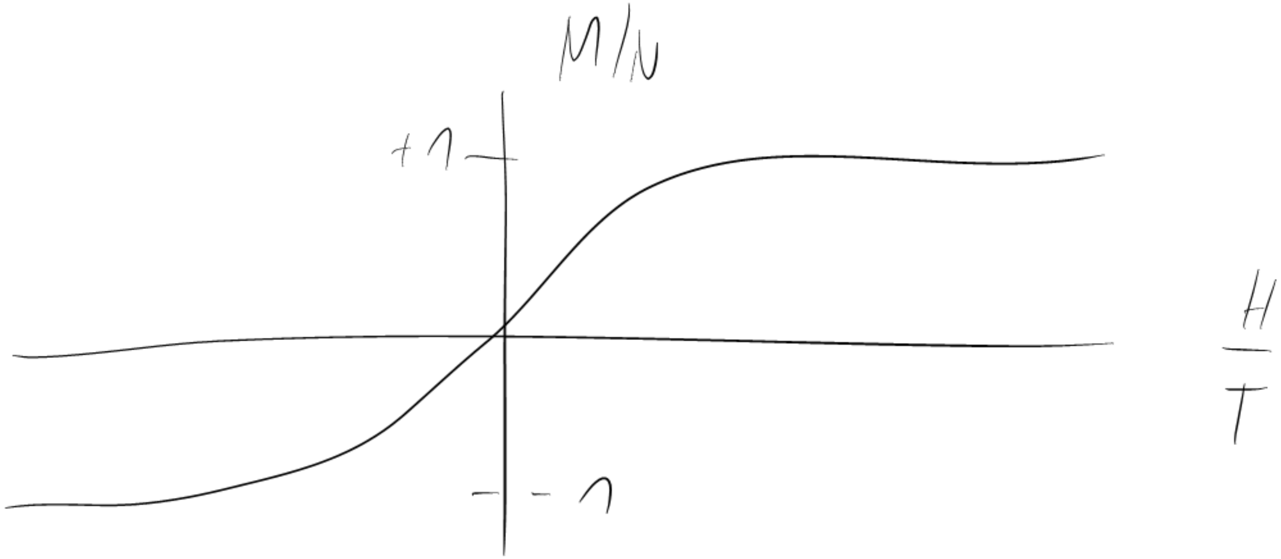
(ii) $T \to 0$: $\frac{c_V}{N} = \left(\frac{H/T}{\cosh \frac{H}{T}} \right)^2$

$1/T \to \infty \quad \Rightarrow C_V \to 0 \quad e^{-\text{const.}/T}$

$dF = -S\,dT - M\,dH \qquad F = -NT\ln 2 - NT \ln\cosh\frac{H}{T}$

$$M = -\frac{\partial F}{\partial H} = +NT\frac{\partial}{\partial H}\ln\cosh\frac{H}{T} =$$

$$= NT\frac{1}{\cosh\frac{H}{T}}\sinh\frac{H}{T}\left(\frac{1}{T}\right) \Rightarrow \boxed{\frac{M}{N} = \tanh\frac{H}{T}}$$



$$\chi N = \frac{\partial M}{\partial H} \Rightarrow \chi = \frac{\partial}{\partial H}\left(\frac{M}{N}\right) = \frac{\partial}{\partial H} \tanh \frac{H}{T} =$$

$$= \frac{1}{\cosh^2 \frac{H}{T}} \frac{1}{T}$$

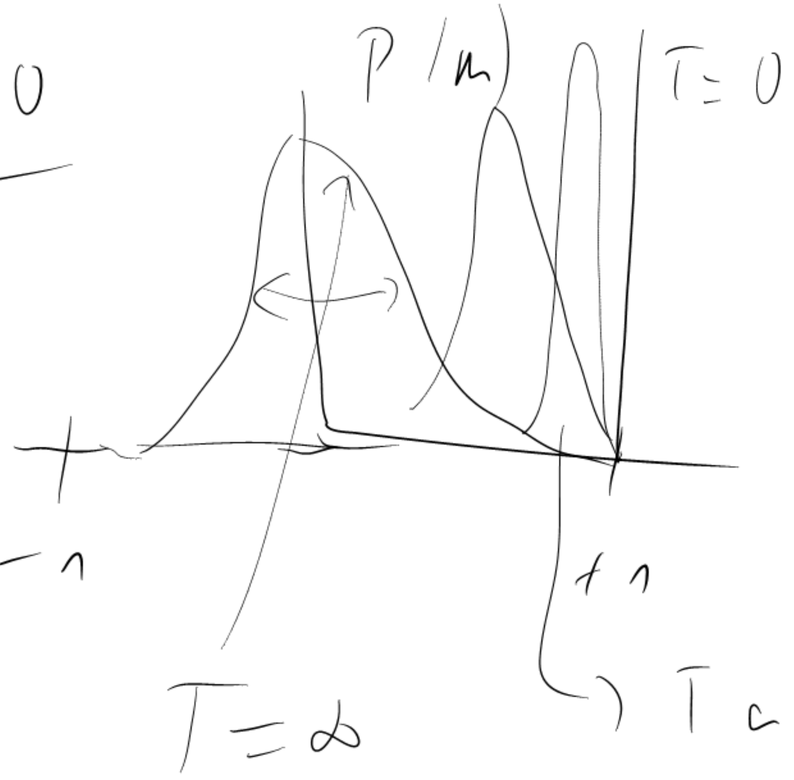
$$H = 0 \Rightarrow \chi = 1/T$$

$$H > 0; \quad T \to \infty \Rightarrow \chi = 1/T$$

$$T \to 0; \quad \chi \to 0$$

$$\chi = \frac{1}{NT}\left\{ \underbrace{\langle M^2 \rangle - \langle M \rangle^2}_{\text{saturates for } T \to \infty} \right\}$$

<u>$H > 0$</u>

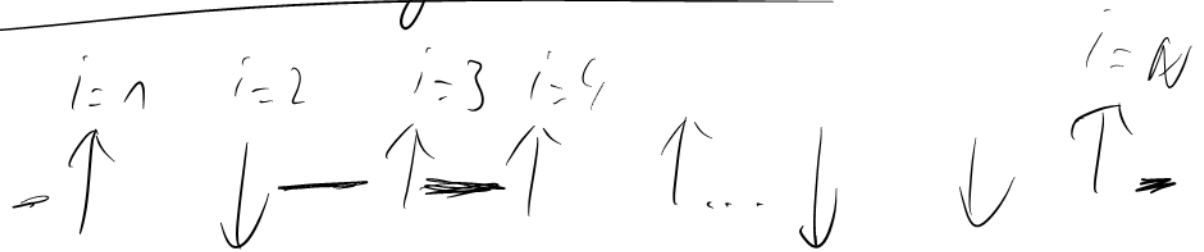


$m = M/N$

$\mathcal{H} = -HM$

The 1D Ising-Model

$i = 1, \dots, N$



$S_i = \pm 1$

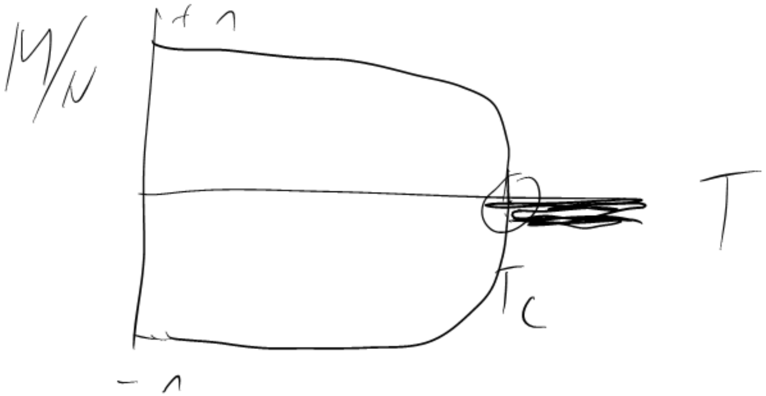
$$\mathcal{H} = -J \sum_{i=1}^{N} S_i S_{i+1} - H \sum_i S_i$$

$S_{N+1} \equiv S_1$

periodic boundary conditions

$J > 0$ ferromagnetic

<u>$H=0$</u>



$(H=0,\ T=T_c)$: F singular

$$-\beta\mathcal{H} = +\underbrace{\beta J}_{K}\sum_i S_i S_{i+1} + \underbrace{\beta H}_{h}\sum_i S_i$$

$$= K\sum_i S_i S_{i+1} + \frac{h}{2}\sum_i (S_i + S_{i+1})$$

$$Z = \sum_{S_1=\pm1}\sum_{S_2=\pm1}\cdots\sum_{S_N=\pm1} \exp\left\{K S_1 S_2 + \frac{h}{2}(S_1+S_2)\right\}$$

$$\exp\left\{K S_2 S_3 + \frac{h}{2}(S_2+S_3)\right\}$$

$$\vdots$$

$$\exp\left\{K S_N S_1 + \frac{h}{2}(S_N+S_1)\right\}$$

Excursion Bras and kets

vector $\vec{x} \longrightarrow |x\rangle$ "ket"

$\vec{x}^{\dagger} = \vec{x}^{T*} \longrightarrow \langle x|$ "bra"

↳ transposed, complex conjugate

$\underbrace{\langle x|y\rangle}_{\text{bra-ket}} \mathrel{\widehat{=}} \vec{x}^{\dagger}\,\vec{y}$ scalar product

bra-ket

= bracket

basis $\quad \vec{x} = \sum_i x_i \vec{e}_i$ basis vectors

basis vectors form an orthonormal basis:

$$\langle e_j | e_i \rangle = \delta_{ij}$$

$$|x\rangle = \sum_i x_i |e_i\rangle \qquad | \langle e_j|$$

$$\underbrace{\langle e_j | x \rangle}_{\text{projection of } |x\rangle \text{ onto } |e_j\rangle} = \sum_i x_i \underbrace{\langle e_j | e_i \rangle}_{\delta_{ij}} = x_j$$

$$|x\rangle = \sum_i x_i |e_i\rangle = \sum_i \langle e_i|x\rangle |e_i\rangle =$$

$$= \underbrace{\left(\sum_i |e_i\rangle\langle e_i|\right)}_{= \mathbb{1} \text{ unit operator}} |x\rangle \qquad \mathbb{1} = \sum_i \underbrace{|e_i\rangle\langle e_i|}_{\text{projection operator}}$$

"completeness relation"

linear operator:

$$|x\rangle \longrightarrow \hat{T}|x\rangle$$

$\hat{T}$ → operator

$$\langle e_i|\hat{T}|e_j\rangle = \text{number} = T_{ij}$$

(matrix element)

$$\sum_j T_{ij} x_j = \sum_j \langle e_i|\hat{T}|e_j\rangle\langle e_j|x\rangle =$$

$$= \langle e_i|\hat{T}\underbrace{\Big(\sum_j |e_j\rangle\langle e_j|\Big)}_{\mathbb{1}}|x\rangle =$$

$$= \langle e_i|\underbrace{\hat{T}|x\rangle}_{\text{image of } |x\rangle}$$

i-component of the image

$$\exp\left\{ K S_i S_{i+1} + \frac{h}{2}\left(S_i + S_{i+1}\right)\right\}$$

"transfer matrix" $\hat{T}$

$$\langle \sigma | \hat{T} | \tau \rangle = \exp\left\{ K \sigma \tau + \frac{h}{2}(\sigma + \tau)\right\} \qquad \begin{array}{l} \sigma = \pm 1 \\ \tau = \pm 1 \end{array}$$

$$Z = \sum_{S_1} \sum_{S_2} \cdots \sum_{S_N} \langle S_1 | \hat{T} | S_2 \rangle \langle S_2 | \hat{T} | S_3 \rangle$$

$$\langle S_3 | \hat{T} | S_4 \rangle \cdots \langle S_{N-1} | \hat{T} | S_N \rangle \langle S_N | \hat{T} | S_1 \rangle$$

$$\sum_{S_i} | S_i \rangle \langle S_i | = \mathbb{1}$$

$$Z = \sum_{S_1} \langle S_1 | \hat{T}\hat{T}\hat{T}\dots\hat{T} | S_1 \rangle$$

$$= \sum_{S_1} \langle S_1 | \hat{T}^N | S_1 \rangle = \underline{\underline{\mathrm{trace}(\hat{T}^N)}}$$

diagonalize $\hat{T} \to \lambda_+, \lambda_-$

$\hat{T}^N$ in diagonal representation: $\begin{pmatrix} \lambda_+^N & 0 \\ 0 & \lambda_-^N \end{pmatrix}$

trace is invariant

$$\boxed{Z = \lambda_+^N + \lambda_-^N}$$

$\lambda_+ = ?$

$\lambda_- = ?$

$$(T)_{ij} = \begin{pmatrix} e^{k+h} & e^{-k} \\ e^{-k} & e^{k-h} \end{pmatrix}$$

$$0 = \det \begin{pmatrix} e^{k+h} - \lambda & e^{-k} \\ e^{-k} & e^{k-h} - \lambda \end{pmatrix} \Rightarrow \ldots \Rightarrow$$

$$\lambda_{\pm} = e^{k} \cosh h \pm \sqrt{(e^{k} \cosh h)^2 - 2 \sinh 2k}$$

$$= e^{k} \cosh h \left\{ 1 \pm \sqrt{1 - \frac{2 \sinh 2k}{(e^{k} \cosh h)^2}} \right\}$$

$$\lambda_+ > \lambda_- \Rightarrow \lambda_+^N \gg \lambda_-^N$$

thermodyn. lim. $\Rightarrow$ neglect λ_-

$$z = \lambda_+^N \Rightarrow F = -NT\ln\lambda_+$$

$$\ln\lambda_+ = K + \ln\cosh h + \ln\left\{1 + \left[1 - \frac{1-e^{-4K}}{\cosh^2 h}\right]^{1/2}\right\}$$

$$\chi N = -\frac{\partial^2 F}{\partial H^2} \Rightarrow \chi T = -\frac{\partial^2}{\partial H^2}\left(\frac{F \cdot T}{N}\right) = \frac{\partial^2}{\partial H^2}\left(T^2 \ln\lambda_+\right)$$

$$= \frac{\partial^2}{\partial h^2} \ln \lambda_+ = \chi T \qquad \text{MAPLE}$$

$$\chi T = e^{+2K} \qquad \underline{\underline{\text{at } H = 0}}$$

$$\chi = \frac{1}{T} \exp\left(2 \frac{J}{T}\right)$$

$$T \to \infty : \quad \chi = 1/T$$

$$T \to 0 : \quad \chi \to \infty$$

"phase transition" at $T = 0$