Statistical Mechanics HW4.

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1. Gibbs variational principle.

$$A(\rho) = E - TS = \mathrm{Tr}(\rho H) + k_B T\,\mathrm{Tr}(\rho \ln \rho)$$

$\boxed{H_{Ising} = -J\sum_{\langle ij\rangle} S_i S_j - B\sum_i S_i}$

→ minimize free energy → canonical density matrix

ref. Kardar prob 10.6.

ⓐ Consider Ising model in d-dim.

Diagonal density fn : $\rho(S_1, \cdots, S_N) = g(S_1)\cdots g(S_N)$

$\begin{cases} g(+1) = g_+ , & \to \text{DOS of spin} \uparrow \\ g(-1) = g_- & \to \text{DOS of spin} \downarrow . \end{cases}$

$\therefore \langle S\rangle = g_+ - g_-$

normalization of density matrix

$$\mathrm{Tr}\,\rho = 1$$

$$= \sum_{\{S_i\}} g_1 \cdots g_N = (g_+ + g_-)^N = 1$$

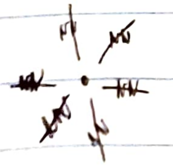
thermodynamic limit $N \to \infty$

$$g_+ + g_- = 1.$$

$$\therefore \boxed{\begin{cases} g_+ = \frac{1}{2}(1+\langle S\rangle) \\ g_- = \frac{1}{2}(1-\langle S\rangle) \end{cases}}$$

ⓑ. using Gibbs principle, the generalized free energy is

$$A(\rho) = \mathrm{Tr}(\rho H) + k_B T\,\mathrm{Tr}(\rho \ln \rho)$$



In d-dim

NN is 2d.

$\begin{cases} \bullet\ \mathrm{Tr}(\rho H) \\ = \sum_{\{S_i\}} g(S_1)\cdots g(S_N)\left(-J\sum_{\langle ij\rangle} S_i S_j - B\sum_i S_i\right) \\ \simeq -J\,2dN\langle S\rangle^2 - BN\langle S\rangle . \\ \bullet\ k_B T\,\mathrm{Tr}(\rho \ln \rho)) \\ k_B T \sum_i (g_1 g_2 \cdots g_N \ln g_1 \cdots g_N) \end{cases}$

$$= k_BT \sum (g_2 \cdots g_N)(g_1 \ln g_1) + (g_1 g_3 \cdots g_N)(g_2 \ln g_2) + \cdots$$

$$= N k_BT \overbrace{\sum_{s_i \neq 1} g_2 \cdots g_N}^{1} \sum_{s_1} g(s_1) \ln g(s_1)$$

$$= N k_BT \left(\frac{1}{2}(1+\langle s\rangle) \ln \frac{1+\langle s\rangle}{2} + \frac{1}{2}(1-\langle s\rangle) \ln \frac{1-\langle s\rangle}{2} \right).$$

$$A(\langle s\rangle) = -2dJN\langle s\rangle^2 - BN\langle s\rangle + \frac{Nk_BT}{2}\left((1+\langle s\rangle)\ln\frac{1+\langle s\rangle}{2} + (1-\langle s\rangle)\ln\frac{1-\langle s\rangle}{2} \right)$$

$$= -2dJN\langle s\rangle^2 - BN\langle s\rangle + N\frac{k_BT}{2}\Big((1+\langle s\rangle)\ln(1+\langle s\rangle) + (1-\langle s\rangle)\ln(1-\langle s\rangle) - 2\ln 2 .\Big)$$

$$= N\left(-2dJ\langle s\rangle^2 - B\langle s\rangle + \frac{k_BT}{2}\big((1+\langle s\rangle)\ln(1+\langle s\rangle) + (1-\langle s\rangle)\ln(1-\langle s\rangle) \big) - k_BT\ln 2 \right)$$

Free energy per site $a = \frac{A}{N}$.

Minimize the free energy

$$\frac{\partial a(\langle s\rangle)}{\partial\langle s\rangle} = \left(-4dJ\langle s\rangle - B + \frac{k_BT}{2}\big(\ln(1+\langle s\rangle) + 1 - \ln(1-\langle s\rangle) - 1\big) \right)$$

Thus, $-4dJ\langle s\rangle^* - B + \frac{k_BT}{2}\ln\frac{1+\langle s\rangle^*}{1-\langle s\rangle^*} = 0.$ where $\langle s\rangle^*$ is the solution of Gibbs variational principle.

$$\frac{k_BT}{2}\ln\frac{1+\langle s\rangle^*}{1-\langle s\rangle^*} = 4dJ\langle s\rangle^* + B.$$

$$\ln\frac{1+\langle s\rangle^*}{1-\langle s\rangle^*} = \frac{2}{k_BT}\left(4dJ\langle s\rangle^* + B\right)$$

$$\boxed{\therefore \langle s\rangle^* = \tanh\left(\frac{1}{k_BT}\left(4dJ\langle s\rangle^* + B\right)\right).}$$

$$\frac{1+x}{1-x} = e^y.$$

$$-1 + \frac{2}{1-x} = e^y$$

$$\frac{2}{1-x} = e^y + 1$$

$$\frac{1-x}{2} = \frac{1}{e^y+1} \qquad x = \frac{e^y-1}{e^y+1} = \tanh(y/2)$$

c This is exactly equivalent to mean field approximation

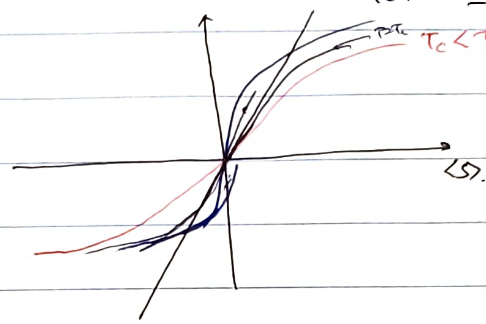
2. Ising model in d dim in mean-field approx.

ⓐ zero external field ($B=0$).

$$\langle s\rangle^* = \tanh\left(\frac{1}{k_B T}\left(4dJ\langle s\rangle^*\right)\right)$$ where free energy per site is

$$a(B=0,T) = -2dJ\langle s\rangle^2 - B\langle s\rangle + \frac{k_BT}{2}\left((1+\langle s\rangle)\ln(1+\langle s\rangle) + (1-\langle s\rangle)\ln(1-\langle s\rangle)\right)$$

say, $4dJ = k_B T_c$.



$$\langle s\rangle^* = \tanh\left(\frac{T_c}{T}\langle s\rangle^*\right)$$

$T > T_c$. $\langle s\rangle^* = 0$

$T < T_c$ $\langle s\rangle^* = 0, \pm s_0$

exists three solutions.

Near T_c, $\left(\frac{T_c - T}{T_c} = \varepsilon\right)$ $0 < \varepsilon \ll 1$

$0 < s_0 \ll 1$

$1 - \delta = \varepsilon$

(Taylor expansion of $\tanh x = x - \frac{x^3}{3} + \cdots$)

ref. Ising model and phase transitions by Alessandro Codello.

$$\therefore\ s_0 \simeq \frac{T_c}{T}s_0 - \frac{1}{3}\left(\frac{T_c}{T}s_0\right)^3$$

$$\frac{1}{3}\left(\frac{T_c}{T}s_0\right)^3 \simeq \frac{T_c - T}{T}s_0$$

$$s_0^3 \simeq \frac{3T^2}{T_c^3}(T_c - T)s_0$$

$$s_0^2 \sim \frac{3T^2}{T_c^2}\left(\frac{T_c - T}{T_c}\right)$$

$$= 3(1-\varepsilon)^2\varepsilon \sim 3(1-2\varepsilon)\varepsilon \sim 3\varepsilon = 3\left(\frac{T_c - T}{T_c}\right).$$

Hence,

$$\langle s\rangle \begin{cases} 0 & (T > T_c) \\ \left(3\left(\frac{T_c - T}{T_c}\right)\right)^{1/2} & (T < T_c) \end{cases}$$

$\boxed{k_B T_c = 4dJ.}$

$\therefore$ Magnetization critical exponent $\beta_{MF} = 1/2$.

(b) with field,

$$\langle S\rangle(T,B) = \tanh\left(\frac{T_c}{T}\langle S\rangle(T,B) + \frac{B}{T}\right).$$

around T_c, magnetization is small

$$\langle S\rangle(T,B) \sim \left(\frac{T_c}{T}\langle S\rangle(T,B) + \frac{B}{T}\right) - \frac{1}{3}\left(\frac{T_c}{T}\langle S\rangle(T,B) + \frac{B}{T}\right)^3.$$

magnetic susceptibility

$$\chi = \left.\frac{\partial\langle S\rangle}{\partial B}\right| = \frac{1}{\cosh^2\left(\frac{T_c}{T}\langle S\rangle + \frac{B}{T}\right)}\left(\frac{T_c}{T}\frac{\partial\langle S\rangle}{\partial B} + \frac{1}{T}\right).$$

$$\therefore \quad \chi = \frac{1}{ch^2\left(\frac{T_c}{T}\langle S\rangle + \frac{B}{T}\right)}\left(\frac{T_c}{T}\chi + \frac{1}{T}\right).$$

$$\frac{ch^2\left(\frac{T_c}{T}\langle S\rangle + \frac{B}{T}\right) - \frac{T_c}{T}}{\cancel{ch^2\left(\frac{T_c}{T}\langle S\rangle + \frac{B}{T}\right)}}\chi = \frac{1}{T}\frac{1}{\cancel{ch^2\left(\frac{T_c}{T}\langle S\rangle + \frac{B}{T}\right)}}$$

$$\chi = \frac{1}{T}\frac{1}{ch^2\left(\frac{T_c}{T}\langle S\rangle + \frac{B}{T}\right) - \frac{T_c}{T}}$$

For $T > T_c$, $\langle S\rangle = 0$,

$$\therefore \chi = \frac{1}{T}\frac{1}{ch^2\left(\frac{B}{T}\right) - \frac{T_c}{T}}$$

$$\left(\frac{e^x+e^{-x}}{2}\right)^2 \qquad \frac{e^{2x}+e^{-2x}+2}{4}$$

$$\chi\big|_{B=0} = \frac{1}{T - T_c}$$

$\therefore$ mean field susceptibility critical exponent $\gamma_{MF} = 1$

ⓒ. $\cancel{a_{B=0} = -2dJ\langle s\rangle^2}$

$$a(B=0,T) = -2dJ\langle s\rangle^2 + \frac{k_BT}{2}\left((1+\langle s\rangle)\ln(1+\langle s\rangle) + (1-\langle s\rangle)\ln(1-\langle s\rangle)\right) - k_BT\ln 2$$

$$= -2dJ\langle s\rangle^2 + \frac{k_BT}{2}\ln(1-\langle s\rangle^2) + \underbrace{\frac{k_BT}{2}\langle s\rangle\ln\frac{1+\langle s\rangle}{1-\langle s\rangle}}_{4dJ\langle s\rangle} - k_BT\ln 2$$

$$= 2dJ\langle s\rangle^2 + \frac{k_BT}{2}\ln\frac{1-\langle s\rangle^2}{4}$$

$$= \frac{k_BT_c}{2}\langle s\rangle^2 + \frac{k_BT}{2}\ln\frac{1-\langle s\rangle^2}{4}$$

$$a(B=0,T)\begin{cases} T>T_c \\ (\langle s\rangle=0) & \boxed{\left(\frac{k_BT}{2}\ln\frac{1}{4}\right)} \\ T<T_c \\ (\langle s\rangle^2 \simeq 3\left(\frac{T_c-T}{T_c}\right)) & \frac{k_BT_c}{2}3\left(\frac{T_c-T}{T_c}\right) + \frac{k_BT}{2}\ln\frac{1-3(1-\frac{T}{T_c})}{4} \end{cases}$$

$$= \frac{k_BT_c}{2}3\left(\frac{T_c-T}{T_c}\right) + \frac{k_BT}{2}\ln\left(\frac{3\frac{T}{T_c}-2}{4}\right).$$

near T_c.

$$\rightarrow \frac{k_BT_c}{2}3(\varepsilon) + \frac{k_BT}{2}\left(\ln(1-3\varepsilon) - \ln 4\right).$$

$$\sim \frac{k_BT_c}{2}3\varepsilon + \frac{k_BT}{2}\left(-3\varepsilon - \ln 4\right).$$

$$\frac{3}{2}k_B\varepsilon(T_c-T) - k_BT\ln 2$$

$$= \boxed{\frac{3}{2}k_B\frac{(T_c-T)^2}{T_c} - k_BT\ln 2.}$$

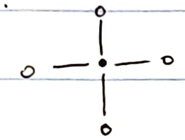
from $da = -s\,dT - P\,dv$

$$C_v = -T\frac{\partial^2 a}{\partial T^2} = \begin{cases} T>T_c & : 0 \\ T<T_c & : 3k_B. \end{cases}$$

Meanfield specific heat critical exponent $\alpha_{MF} = 0$.

3. Ising model in a d-dim using mean-field approx.

ⓐ.



$V(|\vec{r}_i-\vec{r}_j|)$

$\begin{cases} N: \text{total \# of lattice sites} \\ N_a: \text{total \# of atom} \\ N_{aa}: \text{total \# of NN atom.} \end{cases}$

total E. of lattice gas

$E_G = -\epsilon_0 N_{aa}$.

Partition fn.

$$\begin{cases} Z(N_a,T) = \frac{1}{N_a!}\sum_{\text{atoms}}^{N} e^{\beta\epsilon_0 N_{aa}} \\ \Xi = \sum_{N_a=0}^{\infty} z^{N_a} Z(N_a,T) \end{cases} = \sum_{N_a=0}^{\infty} z^{N_a}\frac{1}{N_a!}\sum_{\text{atoms}}^{N} e^{\beta\epsilon_0 N_{aa}}$$

N: ~volume of the system.

$$= \boxed{\sum_{N_a=0}^{\infty} z^{N_a}\sum_{a} g(N_a,N_{aa})\, e^{\beta\epsilon_0 N_{aa}}.}$$

Equation of state

$$\begin{cases} \beta P_G = \frac{1}{N}\log \Xi(z,N,T) \\ \frac{1}{v} = \frac{1}{N} z\frac{\partial}{\partial z}\log\Xi(z,N,T). \end{cases}$$

$\left(\sum_{N_a}^{\infty} N_a \log z\right)$

Ising model

$$\begin{cases} N_+: \text{total \# of } \uparrow \text{ spins} \\ N_-: \text{total \# of } \downarrow \text{ spins} \\ \quad = N - N_+. \end{cases}$$

$\left(\underbrace{\text{NN lines}}\ 2d\,\cancel{N_{++}}\right) \to 2\times N_{++} + 1\times N$

$$\begin{pmatrix} N_{++} & \oplus - \oplus \\ N_{--} & \ominus - \ominus \\ N_{+-} & \oplus - \ominus \end{pmatrix}$$

$$\begin{pmatrix} 2dN_+ = 2N_{++} + N_{+-} \\ 2dN_- = 2N_{--} + N_{+-} \\ N = N_+ + N_- \end{pmatrix}$$

$\Downarrow$

$$\boxed{\begin{cases} N_{+-} = 2dN_+ - 2N_{++} \\ N_- = N - N_+ \\ N_{--} = dN - 2dN_+ + N_{++} \end{cases}}$$

$dN_- - \frac{N_{+-}}{2}$

$d\,N-N_+$

$$\begin{cases} \therefore \sum_{\langle ij\rangle} S_iS_j = N_{++} + N_{--} - N_{+-} = N_{++} + dN - 2dN_+ + N_{++} - 2dN_+ + 2N_{++} \\ \qquad = 4N_{++} - 4dN_+ + dN. \\ \sum_i S_i = N_+ - N_- = 2N_+ - N. \end{cases}$$

$$E_I(N_+,N_{++}) = -J\sum_{\langle ij\rangle} s_i s_j - B\sum_i s_i = -J(4N_{++} - 4dN_+ + dN) - B(2N_+ - N)$$

$$= -4JN_{++} + 2(2dJ - B)N_+ - (dJ - B)N.$$

$$Z(B,T) = \sum_{\{s_1 \cdots s_N\}} e^{-\beta E_I}$$

$$= \sum_{\{s_1 \cdots s_N\}} e^{-\beta(-4JN_{++} + 2(2dJ - B)N_+ - (dJ - B)N)}$$

$$= e^{-\beta A_I(B,T)} = e^{N\beta(dJ - B)} \sum_{\{s_1 \cdots s_N\}} e^{\beta 4JN_{++}} e^{-2\beta(2dJ - B)N_+}$$

$$= e^{N\beta(dJ - B)} \sum_{N_+=0}^{N} e^{-2\beta(2dJ - B)N_+} \sum_{N_{++}=0}{}' g(N_+, N_{++})\, e^{4\beta JN_{++}}.$$

	Ising model	lattice model
	N_+	N_a
	$N - N_+$	$N - N_a$
partition fn	$e^{N\beta(dJ-B)} \sum_{N_+=0}^{N} e^{-2\beta(2dJ-B)N_+} \sum_{N_{++}=0}{}' g(N_+,N_{++}) e^{4\beta JN_{++}}$	$\sum_{N_+} z^{N_+} \sum_{N_{++}}{}' g(N_+,N_{++})\, e^{\beta\epsilon N_{++}}$
	$\parallel$	$\parallel$
	$e^{-\beta A_I(B,T)}$	$e^{\beta N p_G}.$
	$4J$	ϵ
	$e^{-2\beta(2dJ-B)}$	z
	$-\left(\frac{A_I}{N} + dJ - B\right)$	p_G
	$\frac{1}{2}(\langle s\rangle + 1)$	$\frac{1}{v}.$

(b)

$$P_G = -\frac{A_I}{N} - dJ + B.$$

$$= -\left(-2dJ\langle s\rangle^2 - B\langle s\rangle + \frac{k_BT}{2}\left((1+\langle s\rangle)\ln(1+\langle s\rangle) + (1-\langle s\rangle)\ln(1-\langle s\rangle)\right) - k_BT\ln 2\right) - dJ + B.$$

$$= -\left(-2dJ\langle s\rangle^2 - \cancel{B\langle s\rangle} + \frac{k_BT}{2}\ln(1-\langle s\rangle^2) + \frac{k_BT}{2}\langle s\rangle \underbrace{\ln\frac{1+\langle s\rangle}{1-\langle s\rangle}}_{\frac{2}{k_BT}(4dJ\langle s\rangle \cancel{+B})} - k_BT\ln 2\right) - dJ + B.$$

$$= -\left(+2dJ\langle s\rangle^2 + \frac{k_BT}{2}\ln\left(\frac{1-\langle s\rangle^2}{4}\right)\right) - dJ + B.$$

$$= B - dJ(1+2\langle s\rangle^2) - \frac{k_BT}{2}\ln\frac{1-\langle s\rangle^2}{4}$$

$P_G =$

$T > T_c$ $\langle s\rangle = 0.$

$$P_G = B - 2dJ\left(\frac{1}{2} + \langle s\rangle^2\right) - \frac{k_BT}{2}\ln\frac{1-\langle s\rangle^2}{4}$$

$$= B - \frac{k_BT_c}{2}\left(\frac{1}{2} + \langle s\rangle^2\right) - \frac{k_BT}{2}\ln\left(\frac{1-\langle s\rangle^2}{4}\right).$$

$$= B - \frac{k_BT_c}{2}\left(\frac{1}{2}\right) - \frac{k_BT}{2}\ln\frac{1}{4}.$$

$$= B - \frac{k_BT_c}{2}\left(\frac{1}{2} + \frac{T}{T_c}\ln\frac{1}{4}\right).$$

$T < T_c$ $\langle s\rangle^2 = 3\left(\frac{T_c - T}{T_c}\right).$

$$P_G = B - \frac{k_BT_c}{2}\left(\frac{1}{2} + 3\left(\frac{T_c-T}{T_c}\right)\right) - \frac{k_BT}{2}\ln\frac{1}{4}\left(1 - 3\left(\frac{T_c-T}{T_c}\right)\right)$$

$$= B - \frac{k_BT_c}{2}\left(\frac{1}{2} + 3\left(\frac{T_c-T}{T_c}\right)\right) - \frac{k_BT}{2}\left(\ln\left(1 - 3\left(\frac{T_c-T}{T_c}\right)\right) - \ln 4\right).$$