41) Lattice Gas

a) Show if 
$$N_i = \frac{(S_i+1)}{2}$$
 with  $S_i = \pm 1$ ,

Qm (N, T, H')

Determine C, H', J in terms of E, u for a lattice that has a - nearest neighbors.

$$= \frac{1}{2} \sum_{i=1}^{N-1} \sum_{s=1}^{N-1} \sum_{s=1}^{N-1} \exp \left( \frac{s}{2s} \sum_{i=1}^{N} \frac{(s+1)}{2s} + \frac{s}{2s} \sum_{s=1}^{N-1} \frac{(s+1)}{2s} \right)$$

$$= \sum_{S=\pm 1} \sum_{N=\pm 1} \exp\{\pm \beta 2 \left(\sum_{i=1}^{N} (S_{i} + N) + \pm \beta E \left(\sum_{i=1}^{N} (S_{i} + S_{i} + S_{i}$$

If there are 9 nearest neighbors for Si, then

$$\sum_{(i,j)} (S_i + S_j + I) = \left(\sum_{(i,j)} S_i + \sum_{(i,j)} S_j + \sum_{(i,j)} S_j$$

$$=\frac{1}{2}(2953+8N)$$

to avoid double counting.

Recogniting:
$$C = \exp\{\frac{1}{2}BuN + \frac{9}{8}BEN\}$$

$$J = \frac{4}{4}$$

$$H' = \frac{4}{2} + \frac{9}{4}$$

$$k_T = \frac{1}{P} \left( \frac{\partial P}{\partial P} \right)_T = \frac{|-P|}{Pk_B T - 9 \epsilon P^2 (|-P|)}$$

Then: 
$$\mathcal{H}_{LG} - uN = \mathcal{H}_{IM} - \frac{1}{2}uN - \frac{2}{8}EN$$

So  $(\mathcal{H}_{LG} - uN)_{MF} = (\mathcal{H}_{IM} - \frac{1}{2}uN - \frac{2}{8}EN)_{MF}$ 

then  $\Xi_{LG} = \exp([\frac{1}{2}u + \frac{2}{8}E)BN] G_{IM}$ 
 $\Rightarrow \ln \Xi_{LG}^{MF} = \ln Q_{IM}^{MF} + (\frac{1}{2}uN + \frac{2}{8}EN)B$ 

Derive  $\mathcal{H}_{IM}^{MF}$  and  $Q_{IM}^{MF}$ :

 $\mathcal{H}_{IM} = -H' \sum_{i=1}^{N} S_{i} - J \sum_{i=1}^{N} S_{i} S_{i} = -\sum_{i=1}^{N} H_{i}S_{i}$ 
 $A_{i}PPnx_{i}mete: S_{i}S_{i} = (\langle S_{i}\rangle + 8S_{i})(\langle S_{i}\rangle + S_{i})$ 
 $= \langle S_{i}\rangle \times S_{i}\rangle + \langle S_{i}\rangle \times (S_{i} - \langle S_{i}\rangle + \langle S_{i}\rangle \times (S_{i} - \langle S_{i}\rangle)$ 
 $S_{i}S_{i} = \langle S_{i}\rangle + \langle S_{i}\rangle + \langle S_{i}\rangle \times (S_{i} - \langle S_{i}\rangle + \langle S_{i}\rangle \times (S_{i} - \langle S_{i}\rangle \times (S_{i}) + \langle S_{i}\rangle \times (S_{i} - \langle S_{i}\rangle \times (S_{i}) + \langle S_{i}\rangle \times (S_{i}) \times (S_{i}) + \langle S_{i}\rangle \times (S_{i}) \times$ 

Then 
$$Q_{IM} = \sum exp\{-\beta_1 H_{IM}^{hm}\}$$

$$= \sum_{S=1}^{N} \sum_{S=1}^{N} exp\{-\beta_1 H_{IM}^{hm}\}$$

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$$Since exis = p = \frac{S_1}{2} + \frac{1}{2} = \frac{m+1}{2}$$

$$or m = (2p-1)$$

$$Q_{IM}^{MF} = exp\{-\beta_1 H_{IM}^{hm}\} \sum_{S=1}^{N} ..... \sum_{S=1}^{N} exp\{-\beta_1 H_{I}^{hm} + J_{2}(2p-1)\} \sum_{i=1}^{N} \sum_{i=1}^{N} exp\{-\beta_1 H_{I}^{hm} + J_{2}(2p-1)\} \sum_{i=1}^{N} exp\{-\beta_1 H_{I}^{h$$

Since 
$$m = \tanh(\beta H' + \beta J f m)$$

$$2P - 1 = \tanh(\beta (\frac{M}{2} + \frac{16}{4} + \frac{96}{4} (2P - 1)))$$

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$$4 = \frac{2}{8} \tanh(\beta (\frac{M}{2} + \frac{96}{2} + \frac{9}{2}))$$

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$$4 = \frac{1}{8} \ln(\beta - 1) - 96$$

$$4 = \frac{1}{8} \ln($$

Using himt given in question:

$$P = \frac{k_BT}{N} \ln \frac{1}{2}$$

$$P = -k_BT \ln (1-p) - \frac{92}{2} p^2$$

$$K_{T} = \frac{1}{P} \left( \frac{\partial P}{\partial P} \right)_{T} = \frac{1}{P} \left( \frac{\partial P}{\partial P} \right)_{T}$$

$$= \frac{1}{P} \left[ \frac{k_{B}T}{1-P} - 9EP \right]^{-1}$$

$$= \frac{1}{P} \left[ \frac{k_{B}T - 9EP (1-P)}{1-P} \right]^{-1}$$

$$= \frac{1}{P} \left[ \frac{1-P}{1-P} \right]$$

c) Show near critical point, 
$$K_T \rightarrow \frac{1}{k_B} (T-T_c)^{-1}$$

At critical point, 
$$(\frac{\partial P}{\partial P})_T = (\frac{\partial^2 P}{\partial P^2})_T = 0$$

$$(2) \left(\frac{3^{2}}{3\rho^{2}}\right)_{T} = \frac{k_{B}T}{(1-\rho)^{2}} - 9\varepsilon = 0$$

Combine 1 and 2:

$$(1-l_c)$$
 let  $(1-l_c)^2$  let then  $l_c = 1/2$ 

$$||_{k_BT_c=(1-\frac{1}{2})2\xi_2^{\frac{1}{2}}} = \frac{q\xi}{4}$$

$$k_T = \frac{1-\rho}{\rho} \frac{1}{\text{KBT} - 92\rho(1-\rho)}$$

$$f = f_c = \frac{1}{2}$$
 $k_T(f = f_c, T) = \frac{1 - \frac{1}{2}}{\frac{1}{2}}$ 
 $k_B T - g_E = \frac{1}{2}(1 - \frac{1}{2})$ 

but 
$$k_BT_c = \frac{9}{4}$$
 $= \frac{1}{k_BT} - \frac{9}{2} \frac{1}{k_BT}$ 
 $= \frac{1}{k_BT} \left(T - T_c\right)^{-1}$ 

Since  $k_T < T_c$  we see  $s = 1$ 

42) Monte-Carlo:

$$E = \sum_{i=1}^{N} b_{i} t_{i} w_{i}$$

a) Calculate  $Q_{i}$ , determine  $T$  such  $\langle E \rangle = 3678 \text{ cm}^{-1}$ , also find  $\langle SE|^{2} \rangle$ 

$$Q_{i} = \sum_{i=1}^{N} \exp\{-\beta t_{i} w_{i} v_{i}\}\}$$

Partition  $S = \sum_{i=1}^{N} \exp\{-\beta t_{i} w_{i}\}^{N}$ 

Then  $Q = \prod_{i=1}^{N-2} Q_{i}$ 

$$= \prod_{i=1}^{N-2} \prod_{i=1}^{N-2} \frac{1}{1-\exp\{-\beta t_{i} w_{i}\}}$$

$$\langle E \rangle = -\frac{3}{3} (\ln Q)_{N,N} = 3678 \text{ cm}^{-1}$$

$$= \sum_{i=1}^{N-2} \sum_{i=1}^{N} \ln (1-\exp\{-\beta t_{i} w_{i}\})$$

$$= \sum_{i=1}^{N-2} \frac{3}{3} \ln (1-\exp\{-\beta t_{i} w_{i}\})$$

$$\langle E \rangle = \sum_{i=1}^{N-2} t_{i} w_{i} \frac{1}{1-\exp\{-\beta t_{i} w_{i}\}} = 3678 \text{ cm}^{-1}$$

Solve using code, and find 
$$T=870.6k$$

$$\langle (SE)^2 \rangle = \langle (E-\langle E \rangle)^2 \rangle = \frac{3^2 \ln \Omega}{3B^2}$$

$$\downarrow = \frac{3}{2B} \left( \frac{3 \ln \Omega}{3B} \right)$$

$$= -\frac{3}{2B} \left( \frac{3 \ln \Omega}{3B}$$

c) see orde.

$$\frac{dP_i}{dt} = \sum_{j} \left[ w_{i \leftarrow j} P_j - w_{j \leftarrow i} P_i \right]$$

- => P: State occupation probabilities
- => Wij: transition matrix elements, rate from j-state to i-state
- =) assume Wij = Wii , Symmetric.

a) Show 
$$\sum_{i} P_{i} = 1$$
 is conserved by time evolution.

$$\frac{d}{dt}(\sum_{i} P_{i}) = \sum_{i} \frac{d}{dt} P_{i}$$

$$= \sum_{j} \sum_{i} w_{ij} P_{j} - \sum_{j} \sum_{i} w_{ji} P_{i}$$

$$= \sum_{j} (w_{j} P_{j})_{i} - \sum_{j} (w_{j} P_{j})_{j} \quad \text{with } i \neq j, so they're equal}$$

b) show 
$$\frac{dP_i}{dt} = \sum [W_{ij} P_j - W_{ii} P_i]$$
 is consistent with second law.

$$S = -k_{B} \sum_{i} P_{i} \ln P_{i}$$

$$\frac{dS}{dt} = -k_{B} \sum_{i} \frac{dP_{i} \ln P_{i} + dP_{i}}{dt}$$

$$= -k_{B} \sum_{i} \frac{dP_{i} \ln P_{i} + \sum_{i} P_{i}}{dt}$$

$$= -k_{B} \sum_{i} \left(\sum_{j} \left(W_{ij}P_{j} - W_{ji}P_{i}\right) \ln P_{i}\right)$$

$$= -k_{B} \sum_{i} \left(\sum_{j} \left[W_{ij}(P_{j} - P_{i})\right] \ln P_{i}\right)$$

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$$= -k_{B} \sum_{j} \left(\sum_{j} \left[W_{ij}(P_{j} - P_{i})\right] \ln P_{i}\right)$$

then only contributing terms are off-diagonal,

- =) Now if we observe two adjacent pair, (i=1,j=2) and (i=2,j=1)We will sum them up first:
  - 1) ds = KB W12 (P2-P1) In P1
  - 2)  $\frac{dS}{dt}\Big|_{i=2,\bar{v}=1} = -k_B w_{21}(P_1 P_2) \ln P_2 = -k_B w_{21}(P_2 P_1)(-\ln P_2)$

but if 
$$W_{21}=W_{12}$$
, then

$$\frac{dS}{dt}|_{U_2} + \frac{dS}{dt}|_{z_1} = -k_{12} W_{12}(P_2-P_1)(\ln P_1-\ln P_2)$$

Case 1: if  $P_2 \geq P_1$ :

then  $P_2-P_1 \geq 0$ 

So  $(P_2-P_1)(\ln P_1-\ln P_2) \leq 0$ 

and  $\ln P_1-\ln P_2 \leq 0$ 

So  $(P_2-P_1)(\ln P_1-\ln P_2) \leq 0$ 

(ase 2: if  $P_2 \leq P_1$ :

then  $P_2-P_1 \leq 0$  ) we still have and  $P_1-\ln P_2 \geq 0$ 

and  $P_1-\ln P_2 \geq 0$  )  $P_2-P_1(\ln P_1-\ln P_2) \leq 0$ 
 $P_3-P_1(\ln P_1-\ln P_2) \leq 0$ 

and  $P_3-\ln P_2 \leq 0$  ) we still have and  $P_3-\ln P_3 \leq 0$ 
 $P_3-P_1(\ln P_1-\ln P_2) \leq 0$ 

(ase 2: if  $P_2 \leq P_1$ :

then  $P_3-P_1 \leq 0$  ) we still have and  $P_3-P_1(\ln P_1-\ln P_2) \leq 0$ 
 $P_3-P_1(\ln P_1-\ln P_2) \leq 0$ 
 $P_3-P_1(\ln P_1-\ln P_2) \leq 0$ 

So  $(P_2-P_1)(\ln P_1-\ln P_2) \leq 0$ 
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So  $(P_3-P_1)(\ln P_1-\ln P_2) \leq 0$ 
 $P_3-P_1(\ln P_1-\ln P_2) \leq$ 

c) consider two-level system, 
$$P_1(t_0)=1$$
,  $P_2(t_0)=0$   
 $W_{12}=W_{21}=\frac{1}{T}$ , find  $P_1(t)$  and  $P_2(t)$ 

$$\frac{dP_1}{dt} = \frac{1}{7} \left( P_2 - P_1 \right)$$

$$\frac{dP_2}{dt} = \frac{1}{7} (P_1 - P_2)$$

$$\frac{d}{dt}\begin{pmatrix} P_1 \\ P_2 \end{pmatrix} = \frac{1}{\Upsilon}\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} P_1 \\ P_2 \end{pmatrix}$$

$$\begin{vmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & -1 & 1 \end{vmatrix} = \begin{vmatrix} 1 & -(1+\lambda) & 1 \\ 1 & -(1+\lambda) & 1 \end{vmatrix} = 0$$

$$4\left(\frac{1}{7}\right)^{2}\left[\left(\frac{1}{1+\lambda}\right)^{2}-1\right]=\left(\frac{1}{7}\right)^{2}\left[\lambda^{2}+2\lambda\right]$$

$$= \left(\frac{1}{T}\right)^2 \lambda (\lambda + 2) = 0$$

then 
$$\lambda=0$$
 or  $\lambda=-2/\gamma$ 

$$\left(\frac{1}{1}\right)\left(\frac{-1}{1}\right)\left(\frac{q^{+}}{q^{+}_{2}}\right)=0.$$

$$\frac{1}{7}\left(\begin{array}{c}-(1-2) & 1\\ 1 & -(1-2)\end{array}\right) = \frac{1}{7}\left(\begin{array}{c}1 & 1\\ 1 & 1\end{array}\right)$$

Then: 
$$P_i = A \begin{pmatrix} 1 \\ 1 \end{pmatrix} + B \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \stackrel{?}{\Rightarrow} t$$

then 
$$\binom{P_1}{P_2} = \frac{1}{2} \binom{1}{1} + \frac{1}{2} \binom{1}{-1} e^{-\frac{\lambda}{2}(t-t)}$$