Session 3 : solutions

Exercise 1

Recall that

$$m(h) = \sinh(\beta h)\, \frac{e^{\beta J} + e^{2\beta J}\cosh(\beta h)\left(e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}\right)^{-1/2}}{e^{\beta J}\cosh(\beta h) + \sqrt{e^{2\beta J}\sinh^2(\beta h) + e^{-2\beta J}}}$$

then take $\beta \to \infty$ $(T \to 0)$

* for $h > 0$

$$\cosh(\beta h) \to \frac{1}{2} e^{\beta h} \qquad \sinh(\beta h) \to \frac{1}{2} e^{\beta h} \qquad e^{-2\beta J} \to 0$$

then

$$m(h) \underset{\beta\to\infty}{\simeq} \frac{1}{2} e^{\beta h}\, \frac{e^{\beta J} + e^{\cancel{2}\beta J}\, \cancel{\tfrac{1}{2}}\, \cancel{e^{\beta h}} \cdot \left(\cancel{e^{\beta J}}\, \cancel{\tfrac{1}{2}}\, \cancel{e^{\beta h}}\right)^{-1}}{e^{\beta J}\, \frac{1}{2} e^{\beta h} + e^{\beta J}\, \frac{1}{2} e^{\beta h}} =$$

$$= \frac{1}{2} e^{\beta h}\, \frac{2 e^{\beta J}}{e^{\beta(J+h)}} = \frac{e^{\beta h + \beta J}}{e^{\beta J + \beta h}} = 1$$

$$\lim_{h\to 0^+} m(h) = 1 \quad \text{at } T = 0$$

* for $h < 0$

$$\cosh(\beta h) \to \frac{1}{2} e^{-\beta h} \qquad \sinh(\beta h) \to -\frac{1}{2} e^{-\beta h}$$

then

$$m(h) \underset{\beta\to\infty}{\simeq} -\frac{1}{2} e^{-\beta h}\, \frac{e^{\beta J} + e^{2\beta J}\, \frac{1}{2} e^{-\beta h} \left(e^{\beta J}\, \frac{1}{2} e^{-\beta h}\right)^{-1}}{e^{\beta J - \beta h}} =$$

$$= -1$$

!!!

Exercise 2

Remember that

$$F = \langle E \rangle + k_B T \langle \ln P \rangle =$$

$$= \sum_{\{s_i\}} \left[-J \sum_i s_i s_{i+1} - h \sum_i s_i \right] P(\{s_i\}) +$$

$$+ k_B T \sum_{\{s_i\}} P(\{s_i\}) \ln P(\{s_i\}$$

By tracing over the variables that do not appear in each term of the energy, we obtain for the first term

$$\langle E \rangle = \sum_i \left\{ -J \sum_{s_i = \pm 1} \sum_{s_{i+1} = \pm 1} s_i s_{i+1} P(s_i, s_{i+1}) - h \sum_{s_i = \pm 1} s_i P(s_i) \right\}$$

How do we simplify the structure of the probability?

We postulate that

$$P(s_1, \dots, s_N) = P(s_N | s_{N-1}, \dots s_1) P(s_{N-1}, \dots, s_1) =$$

$$\simeq \underbrace{P(s_N | s_{N-1})}_{\substack{s_N \text{ depends} \\ \text{only on } s_{N-1}}} P(s_{N-1}, \dots, s_1) =$$

$$= P(s_N | s_{N-1}) P(s_{N-1} | s_{N-2}) \dots P(s_2 | s_1) P(s_1)$$

by iterating the argument

Now use

$$P(x|y) = P(x,y)/p(y) \qquad \text{Bayes}$$

to obtain

$$P(\{s_i\}) \approx \underbrace{\prod_{i=1}^{N} P(s_i, s_{i+1})}_{\text{here we added } p(s_N, s_{N+1}) = p(s_N, s_1) \text{ periodic boundary conditions}} \underbrace{\left(\prod_{i=1}^{N} p(s_i)\right)^{-1}}_{\text{here we have added, by necessity, also } p(s_1)}$$

The entropy term becomes

$$\sum_{\{s_i\}} P(\{s_i\}) \left[\sum_{i=1}^{N} \ln P(s_i, s_{i+1}) - \sum_{i=1}^{N} \ln p(s_i) \right] =$$

$$= \sum_{i=1}^{N} \sum_{\{s_i\}} P(\{s_i\}) \ln P(s_i, s_{i+1}) - \sum_{i=1}^{N} \sum_{\{s_i\}} P(\{s_i\}) \ln p(s_i) =$$

$$= \sum_{i=1}^{N} P(s_i, s_{i+1}) \ln P(s_i, s_{i+1}) - \sum_{i=1}^{N} p(s_i) \ln p(s_i)$$

Then using $p(s_i, s_{i+1}) = p(s,s') \quad \forall i$

$$F_N = N\left\{ -J \sum_{s,s'} ss' P(s,s') - h \sum_s s\,p(s) + \right.$$

$$\left. + k_B T \sum_{s,s'} p(s,s') \ln p(s,s') - k_B T \sum_s p(s) \ln p(s) \right\}$$

Now we use

$p(+,+) + p(-,-) - p(+,-) - p(-,+) = c$ correlation

$p(+) = p(+,+) + p(+,-) \qquad p(-) = p(-,+) + p(-,-)$

$p(+,+) + p(+,-) - p(-,+) - p(-,-) = m$ magnetization

by symmetry $\quad p(+,-) = p(-,+)$

and normalization $\quad p(+,+) + p(-,-) + 2p(+,-) = 1$

Then we have the system

$$\begin{cases} P_{++} + P_{--} - 2P_{+-} = c \\ P_{++} + P_{--} + 2P_{+-} = 1 \\ P_{++} - P_{--} = m \end{cases}$$

$$\Rightarrow \quad P_{+-} = \frac{1}{4}(1-c)$$

$$\begin{cases} P_{++} + P_{--} = \frac{1}{2}(1+c) \\ P_{++} - P_{--} = m \end{cases} \Rightarrow \begin{cases} P_{++} = \frac{1}{4}(1+c) + \frac{1}{2}m \\ P_{--} = \frac{1}{4}(1+c) - \frac{1}{2}m \end{cases}$$

Thus we have

$$\begin{cases} P_{+-} = \frac{1}{4}(1-c) \\ P_{++} = \frac{1}{4}(1+c) + \frac{1}{2}m \\ P_{--} = \frac{1}{4}(1+c) - \frac{1}{2}m \end{cases} \qquad P_+ = \frac{1+m}{2} \qquad P_- = \frac{1-m}{2}$$

The free energy is then

$$\frac{F_N}{N} = f = -Jc - hm + k_BT\Big[\left(\frac{1}{4}(1+c)+\frac{1}{2}m\right)\ln\left(\frac{1}{4}(1+c)+\frac{1}{2}m\right) +$$

$$+ \left(\frac{1}{4}(1+c)-\frac{1}{2}m\right)\ln\left(\frac{1}{4}(1+c)-\frac{1}{2}m\right) +$$

$$+ 2\,\frac{1}{4}(1-c)\ln\left(\frac{1}{4}(1-c)\right)\Big] - k_BT\left[\frac{1+m}{2}\ln\frac{1+m}{2} + \frac{1-m}{2}\ln\frac{1-m}{2}\right]$$

Now we must minimize with respect to m and c

$$\frac{\partial f}{\partial c} = -J + k_BT\Big[\frac{1}{4}\ln\left(\frac{1}{4}(1+c)+\frac{1}{2}m\right) + \cancel{\frac{1}{4}} +$$

$$+ \frac{1}{4}\ln\left(\frac{1}{4}(1+c)-\frac{1}{2}m\right) + \cancel{\frac{1}{4}} - \frac{1}{2}\ln\left(\frac{1}{4}(1-c)\right) - \cancel{\frac{1}{2}}\Big] =$$

$$= -J + \frac{k_BT}{4}\ln\left[\left(\frac{1}{4}(1+c)\right)^2 - \frac{1}{4}m^2\right] - \frac{k_BT}{2}\ln\left(\frac{1}{4}(1-c)\right) = 0$$

$$\frac{\partial f}{\partial m} = -h + k_BT\Big[\frac{1}{2}\ln\left(\frac{1}{4}(1+c)+\frac{1}{2}m\right) + \cancel{\frac{1}{2}} - \frac{1}{2}\ln\left(\frac{1}{4}(1+c)-\frac{1}{2}m\right) +$$

$$-\cancel{\frac{1}{2}}\Big] - k_BT\left[\frac{1}{2}\ln\frac{1+m}{2} + \cancel{\frac{1}{2}} - \frac{1}{2}\ln\frac{1-m}{2} - \frac{1}{2}\right] =$$

$$= -h + k_B T \frac{1}{2} \ln \frac{\frac{1}{4}(1+c) + \frac{1}{2}m}{\frac{1}{4}(1+c) - \frac{1}{2}m} - k_B T \frac{1}{2} \ln \frac{1+m}{1-m} = 0$$

Putting the two equations together:

$$\begin{cases} -J + \frac{k_B T}{4} \ln\left[\left(\frac{1}{4}(1+c)\right)^2 - \frac{1}{4}m^2\right] - \frac{k_B T}{2} \ln\left(\frac{1}{4}(1-c)\right) = 0 \\ -h + k_B T \frac{1}{2} \ln \frac{\frac{1}{4}(1+c) + \frac{1}{2}m}{\frac{1}{4}(1+c) - \frac{1}{2}m} - k_B T \frac{1}{2} \ln \frac{1+m}{1-m} = 0 \end{cases}$$

$$\begin{cases} \frac{(1+c)^2 - 4\, m^2}{(1-c)^2} = e^{4\beta J} \\ \frac{(1+c) + 2\, m}{(1+c) - 2\, m} \cdot \frac{1-m}{1+m} = e^{2\beta h} \end{cases}$$

Using the second equation we get

$$c = 2m \frac{ch(\beta h) + sh(\beta h)\, m}{sh(\beta h) + ch(\beta h)\, m} - 1$$

and plugging it back into the first equation we obtain, after some tedious but trivial calculations, that

$$m = \frac{e^{2\beta J} \sinh(\beta h)}{\sqrt{1 + e^{4\beta J} \sinh^2(\beta h)}}$$

which is identical to the exact solution obtained using the transfer matrix (after some lengthy rearrangements)

$$1+c = 2m\,\frac{ch(\beta h)+sh(\beta h)\,m}{sh(\beta h)+ch(\beta h)\,m}$$

$$c = 2m\,\frac{ch(\beta h)+sh(\beta h)\,m}{sh(\beta h)+ch(\beta h)\,m} - 1$$

$$1-c = 2 - 2m\,\frac{ch(\beta h)+sh(\beta h)\,m}{sh(\beta h)+ch(\beta h)\,m}$$

$$(1+c)^2 = 4m^2\,\frac{ch^2+sh^2 m^2+2\,ch\,sh\,m}{sh^2+ch^2 m^2+2\,ch\,sh\,m}$$

$$(1+c)^2 - 4m^2 =$$

$$= \frac{4m^2\left[(ch^2-sh^2)+(sh^2-ch^2)m^2\right]}{sh^2+ch^2 m^2+2\,ch\,sh\,m} =$$

$$= 4m^2\,\frac{1-m^2}{sh^2+ch^2 m^2+2\,ch\,sh\,m}$$

$$(1-c)^2 \doteq 4 \cdot \left\{ 1 + m^2 \frac{ch^2 + sh^2 m^2 + 2\,ch\,sh\,m}{sh^2 + ch^2 m^2 + 2\,ch\,sh\,m} + \right.$$

$$\left. -2m \frac{ch + sh\,m}{sh + ch\,m} \right\}$$

$$4m^2 \frac{1-m^2}{sh^2 + ch^2 m^2 + 2\,ch\,sh\,m} =$$

$$= e^{4\beta J} 4 \left\{ \qquad \right\}$$

$$m^2(1-m^2) = e^{4\beta J} \left\{ sh^2 + ch^2 m^2 + 2\,ch\,sh\,m + \right.$$

$$+ m^2 \left(ch^2 + sh^2 m^2 + 2\,ch\,sh\,m \right) +$$

$$\left. -2m (ch + sh\,m)(sh + ch\,m) \right\}$$

$$m^2(1-m^2) = e^{4\beta J}\Big\{ sh^2 + ch^2 m^2 + 2ch\, sh\, m +$$

$$+ m^2\left(ch^2 + sh^2 m^2 + 2ch\, sh\, m\right) +$$

$$- 2m\left(ch + sh\, m\right)\left(sh + ch\, m\right)\Big\}$$

$$m^2(1-m^2) = e^{4\beta J}\Big\{ sh^2 + ch^2 m^2 + \cancel{2ch\, sh\, m} - \cancel{2m\, ch\, sh} - 2m^2 ch^2 +$$

$$- 2m^2 sh^2 + \cancel{2m^3 sh\, ch} +$$

$$+ m^2 ch^2 + m^4 sh^2 + \cancel{2m^3 ch\, sh}\Big\}$$

$$m^2(1-m^2) = e^{4\beta J}\Big\{ m^4 sh^2 + m^2\left(\cancel{ch^2} - \cancel{2ch^2} - 2 sh^2 + \cancel{ch^2}\right) + sh^2\Big\} =$$

$$= e^{4\beta J}\Big\{ sh^2 m^4 - 2m^2 sh^2 + sh^2\Big\} = e^{4\beta J} sh^2 (m^2-1)^2$$

$$m^2(1-m^2) = e^{4\beta J}(1-m^2)^2\, sh^2(\beta h)$$

$$m^2 = e^{4\beta J} sh^2(\beta h)\,(1-m^2)$$

$$m^2\left[1 + e^{4\beta J} sh^2(\beta h)\right] = e^{4\beta J} sh^2 \beta h$$

$$m = \frac{e^{2\beta J}\, sh(\beta h)}{\sqrt{1 + e^{4\beta J}\, sh^2(\beta h)}}$$