

Phys 504 hw 6 solution

I. THE ONE DIMENSIONAL CLASSICAL ISING MODEL

1,

$$\begin{aligned} Z &= \sum_{\sigma} e^{-\beta E[\sigma]} \\ &= \sum_{\sigma} \prod_{i=1}^N \exp(\beta J \sigma_i \sigma_{i+1} + \beta H \sigma_i) \\ &= \text{tr} \left(\prod_{i=1}^N \exp(\beta \sigma_i \sigma_{i+1} + \frac{\beta H}{2} (\sigma_i + \sigma_{i+1})) \right) \end{aligned}$$

Let $\langle \sigma_i | T | \sigma_j \rangle = \exp(\beta J \sigma_i \sigma_j + \frac{\beta H}{2} (\sigma_i + \sigma_{i+1}))$

Then

$$\begin{aligned} Z &= \text{tr} [\langle \sigma_1 | T | \sigma_2 \rangle \langle \sigma_2 | T | \sigma_3 \rangle \cdots \langle \sigma_N | T | \sigma_1 \rangle] \\ &= \text{tr} [T^N] \end{aligned} \tag{1}$$

The transfer matrix is therefore

$$T = \begin{pmatrix} e^{\beta(J+H)} & e^{-\beta J} \\ e^{-\beta J} & e^{\beta(J-H)} \end{pmatrix} \tag{2}$$

2, The transfer matrix has eigenvalues

$$t_{\pm} = e^{\beta J} \cosh \beta H \pm \sqrt{e^{2\beta J} \cosh^2 \beta H - 2 \sinh 2\beta J} \tag{3}$$

$$= e^{\beta J} \left(\cosh(\beta H) \pm \sqrt{\sinh^2 \beta H + e^{-4\beta J}} \right) \tag{4}$$

3, The partition function can be written as

$$Z = t_+^N + t_-^N \tag{5}$$

The free energy is therefore

$$\begin{aligned} F_N &= -kT \ln Z \\ &= -kT \ln(t_+^N + t_-^N) \end{aligned} \tag{6}$$

4, In the thermodynamic limit $N \rightarrow \infty$ the free energy becomes

$$F_N = -kT \left\{ N \ln t_+ + \ln \left(1 + \left(\frac{t_-}{t_+} \right)^N \right) \right\}$$

$$\rightarrow -NkT \ln t_+ \quad (7)$$

which is determined by the behavior at large t_+ . Since F_N is proportional to N , it is extensive. In the no-field limit $H \rightarrow 0$, the free energy beomes

$$F_N \rightarrow -NkT \ln(2 \cosh \beta J) \quad (8)$$

By direct differentiation

$$\frac{1}{Nk} \frac{\partial F_\infty}{\partial T} = -\ln(2 \cosh \beta J) + \beta J \tanh(\beta J) \quad (9)$$

$$\frac{1}{Nk^2} \frac{\partial^2 F_\infty}{\partial T^2} = -\beta^3 J^2 \operatorname{sech}^2 \beta J \quad (10)$$

which is differentiable for the 2nd order for $T > 0$. No phase transition for it.

5,

In the low temperature limit with $\beta J \geq 1$ and $\beta H \geq 1$

$$t_+ = e^{\beta J} \left(\cosh \beta H + \sqrt{\sinh^2 \beta H + e^{-4\beta J}} \right)$$

$$\rightarrow e^{\beta(J+H)} (1 + e^{-\beta(4J+2H)}) \quad (11)$$

On the other hand, expand it in the high temperature limit with small β

$$t_+ \approx 2 + (\beta H)^2 + (\beta J)^2 \quad (12)$$

So

$$\ln t_+ \approx \ln 2 + \frac{\beta^2}{2} (H^2 + J^2) \quad (13)$$

a) From $F_\infty = -NkT \ln t_+$, the average magnetization per site is

$$m(T, J, H) = \frac{1}{N} \frac{1}{\beta} \frac{1}{Z} \frac{\partial Z}{\partial H}$$

$$= -\frac{1}{N} \frac{\partial F_\infty}{\partial H}$$

$$= kT \frac{1}{t_+} \left(e^{\beta J} \beta \sinh \beta H + \frac{e^{2\beta J} \beta \sinh \beta H \cosh \beta H}{\sqrt{e^{2\beta J} \sinh^2 \beta H + e^{-2\beta J}}} \right)$$

$$= \frac{e^{\beta J} \sinh \beta H}{t_+} \left(1 + \frac{e^{\beta J} \cosh \beta H}{\sqrt{e^{2\beta J} \sinh^2 \beta H + e^{-2\beta J}}} \right) \quad (14)$$

In the low temperature,

$$\begin{aligned} m(T, J, H) &\rightarrow kT \frac{\partial}{\partial H} (\beta(J + H) + e^{-\beta(4J+2H)}) \\ &= 1 - 2e^{-\beta(4J+2H)} \end{aligned} \quad (15)$$

The system approaches the configuration with all spins aligned with the magnetic field as the temperature decrease. In the high temperature limit

$$\begin{aligned} m(T, J, H) &\rightarrow kT \frac{\partial}{\partial H} (\ln 2 + \frac{\beta^2}{2}(H^2 + J^2)) \\ &= \beta H \end{aligned} \quad (16)$$

So the system approaches the completely disordered configuration as the temperature increases.

b) The magnetic susceptibility is

$$\chi(T, J, H) = \frac{\partial m}{\partial H} \quad (17)$$

In the low temperature limit,

$$\chi(T, J, H) \rightarrow 4\beta e^{-\beta(4J+2H)} \quad (18)$$

and in the high temperature limit

$$\chi(T, J, H) \rightarrow \beta \quad (19)$$

c) The entropy is

$$S = -\frac{\partial F}{\partial T} \quad (20)$$

In the low temperature limit,

$$\begin{aligned} S &\rightarrow N \frac{\partial}{\partial T} (kT\beta(J + H) + kTe^{-\beta(4J+2H)}) \\ &\approx \frac{N}{T} (4J + 2H) e^{-\beta(4J+2H)} \end{aligned} \quad (21)$$

In the high temperature limit

$$\begin{aligned} S &\rightarrow N \frac{\partial}{\partial T} (kT \ln 2 + kT \frac{\beta^2}{2}(H^2 + J^2)) \\ &= N(k \ln 2 - \frac{1}{2kT^2}(H^2 + J^2)) \end{aligned} \quad (22)$$

d) The specific heat

$$c = \frac{T}{N} \frac{\partial S}{\partial T} \quad (23)$$

In the low temperature limit

$$\begin{aligned} c &\rightarrow (4J + 2H) \frac{\partial}{\partial T} e^{-\beta(4J+2H)} \\ &= (4J + 2H)^2 \frac{1}{kT^2} e^{-\beta(4J+2H)} \end{aligned} \quad (24)$$

while in the high temperature limit

$$\begin{aligned} c &\rightarrow T \frac{\partial}{\partial T} \left(-\frac{1}{2kT^2} (H^2 + J^2) \right) \\ &= \frac{1}{kT^2} (H^2 + J^2) \end{aligned} \quad (25)$$

II. MEAN FIELD THEORY

1) Under $\sigma \rightarrow -\sigma$

$$H[-\sigma] = -J \sum_{r_A, r_B} \sigma(r_A) \sigma(r_B) + h \sum_{r_A} \sigma(r_A) - h \sum_{r_B} \sigma(r_B)$$

This Hamiltonian will give the same free energy as $H[\sigma]$ since the A and B sublattices are equivalent.

2. The antiferromagnetic state $\sigma(r_A) = \sigma(r_B) = 1$ has energy

$$H_{af} = -2NJ \quad (26)$$

while the ferromagnetic state $\sigma(r_A) = -\sigma(r_B) = 1$

$$H_f = 2NJ - Nh \quad (27)$$

Therefore, there is a ground state phase transition when $H_{af} = H_f$ at the critical field $h_c = 4J$

3.

$$F \leq \tilde{F} = F_0 + \langle H - H_0 \rangle \quad (28)$$

$$H - H_0 = [-J \sum_{r_A, r_B} \sigma(r_A)\sigma(r_B) - h \sum_{r_A} \sigma(r_A) + h \sum_{r_B} \sigma(r_B)] - [-h_A \sum_{r_A} \sigma(r_A) - h_B \sum_{r_B} \sigma(r_B)] \quad (29)$$

$$= -J \sum_{r_A, r_B} \sigma(r_A)\sigma(r_B) - (h - h_A) \sum_{r_A} \sigma(r_A) + (h + h_B) \sum_{r_B} \sigma(r_B) \quad (30)$$

In addition

$$\langle H - H_0 \rangle_0 = \langle H \rangle_0 - \langle H_0 \rangle_0 \quad (31)$$

$$\langle H_0 \rangle_0 = -2NJ \langle \sigma_A \rangle_0 \langle \sigma_B \rangle_0 - \frac{h}{2} N \langle \sigma_A \rangle_0 + \frac{h}{2} N \langle \sigma_B \rangle_0 \quad (32)$$

$$\langle H_0 \rangle_0 = -\frac{N}{2} [h_A \langle \sigma_A \rangle_0 + h_B \langle \sigma_B \rangle_0] \quad (33)$$

Therefore

$$\langle H - H_0 \rangle_0 = -2NJ \langle \sigma_A \rangle_0 \langle \sigma_B \rangle_0 + \frac{N}{2} \langle \sigma_A \rangle_0 (h_A - h) + \frac{N}{2} \langle \sigma_B \rangle_0 (h_0 - h) \quad (34)$$

Therefore

$$\tilde{F} = F_0(\beta h_A, \beta h_B) - 2NJ \langle \sigma_A \rangle_0 \langle \sigma_B \rangle_0 - \frac{Nh}{2} (\langle \sigma_A \rangle_0 - \langle \sigma_B \rangle_0) + \frac{N}{2} (h_A \langle \sigma_A \rangle_0 + h_B \langle \sigma_B \rangle_0) \quad (35)$$

Note that the two sublattices in H_0 are non interacting, we can write

$$\begin{aligned} \langle \sigma(r_A)\sigma(r_B) \rangle_0 &= \langle \sigma_H \rangle_0 \langle \sigma_B \rangle_0 \\ &= m_A m_B \end{aligned} \quad (36)$$

where m_A and m_B are the magnetization of the two sublattices.

$$H - H_0 = -J \sum_{\langle r_A, r_B \rangle} \sigma(r_A)\sigma(r_B) + (h_A - h) \sum_{r_A} \sigma(r_A) + (h_B + h) \sum_{r_B} \sigma(r_B) \quad (37)$$

Hence the variational free energy is

$$\tilde{F} = F_0(\beta h_A, \beta h_B) - 2NJ m_A m_B - \frac{1}{2} Nh (m_A - m_B) + \frac{1}{2} N (h_A m_A + h_B m_B) \quad (38)$$

4. With the partition function of H_0 as

$$\begin{aligned} Z_0 &= \sum_{\sigma} e^{-\beta H_0[\sigma]} \\ &= (2 \cosh \beta h_A)^{N/2} (2 \cosh \beta h_B)^{N/2} \end{aligned} \quad (39)$$

we compute the sublattice magnetization

$$\begin{aligned}
m_A &= \frac{1}{Z_0} \sum_{\sigma} \sigma(r_A) e^{-\beta H_0[\sigma]} \\
&= \frac{\sum_{\sigma(r_A)} \sigma(r_A) e^{\beta h_A \sigma(r_A)}}{\sum_{\sigma(r_A)} e^{\beta h_A \sigma(r_A)}} \\
&= \tanh(\beta h_A)
\end{aligned} \tag{40}$$

$$m_B = \tanh(\beta h_B) \tag{41}$$

It follows that

$$\begin{aligned}
F_0 &= -kT \ln Z_0 \\
&= -\frac{1}{2} NkT (\ln(2 \cosh \beta h_A) + \ln(2 \cosh \beta h_B)) \\
&= -\frac{1}{2} NkT \left(\ln \frac{2}{\sqrt{1-m_A^2}} + \ln \frac{2}{\sqrt{1-m_B^2}} \right)
\end{aligned} \tag{42}$$

$$\begin{aligned}
\tilde{F} &= -\frac{1}{2} NkT [2 \ln 2 - \frac{1}{2} \ln(1-m_A^2) - \frac{1}{2} \ln(1-m_B^2)] - 2N J m_A m_B \\
&\quad - \frac{1}{2} N h (m_A - m_B) + \frac{1}{2} NkT (m_A \tanh^{-1} m_A + m_B \tanh^{-1} m_B)
\end{aligned}$$

Then differentiating with respect to m_A and m_B

$$\begin{aligned}
\frac{\partial \tilde{F}}{\partial m_A} &= \frac{1}{2} NkT \tanh^{-1} m_A - 2N J m_B - \frac{1}{2} N h \\
\frac{\partial \tilde{F}}{\partial m_B} &= \frac{1}{2} NkT \tanh^{-1} m_A - 2N J m_B + \frac{1}{2} N h
\end{aligned} \tag{43}$$

we find that \tilde{F} is minimized when

$$\begin{aligned}
m_A &= \tanh(4\beta J m_B + \beta h) \\
m_B &= \tanh(4\beta J m_B - \beta h)
\end{aligned}$$

5.

Notice that $m_A = -m_B$ is always a solution to the set of equations, this correspond to the state with $m = 0$. Summing the two equations gives

$$m = \tanh(\beta h + 4\beta J(m - n)) + \tanh(4\beta J(m + n) - \beta h) \quad (44)$$

We cannot solve this transcendental equation but we do find some useful things. There will be another solution when the slope of the right handside is bigger than 1 In other words, the critical point is given by

$$4\beta_c J[\operatorname{sech}^2(\beta_c h - 4\beta_c J_n) + \operatorname{sech}^2(4\beta_c J_n - \beta_c h)] \quad (45)$$

Therefore

$$8\beta_c J \operatorname{sech}^2(\beta_c h - 4\beta_c J_n) = 1 \quad (46)$$

6. Substitute m_A and m_B for m and n , and expand about small m

$$\begin{aligned} \tilde{F} &= -\frac{1}{2}NkT(2 \ln 2 - \frac{1}{2} \ln(1 - m_A^2) - \frac{1}{2} \ln(1 - m_B^2)) \\ &\quad - 2NJm_A m_B - \frac{1}{2}Nh(m_A - m_B) \frac{1}{2}NkT(m_A \tanh^{-1} m_A + m_B \tanh^{-1} m_B) \end{aligned} \quad (47)$$

$$\approx -\frac{1}{2}NkT[2 \ln 2 - \frac{1}{2} \ln(1 - 2n^2 + n^4) + \frac{1 + n^2}{(1 - n^2)^2}m^2 + \frac{1 + 6n^2 + n^4}{2(1 - n^2)^4}m^4] \quad (48)$$

where

$$\begin{aligned} A &= -\frac{1}{2}NkT[2 \ln 2 - \frac{1}{2} \ln(1 - 2n^2 + n^4) - 2n \tanh^{-1} n] + 2NJn^2 - Nhn \\ B &= -2NJ + \frac{1}{2}NkT \frac{1}{1 - n^2} \\ C &= \frac{1}{12}NkT \frac{1 + 2n^2 - 3n^4}{(1 - n^2)^4} \end{aligned} \quad (49)$$