

**PHYSICS 140B W26 : STATISTICAL PHYSICS  
HW ASSIGNMENT #5 SOLUTIONS**

(1) The Dieterici equation of state is

$$p(v - b) = RT \exp\left(-\frac{a}{vRT}\right).$$

(a) Find the critical point  $(p_c, v_c, T_c)$  for this equation of state

(b) Writing  $\bar{p} = p/p_c$ ,  $\bar{v} = v/v_c$ , and  $\bar{T} = T/T_c$ , rewrite the equation of state in the form  $\bar{p} = \bar{p}(\bar{v}, \bar{T})$ .

**Solution :**

(a) We have

$$p = \frac{RT}{v - b} e^{-a/vRT},$$

hence

$$\left(\frac{\partial p}{\partial v}\right)_T = p \cdot \left\{ -\frac{1}{v - b} + \frac{a}{v^2 RT} \right\}.$$

Setting the LHS of the above equation to zero, we then have

$$\frac{v^2}{v - b} = \frac{a}{RT} \Rightarrow f(u) \equiv \frac{u^2}{u - 1} = \frac{a}{bRT},$$

where  $u = v/b$  is dimensionless. Setting  $f'(u^*) = 0$  yields  $u^* = 2$ , hence  $f(u)$  on the interval  $u \in (1, \infty)$  has a unique global minimum at  $u = 2$ , where  $f(2) = 4$ . Thus,

$$v_c = 2b, \quad T_c = \frac{a}{4bR}, \quad p_c = \frac{a}{4b^2} e^{-2}.$$

(b) In terms of the dimensionless variables  $\bar{p}$ ,  $\bar{v}$ , and  $\bar{T}$ , the equation of state takes the form

$$\bar{p} = \frac{\bar{T}}{2\bar{v} - 1} \exp\left(2 - \frac{2}{\bar{v}\bar{T}}\right).$$

(2) Consider an Ising ferromagnet where the nearest neighbor exchange temperature is  $J_{NN}/k_B = 50$  K and the next nearest neighbor exchange temperature is  $J_{NNN}/k_B = 10$  K. What is the mean field transition temperature  $T_c$  if the lattice is:

- (a) square
- (b) honeycomb
- (c) triangular

- (d) simple cubic
- (e) body centered cubic

Hint : As an intermediate step, you might want to show that the mean field transition temperature is given by

$$k_B T_c^{\text{MF}} = z_1 J_{\text{NN}} + z_2 J_{\text{NNN}} ,$$

where  $z_1$  and  $z_2$  are the number of nearest neighbors and next-nearest neighbors of a given lattice site, respectively.

**Solution:**

The mean field transition temperature is given by  $k_B T_c^{\text{MF}} = \hat{J}(0)$ . With only nearest and next-nearest neighbors, we have

$$k_B T_c^{\text{MF}} = \sum_{\mathbf{R}} J(\mathbf{R}) = z_1 J_{\text{NN}} + z_2 J_{\text{NNN}} ,$$

where  $J_{\text{NN}}$  and  $J_{\text{NNN}}$  are the nearest neighbor and next nearest neighbor exchange interaction energies. According to sketches in fig. 1, we have

(a) square lattice :  $z_1 = 4$  and  $z_2 = 4$ . Thus,  $T_c^{\text{MF}} = 240$  K.

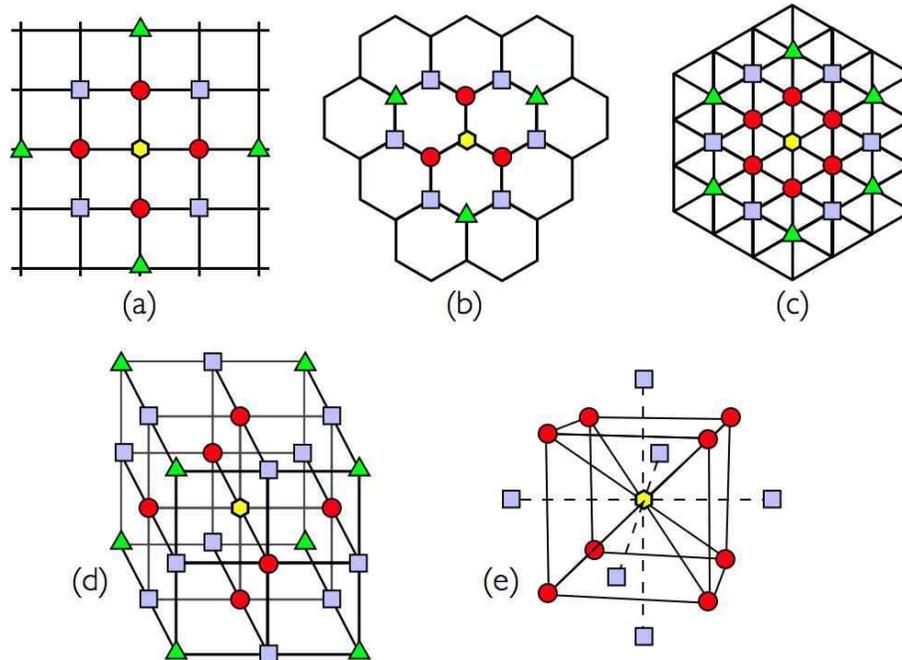


Figure 1: Nearest neighbors (red circles), next nearest neighbors (light blue squares), and some third nearest neighbors (green triangles) for five common lattices. (a) square, (b) honeycomb, (c) triangular, (d) simple cubic, and (e) body centered cubic.

- (b) honeycomb lattice :  $z_1 = 3$  and  $z_2 = 6$ . Thus,  $T_c^{\text{MF}} = 210$  K.  
(c) triangular lattice :  $z_1 = 6$  and  $z_2 = 6$ . Thus,  $T_c^{\text{MF}} = 360$  K.  
(d) simple cubic lattice :  $z_1 = 6$  and  $z_2 = 12$ . Thus,  $T_c^{\text{MF}} = 420$  K.  
(e) body-centered cubic lattice :  $z_1 = 8$  and  $z_2 = 6$ . Thus,  $T_c^{\text{MF}} = 460$  K.

(3) Consider a three state Ising model,

$$\hat{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i,$$

where  $S_i \in \{-1, 0, +1\}$ .

- (a) Writing  $S_i = m + \delta S_i$  and ignoring terms quadratic in the fluctuations, derive the mean field Hamiltonian  $H_{\text{MF}}$ .  
(b) Find the dimensionless mean field free energy density,  $f = F_{\text{MF}}/NzJ$ , where  $z$  is the lattice coordination number. You should define the dimensionless temperature  $\theta \equiv k_B T/zJ$  and the dimensionless field  $h \equiv H/zJ$ .  
(c) Find the self-consistency equation for  $m = \langle S_i \rangle$  and show that this agrees with the condition  $\partial f/\partial m = 0$ .  
(d) Expand  $f(m)$  to fourth order in  $m$  and first order in  $h$ .  
(e) Find the critical temperature  $\theta_c$ .  
(d) Find  $m(\theta_c, h)$ .

**Solution:**

(a) We have

$$\begin{aligned} S_i S_j &= (m + \delta S_i)(m + \delta S_j) \\ &= m^2 + m(\delta S_i + \delta S_j) + \delta S_i \delta S_j \\ &= -m^2 + m(S_i + S_j) + \delta S_i \delta S_j. \end{aligned}$$

We ignore the fluctuation term, resulting in the mean field Hamiltonian

$$H_{\text{MF}} = \frac{1}{2} N z J m^2 - (z J m + H) \sum_i S_i.$$

(b) The effective field is  $H_{\text{eff}} = z J m + H$ . Note that

$$\sum_S e^{H_{\text{eff}} S/k_B T} = 1 + 2 \cosh\left(\frac{z J m + H}{k_B T}\right).$$

It is convenient to adimensionalize, writing  $f = /NzJ$ ,  $\theta = k_B T / zJ$ , and  $h = H / zJ$ . Then we have

$$f(m, \theta, h) = \frac{1}{2}m^2 - \theta \ln \left( 1 + 2 \cosh \left( \frac{m+h}{\theta} \right) \right).$$

(c) Extremizing the free energy  $f(m)$  with respect to  $m$ , we obtain the mean field equation:

$$\frac{\partial f}{\partial m} = 0 \quad \Longrightarrow \quad m = \frac{2 \sinh \left( \frac{m+h}{\theta} \right)}{1 + 2 \cosh \left( \frac{m+h}{\theta} \right)}.$$

The self consistency condition is the same:

$$m = \frac{\sum_S S e^{(m+h)S/\theta}}{\sum_S e^{(m+h)S/\theta}} = \frac{2 \sinh \left( \frac{m+h}{\theta} \right)}{1 + 2 \cosh \left( \frac{m+h}{\theta} \right)}.$$

(d) We have

$$\begin{aligned} f(m) &= \frac{1}{2}m^2 - \theta \ln \left( 3 + \frac{(h+m)^2}{\theta^2} + \frac{(h+m)^4}{12\theta^4} + \dots \right) \\ &= -\theta \ln 3 + \frac{1}{2} \left( 1 - \frac{2}{3\theta} \right) m^2 + \frac{m^4}{36\theta^3} - \frac{2hm}{3\theta} + \dots \end{aligned}$$

(e) The critical temperature is identified as the value of  $\theta$  where the coefficient of the  $m^2$  term in the free energy vanishes. Thus,  $\theta_c = \frac{2}{3}$ .

(f) Setting  $\theta = \theta_c = \frac{2}{3}$ , we extremize  $f(m)$  and obtain the equation

$$f'(m, \theta_c, h) = 0 = \frac{m^3}{9\theta_c^3} - \frac{2h}{3\theta_c} \quad \Longrightarrow \quad m(\theta_c, h) = (6\theta_c^2 h)^{1/3} = \left(\frac{8}{3}h\right)^{1/3}.$$

**(4)** For the O(3) Heisenberg ferromagnet,

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j,$$

find the mean field transition temperature  $T_c^{\text{MF}}$ . Here, each  $\hat{\mathbf{n}}_i$  is a three-dimensional unit vector, which can be parameterized using the usual polar and azimuthal angles:

$$\hat{\mathbf{n}}_i = (\sin \theta_i \cos \phi_i, \sin \theta_i \sin \phi_i, \cos \theta_i).$$

The thermodynamic trace is defined as

$$\text{Tr} A(\hat{\mathbf{n}}_1, \dots, \hat{\mathbf{n}}_N) = \int \prod_{i=1}^N \frac{d\hat{\mathbf{n}}_i}{4\pi} A(\hat{\mathbf{n}}_1, \dots, \hat{\mathbf{n}}_N),$$

where

$$d\hat{\mathbf{n}}_i = \sin \theta_i d\theta_i d\phi_i .$$

*Hint : Your mean field Ansatz will look like  $\hat{\mathbf{n}}_i = \mathbf{m} + \delta\mathbf{n}_i$ , where  $\mathbf{m} = \langle \mathbf{n}_i \rangle$ . You'll want to ignore terms in the Hamiltonian which are quadratic in fluctuations, i.e.  $\delta\mathbf{n}_i \cdot \delta\mathbf{n}_j$ . You can, without loss of generality, assume  $\mathbf{m}$  to lie in the  $\hat{z}$  direction.*

**Solution :**

Writing  $\hat{\mathbf{n}}_i = \mathbf{m} + \delta\mathbf{n}_i$  and neglecting the fluctuations, we arrive at the mean field Hamiltonian

$$H_{\text{MF}} = \frac{1}{2}NzJm^2 - zJ\mathbf{m} \cdot \sum_i \hat{\mathbf{n}}_i ,$$

where  $\mathbf{m} = \langle \hat{\mathbf{n}}_i \rangle$  is assumed to be independent of the site index  $i$ . The partition function is

$$Z = e^{-\frac{1}{2}N\beta zJm^2} \left( \int \frac{d\hat{\mathbf{n}}}{4\pi} e^{\beta zJ\mathbf{m} \cdot \hat{\mathbf{n}}} \right)^N .$$

We once again adimensionalize, writing  $f = F/NzJ$  and  $\theta = k_{\text{B}}T/zJ$ . We then find

$$\begin{aligned} f(\mathbf{m}, \theta) &= \frac{1}{2}m^2 - \theta \ln \int \frac{d\hat{\mathbf{n}}}{4\pi} e^{\mathbf{m} \cdot \hat{\mathbf{n}}/\theta} \\ &= \frac{1}{2}m^2 - \theta \ln \left( \frac{\sinh(m/\theta)}{m/\theta} \right) \\ &= \frac{1}{2}m^2 - \theta \ln \left( 1 + \frac{m^2}{6\theta^2} + \frac{m^4}{120\theta^4} + \dots \right) \\ &= \frac{1}{2} \left( 1 - \frac{1}{3\theta} \right) m^2 + \frac{m^4}{180\theta^3} + \dots \end{aligned}$$

Setting the coefficient of the quadratic term to zero, we obtain  $\theta_c = \frac{1}{3}$ .

(5) The spin lattice Hamiltonian for the three state ( $\mathbb{Z}_3$ ) clock model is written

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\mathbf{n}}_i \cdot \hat{\mathbf{n}}_j ,$$

where each local unit vector  $\hat{\mathbf{n}}_i$  is a planar spin which can take one of three possible values:

$$\hat{\mathbf{n}} = \hat{\mathbf{e}}_1 \quad , \quad \hat{\mathbf{n}} = -\frac{1}{2}\hat{\mathbf{e}}_1 + \frac{\sqrt{3}}{2}\hat{\mathbf{e}}_2 \quad , \quad \hat{\mathbf{n}} = -\frac{1}{2}\hat{\mathbf{e}}_1 - \frac{\sqrt{3}}{2}\hat{\mathbf{e}}_2 \quad .$$

Note that the *internal space* in which each unit vector  $\hat{\mathbf{n}}_i$  exists is distinct from the physical Euclidean space in which the lattice points reside.

(a) Consider the clock model on a lattice of coordination number  $z$ . Make the mean field assumption  $\langle \hat{\mathbf{n}}_i \rangle = m \hat{\mathbf{e}}_1$ . Expanding the Hamiltonian to linear order in the fluctuations, derive the mean field Hamiltonian for this model  $\hat{H}_{\text{MF}}$ .

(b) Rescaling  $\theta = k_B T / zJ$  and  $f = F / NzJ$ , where  $F$  is the Helmholtz free energy and  $N$  is the number of sites, find  $f(m, \theta)$ .

(c) Is the transition second order or first order? Why?

(d) Find the equations which determine the critical temperature  $\theta_c$ .

(e) Show that this model is equivalent to the three state Potts model. Is the  $\mathbb{Z}_4$  clock model equivalent to the four state Potts model? Why or why not?

**Solution :**

(a) We can solve the mean field theory on a general lattice of coordination number  $z$ . The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \frac{1}{2} NzJm^2 - zJm \hat{\mathbf{e}}_1 \cdot \sum_i \hat{\mathbf{n}}_i \quad .$$

(b) We have

$$\begin{aligned} f(m, \theta) &= \frac{1}{2} m^2 - \theta \ln \text{Tr}_{\hat{\mathbf{n}}} \exp(m \hat{\mathbf{e}}_1 \cdot \hat{\mathbf{n}} / \theta) \\ &= \frac{1}{2} m^2 - \theta \ln \left( \frac{1}{3} e^{m/\theta} + \frac{2}{3} e^{-m/2\theta} \right) \\ &= \frac{1}{2} \left( 1 - \frac{1}{2\theta} \right) m^2 - \frac{m^3}{24\theta^2} + \frac{m^4}{64\theta^3} + \mathcal{O}(m^5) \quad . \end{aligned}$$

Here we have defined  $\text{Tr}_{\hat{\mathbf{n}}} = \frac{1}{3} \sum_{\hat{\mathbf{n}}} \text{Tr}$  as the normalized trace. The last line is somewhat tedious to obtain, but is not necessary for this problem.

(c) Since  $f(m, \theta) \neq f(-m, \theta)$ , the Landau expansion of the free energy (other than constants) should include terms of all orders starting with  $\mathcal{O}(m^2)$ . This means that there will in general be a cubic term, hence we expect a first order transition.

(d) At the critical point, the magnetization  $m = m_c$  is finite. We then have to solve two equations to determine  $m_c$  and  $\theta_c$ . The first condition is that the free energy have degenerate minima at the transition, *i.e.*  $f(m = 0, \theta = \theta_c) = f(m = m_c, \theta = \theta_c)$ . Thus,

$$\frac{1}{2} m^2 = \theta \ln \left( \frac{1}{3} e^{m/\theta} + \frac{2}{3} e^{-m/2\theta} \right) \quad .$$

The second is the mean field equation itself, *i.e.*

$$\frac{\partial f}{\partial m} = 0 \quad \Rightarrow \quad m = \frac{e^{m/\theta} - e^{-m/2\theta}}{e^{m/\theta} + 2e^{-m/2\theta}} \quad .$$

These equations for  $(m, \theta) = (m_c, \theta_c)$  are nonlinear and hence we cannot expect to solve them analytically.

If, however, the transition were *very weakly* first order, then  $m_c$  is by assumption small, which means we should be able to get away with the fourth order Landau expansion of

$\varepsilon_{\sigma\sigma'}^{\text{clock}}$	$0^\circ$	$120^\circ$	$240^\circ$
$0^\circ$	$-J$	$\frac{1}{2}J$	$\frac{1}{2}J$
$120^\circ$	$\frac{1}{2}J$	$-J$	$\frac{1}{2}J$
$240^\circ$	$\frac{1}{2}J$	$\frac{1}{2}J$	$-J$

Table 1:  $\mathbb{Z}_3$  clock model energy matrix.

the free energy. For a free energy  $f(m) = \frac{1}{2}am^2 - \frac{1}{3}ym^3 + \frac{1}{4}bm^4$ , setting  $f(m) = f'(m) = 0$  we obtain  $m = 3a/y$  and  $y^2 = 9ab$ . For our system,  $a = 1 - \frac{1}{2\theta}$ ,  $y = \frac{1}{8\theta^2}$ , and  $b = \frac{1}{16\theta^3}$ . We then obtain  $\theta_c = \frac{5}{9}$ . Note that the second order term in  $f(m)$  changes sign at  $\theta^* = \frac{1}{2}$ , so  $\theta_c > \theta^*$  is consistent with the fact that the second order transition is preempted by the first order one. Now we may ask, just how good was our assumption that the transition is weakly first order. To find out, we compute  $m_c = 3a/y = 24\theta_c(\theta_c - \frac{1}{2}) = \frac{20}{27}$  which is not particularly small compared to unity. Hence the assumption that our transition is weakly first order is not justified.

(e) Let  $\varepsilon(\hat{n}, \hat{n}') = -J\hat{n} \cdot \hat{n}'$  be the energy for a given link. The unit vectors  $\hat{n}$  and  $\hat{n}'$  can each point in any of three directions, which we can label as  $0^\circ$ ,  $120^\circ$ , and  $240^\circ$ . The matrix of possible bond energies is shown in Tab. 1.

$\varepsilon_{\sigma\sigma'}^{\text{Potts}}$	A	B	C
A	$-\tilde{J}$	0	0
B	0	$-\tilde{J}$	0
C	0	0	$-\tilde{J}$

Table 2:  $q = 3$  Potts model energy matrix.

Now consider the  $q = 3$  Potts model, where the local states are labeled  $|A\rangle$ ,  $|B\rangle$ , and  $|C\rangle$ . The Hamiltonian is

$$\hat{H} = -\tilde{J} \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j} \quad .$$

The interaction energy matrix for the Potts model is given in Tab. 2.

We can in each case label the three states by a local variable  $\sigma \in \{1, 2, 3\}$ , corresponding, respectively, to  $0^\circ$ ,  $120^\circ$ , and  $240^\circ$  for the clock model and to A, B, and C for the Potts model. We then observe

$$\varepsilon_{\sigma\sigma'}^{\text{clock}}(J) = \varepsilon_{\sigma\sigma'}^{\text{Potts}}\left(\frac{3}{2}J\right) + \frac{1}{2}J \quad .$$

Thus, the free energies satisfy

$$F^{\text{clock}}(J) = \frac{1}{4}NzJ + F^{\text{Potts}}\left(\frac{3}{2}J\right) \quad ,$$

and the models are equivalent. However, the  $\mathbb{Z}_q$  clock model and  $q$ -state Potts model are *not* equivalent for  $q > 3$ . Can you see why? *Hint: construct the corresponding energy matrices for  $q = 4$ .*