PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #4 SOLUTIONS

(1) Consider the equation of state

$$p\sqrt{v^2-b^2} = RT\,\exp\left(-\frac{a}{RTv^2}\right) .$$

(a) Find the critical point (v_c, T_c, p_c).

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

(c) Expanding $\bar{p} = 1 + \pi$, $\bar{v} = 1 + \epsilon$, and $\bar{T} = 1 + t$, find $\epsilon_{\mathrm{liq}}(t)$ and $\epsilon_{\mathrm{gas}}(t)$ for $-1 \ll t < 0$.

Solution :

(a) We write

$$p(T,v) = \frac{RT}{\sqrt{v^2-b^2}}\,e^{-a/RTv^2} \qquad \Rightarrow \qquad \left(\frac{\partial p}{\partial v}\right)_T = \left(\frac{2a}{RTv^3} - \frac{v}{v^2-b^2}\right) p .$$

Thus, setting $\left(\frac{\partial p}{\partial v}\right)_T = 0$ yields the equation

$$\frac{2a}{b^2RT} = \frac{u^4}{u^2-1} \equiv \varphi(u) ,$$

where $u \equiv v/b$. Differentiating $\varphi(u)$, we find it has a unique minimum at $u^* = \sqrt{2}$, where $\varphi(u^*) = 4$. Thus,

$$T_c = \frac{a}{2b^2R} \quad , \quad v_c = \sqrt{2}\,b \quad , \quad p_c = \frac{a}{2eb^2} .$$

(b) In terms of $\bar{p}$, $\bar{v}$, and $\bar{T}$, we have the universal equation of state

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

(c) With $\bar{p} = 1 + \pi$, $\bar{v} = 1 + \epsilon$, and $\bar{T} = 1 + t$, we have from ch. 7 of the Lecture Notes,

$$\epsilon_{\mathsf{L,G}} = \mp\left(\frac{6\,\pi_{\epsilon t}}{\pi_{\epsilon\epsilon\epsilon}}\right)^{1/2}(-t)^{1/2} + \mathcal{O}(t) .$$

From `Mathematica` we find $\pi_{\epsilon t} = -2$ and $\pi_{\epsilon\epsilon\epsilon} = -16$, hence

$$\epsilon_{\mathsf{L,G}} = \mp\tfrac{\sqrt{3}}{2}\,(-t)^{1/2} + \mathcal{O}(t) .$$

(2) Consider an Ising ferromagnet where the nearest neighbor exchange temperature is $J_{\rm NN}/k_{\rm B} = 50\,{\rm K}$ and the next nearest neighbor exchange temperature is $J_{\rm NNN}/k_{\rm B} = 10\,{\rm K}$. What is the mean field transition temperature $T_{\rm c}$ 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

$$k_{\rm B}T_{\rm c}^{\rm MF} = z_1\, J_{\rm NN} + z_2\, J_{\rm NNN}\ ,$$

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 $k_{\rm B}T_{\rm c}^{\rm MF} = \hat{J}(0)$. With only nearest and next-nearest neighbors, we have

$$k_{\rm B}T_{\rm c}^{\rm MF} = \sum_{\boldsymbol{R}} J(\boldsymbol{R}) = z_1\, J_{\rm NN} + z_2\, J_{\rm NNN}\ ,$$

where $J_{\rm NN}$ and $J_{\rm NNN}$ 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 $z_2 = 4 \Rightarrow T_{\rm c}^{\rm MF} = 240\,{\rm K}$.
(b) honeycomb lattice : $z_1 = 3$ and $z_2 = 6 \Rightarrow T_{\rm c}^{\rm MF} = 210\,{\rm K}$.
(c) triangular lattice : $z_1 = 6$ and $z_2 = 6 \Rightarrow T_{\rm c}^{\rm MF} = 360\,{\rm K}$.
(d) simple cubic lattice : $z_1 = 6$ and $z_2 = 12 \Rightarrow T_{\rm c}^{\rm MF} = 420\,{\rm K}$.
(e) body-centered cubic lattice : $z_1 = 8$ and $z_2 = 6 \Rightarrow T_{\rm c}^{\rm MF} = 460\,{\rm K}$.

(3) Consider a three state Ising model,

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

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

(a) Writing $S_i = m + \delta S_i$ and ignoring terms quadratic in the fluctuations, derive the mean field Hamiltonian $H_{\rm MF}$.

(b) Find the dimensionless mean field free energy density, $f = F_{\rm MF}/NzJ$, where z is the lattice coordination number. You should define the dimensionless temperature $\theta \equiv k_{\rm B}T/zJ$ and the dimensionless field $h \equiv B/zJ$.

(c) Find the self-consistency equation for $m = \langle S_i \rangle$ and show that this agrees with the condition $\partial f/\partial m = 0$.

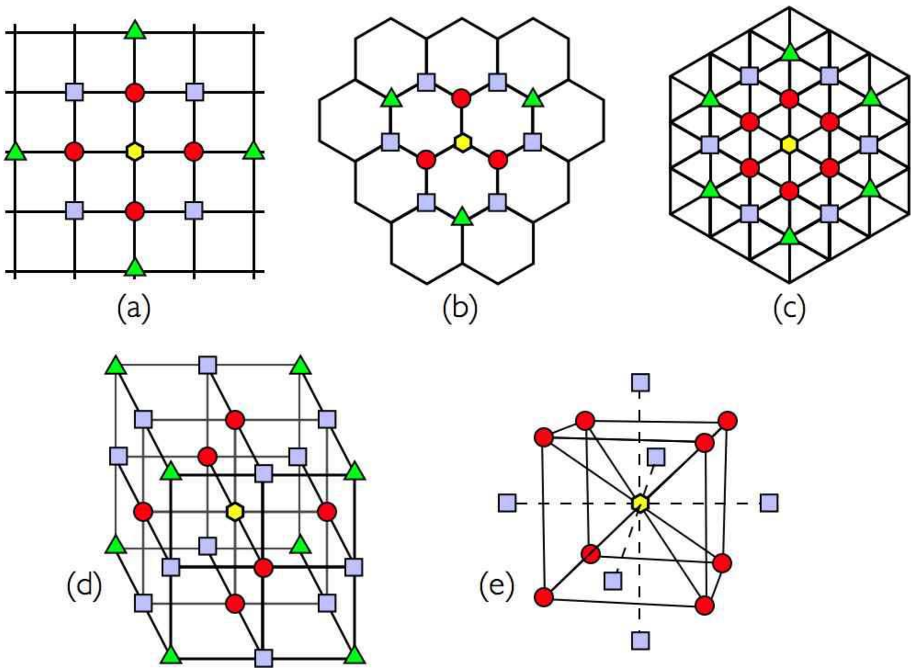

Figure 1: Nearest neighbors (red circles), next nearest neighbors (light blue squares), and some third nearest neighbors (green triangles) for five common lattices. (a) square, (b) honeycomb, (c) triangular, (d) simple cubic, and (e) body centered cubic.

(d) Expand $f(m)$ to fourth order in m and first order in h.

(e) Find the critical temperature θ_{c}.

(f) Find $m(\theta_{\mathrm{c}}, h)$.

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

$$H_{\mathrm{MF}} = \tfrac{1}{2} N z J m^2 - \big(zJm + B\big) \sum_i S_i\ .$$

(b) The effective field is $B_{\mathrm{eff}} = zJm + B$. Note that

$$\sum_S e^{B_{\mathrm{eff}} S / k_{\mathrm{B}} T} = 1 + 2 \cosh\!\left(\frac{zJm + B}{k_{\mathrm{B}} T}\right) .$$

It is convenient to adimensionalize, writing $f = /NzJ$, $\theta = k_{\rm B}T/zJ$, and $h = B/zJ$. Then we have

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

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

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

The self consistency condition is the same:

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

(d) We have

$$\begin{aligned} f(m) &= \tfrac{1}{2}m^2 - \theta \ln\bigg(3 + \frac{(h+m)^2}{\theta^2} + \frac{(h+m)^4}{12\theta^4} + \ldots\bigg) \\ &= -\theta \ln 3 + \tfrac{1}{2}\Big(1 - \frac{2}{3\theta}\Big)\, m^2 + \frac{m^4}{36\theta^3} - \frac{2hm}{3\theta} + \ldots . \end{aligned}$$

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

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

$$f'(m,\theta_{\rm c},h) = 0 = \frac{m^3}{9\theta_{\rm c}^3} - \frac{2h}{3\theta_{\rm c}} \qquad \Longrightarrow \qquad m(\theta_{\rm c},h) = \big(6\,\theta_{\rm c}^2\, h\big)^{1/3} = \big(\tfrac{8}{3}h\big)^{1/3} .$$

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

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

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

$$\hat{\boldsymbol{\Omega}}_i = \big(\sin\theta_i\,\cos\phi_i\,,\,\sin\theta_i\,\sin\phi_i\,,\,\cos\theta_i\big) .$$

The thermodynamic trace is defined as

$$\mathrm{Tr}\, A(\hat{\boldsymbol{\Omega}}_1\,,\,\ldots\,,\,\hat{\boldsymbol{\Omega}}_N) = \int\prod_{i=1}^{N} \frac{d\Omega_i}{4\pi}\, A(\hat{\boldsymbol{\Omega}}_1\,,\,\ldots\,,\,\hat{\boldsymbol{\Omega}}_N) ,$$

where

$$d\Omega_i = \sin\theta_i \, d\theta_i \, d\phi_i \ .$$

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

Solution:

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

$$H_{\text{MF}} = \tfrac{1}{2} N z J \boldsymbol{m}^2 - z J \boldsymbol{m} \cdot \sum_i \hat{\boldsymbol{\Omega}}_i \ ,$$

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

$$Z = e^{-\frac{1}{2} N \beta z J \boldsymbol{m}^2} \left(\int \frac{d\Omega}{4\pi} \, e^{\beta z J \boldsymbol{m} \cdot \hat{\boldsymbol{\Omega}}} \right)^N \ .$$

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

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

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