PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #7 SOLUTIONS

(1) Consider the equation of state

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

(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 $\epsilon_{liq}(t)$ and $\epsilon_{gas}(t)$ for $-1 \ll t < 0$.

Solution :

(a) We write

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

Thus, setting $\big(\frac{\partial p}{\partial v}\big)_T = 0$ 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

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

(c) With $\bar{p} = 1+\pi$, $\bar{v} = 1+\epsilon$, and $\bar{T} = 1+t$, we have from Eq. 7.32 of the Lecture Notes,

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

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 a nearest neighbor two-state Ising *antiferromagnet* on a triangular lattice. The Hamiltonian is

$$\hat{H} = J \sum_{\langle ij \rangle} \sigma_i \sigma_j - \mathsf{H} \sum_i \sigma_i \ ,$$

with $J > 0$.

(a) Show graphically that the triangular lattice is *tripartite*, *i.e.* that it may be decomposed into three component sublattices A, B, and C such that every neighbor of A is either B or C, *etc.*

(b) Use a variational density matrix which is a product over single site factors, where

$$\begin{aligned} \rho(\sigma_i) &= \frac{1+m}{2}\, \delta_{\sigma_i,+1} + \frac{1-m}{2}\, \delta_{\sigma_i,-1} \qquad \text{if } i \in \text{A or } i \in \text{B} \\ &= \frac{1+m_{\text{C}}}{2}\, \delta_{\sigma_i,+1} + \frac{1-m_{\text{C}}}{2}\, \delta_{\sigma_i,-1} \qquad \text{if } i \in \text{C} \ . \end{aligned}$$

Compute the variational free energy $F(m, m_{\text{C}}, T, \mathsf{H}, N)$.

(c) Find the mean field equations.

(d) Find the mean field phase diagram.

(e) While your mean field analysis predicts the existence of an ordered phase, it turns out that $T_{\text{c}} = 0$ for this model because it is so highly frustrated when $h = 0$. The ground state is highly degenerate. Show that for any ground state, no triangle can be completely ferromagnetically aligned. What is the ground state energy? Find a lower bound for the ground state entropy per spin.

Solution :

(a) See fig. 1.

(b) Of the $3N$ links of the lattice, N are between A and B sites, N are between A and C sites, and N are between B and C sites. Thus the mean field energy is

$$E = NJm^2 + 2NJmm_{\text{C}} - \tfrac{2}{3} N\mathsf{H}m - \tfrac{1}{3} N\mathsf{H}m_{\text{C}} \ .$$

The entropy of the A and B sublattices is $S_{\text{A}} = S_{\text{B}} = \frac{2}{3} N s(m)$, while that for the C sublattice is $S_{\text{C}} = \frac{1}{3} N s(m_{\text{C}})$, where

$$s(m) = -\left[\left(\frac{1+m}{2}\right) \ln\left(\frac{1+m}{2}\right) + \left(\frac{1-m}{2}\right) \ln\left(\frac{1-m}{2}\right) \right] .$$

The free energy is $F = E - TS$. We define $f \equiv F/2JN$, $\theta \equiv k_{\text{B}}T/6J$, and $h \equiv \mathsf{H}/6J$. Then

$$f(m, m_{\text{C}}, \theta, h) = \tfrac{1}{2} m^2 + m m_{\text{C}} - 2hm - hm_{\text{C}} - 2\theta s(m) - \theta s(m_{\text{C}}) \ .$$

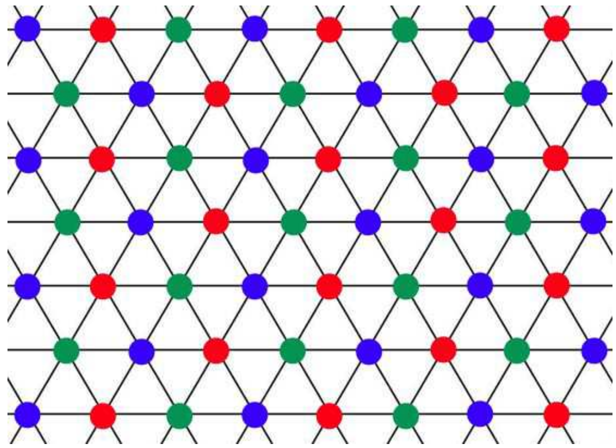

Figure 1: The three triangular sublattices of the (tripartite) triangular lattice.

(c) The mean field equations are

$$\frac{\partial f}{\partial m} = 0 = m + m_{\rm C} - 2h + \theta \ln\!\left(\frac{1+m}{1-m}\right)$$

$$\frac{\partial f}{\partial m_{\rm C}} = 0 = m - h + \tfrac{1}{2}\theta \ln\!\left(\frac{1+m_{\rm C}}{1-m_{\rm C}}\right) .$$

Equivalently,

$$m = \tanh\!\left(\frac{2h - m - m_{\rm C}}{2\theta}\right) \qquad , \qquad m_{\rm C} = \tanh\!\left(\frac{h-m}{\theta}\right) .$$

(d) The order parameter for our model is the difference in sublattice magnetizations, $\varepsilon \equiv m_{\rm C} - m$. Let us first consider the zero temperature limit, $\theta \to 0$, for which the entropy term makes no contribution in the free energy. We compare two competing states: the ferromagnetic state with $m = m_{\rm C} = 1$, and the antiferromagnetic state with $m = 1$ and $m_{\rm C} = -1$. The energies of these two states are

$$e_0(1,1,h) = \tfrac{3}{2} - 3h$$

$$e_0(1,-1,h) = -\tfrac{1}{2} - h .$$

We see that for $h < 1$ the AF configuration wins (*i.e.* has lower energy per site e_0), while for $h > 1$ the F configuration wins. Thus, at $\theta = 0$ there is a first order transition from AF to F at $h_c = 1$.

Next, let us examine the behavior with θ when $h = 0$. We can combine the two mean field equations to give

$$m + \theta \,\ln\!\left(\frac{1+m}{1-m}\right) = \tanh\left(m/\theta\right) .$$

Expanding in powers of m, we equate the coefficient of the linear term on either side to identify θ_c and thus we obtain the equation $2\theta^2 + \theta - 1 = (2\theta - 1)(\theta + 1) = 0$, hence $\theta_c(h=0) = \frac{1}{2}$.

We identify the order parameter as $\varepsilon = m_C - m$, the difference in the sublattice magnetizations. We now seek the phase boundary $h(\theta)$ along which the order parameter vanishes in the (θ, h) plane. To this end, we write the two mean field equations in terms of m and ε, rather than m and m_C. We find

$$m + \tfrac{1}{2}\varepsilon = h - \frac{\theta}{2}\ln\left(\frac{1+m}{1-m}\right)$$
$$m = h - \frac{\theta}{2}\ln\left(\frac{1+m+\varepsilon}{1-m-\varepsilon}\right) .$$

Taking the difference, we obtain

$$\varepsilon = \theta \ln\left(\frac{1+\frac{\varepsilon}{1+m}}{1-\frac{\varepsilon}{1-m}}\right) = \frac{2\varepsilon\theta}{1-m^2} + \mathcal{O}\big(\varepsilon^2\big) .$$

Along the phase boundary, *i.e.* in the $\varepsilon \to 0$ limit, we therefore have

$$\frac{2\theta}{1-m^2} = 1 .$$

We also have the mean field equation for m,

$$m = \tanh\left(\frac{h-m}{\theta}\right) .$$

Putting these together, we obtain the curve

$$h^*(\theta) = \sqrt{1-2\theta} + \frac{\theta}{2}\ln\left(\frac{1+\sqrt{1-2\theta}}{1-\sqrt{1-2\theta}}\right) .$$

The phase boundary is shown in Fig. 2.

If we eliminate m_C through the second mean field equation, we can generate the Landau expansion

$$f(m,\theta,h) = -3\ln(2)\,\theta + \big(\theta - \tfrac{1}{2}\big)\big(\theta^{-1}+1\big)\,m^2 + \tfrac{1}{6}\big(\theta + \tfrac{1}{2}\theta^{-3}\big)\,m^4$$
$$- 2\theta^{-1}\big(\theta - \tfrac{1}{2}\big)\,hm - \tfrac{1}{3}\theta^{-3}hm^3 + \mathcal{O}\big(m^6, hm^5, h^3\big)$$

The full expression $f(m, m_C(m), \theta, h)$ is shown as a function of m for various values of θ and h in fig. 3. Thus, we obtain a Landau theory with a second order transition at $\theta_c = \frac{1}{2}$. We retain the $\mathcal{O}\big(hm^3\big)$ term because the coefficient of hm vanishes at $\theta = \theta_c$. Differentiating with respect to m, we obtain

$$\frac{\partial f}{\partial m} = 0 = 2\theta^{-1}\big(\theta+1\big)\big(\theta - \tfrac{1}{2}\big)\,m + \tfrac{1}{3}\theta^{-3}\big(1+2\theta^4\big)\,m^3 - 2\theta^{-1}\big(\theta - \tfrac{1}{2}\big)\,h - \theta^{-2}hm^2$$

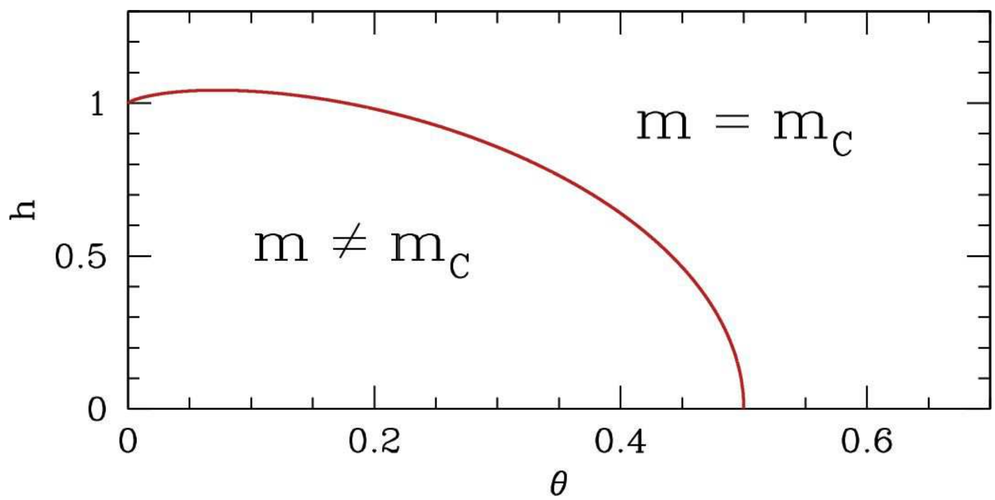

Figure 2: Phase diagram for the mean field theory of problem 2.

Thus,

$$m(\theta, h_c) = \sqrt{2}\,(\theta_c - \theta)_+^{1/2} + \mathcal{O}\big(|\theta - \theta_c|^{3/2}\big)$$

$$m(\theta, h) = \tfrac{2}{3}h + \mathcal{O}(h^3)$$

$$m(\theta_c, h) = \tfrac{4}{3}h + \mathcal{O}(h^3)\ .$$

Note that $h_c = 0$. In the second equation, we have $\epsilon \equiv \theta - \theta_c \to 0$ with $\epsilon \gg h$, while in the third equation we have $h \to 0$ with $\epsilon \equiv 0$, so the two equations represent two different limits. We obtain the exponents $\alpha = 0$, $\beta = \frac{1}{2}$, $\gamma = 0$, $\delta = 1$. This seemingly violates the Rushbrooke scaling law $\alpha + 2\beta + \gamma = 2$, but satisfies the Griffiths relation $\beta + \gamma = \beta\delta$. However, this is because we are using the wrong field. Rather than defining the exponents γ and δ with respect to a uniform field h, we should instead consider a *staggered* field h_s such that $h_A = h_B = h_s$ but $h_C = -h_s$.

(e) With antiferromagnetic interactions and $h = 0$, it is impossible for every link on an odd-membered ring (*e.g.* a triangle) to be satisfied. This is because on a k-site ring (with $(k+1) \equiv 1$), taking the product of $\sigma_j \sigma_{j+1}$ over all links on the ring gives

$$(\sigma_1\sigma_2)(\sigma_2\sigma_3)\cdots(\sigma_k\sigma_1) = 1\ ,$$

If we assume, however, that each link satisfies the antiferromagnetic interaction, then $\sigma_j \sigma_{j+1} = -1$ and the product would be $(-1)^k = -1$ since k is odd. So not all odd-membered rings can be completely satisfied. Clearly the best we can do on any odd-membered ring is to have $k - 1$ of the bonds antiferromagnetically aligned and the remaining bond ferromagnetically aligned.

Now let us decompose the triangular lattice into A, B, and C sublattices. If we place all spins on the A and B sublattices are up ($\sigma = +1$) and all spins on the C sublattice are

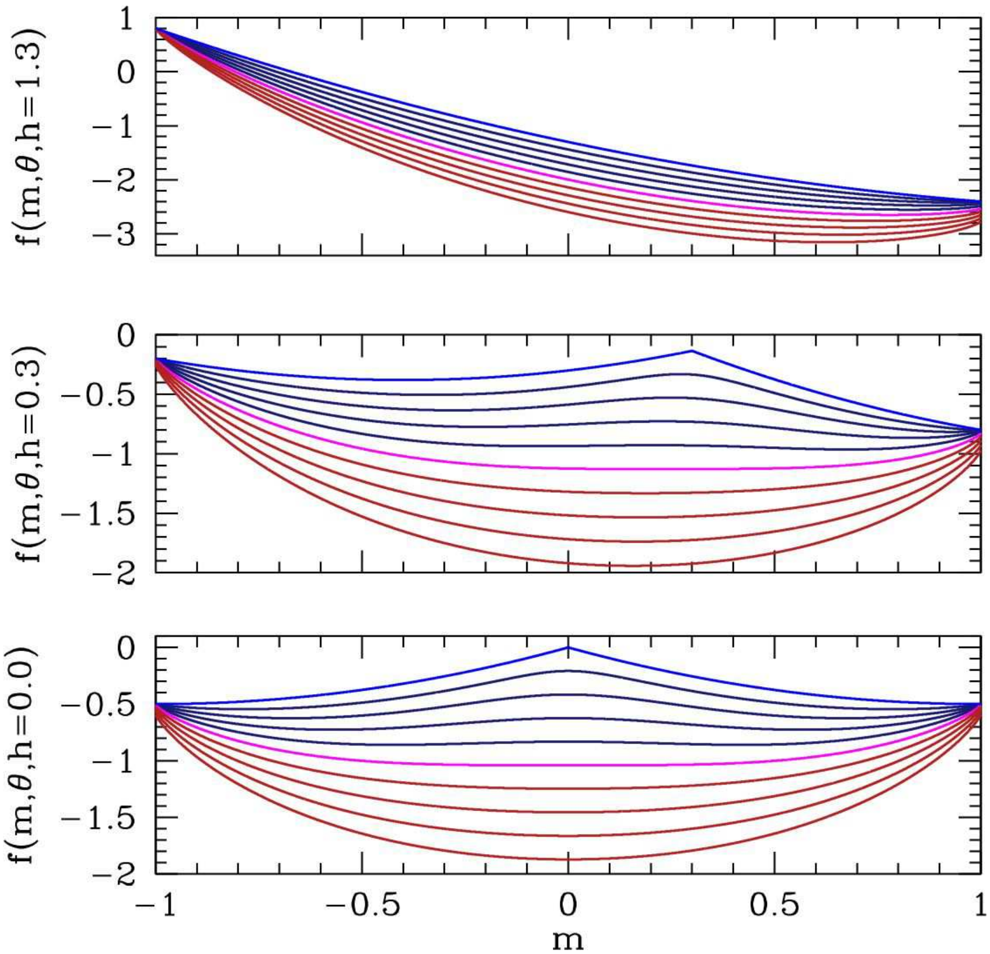

Figure 3: Free energy for the mean field theory of problem 2 at ten equally spaced dimensionless temperatures between $\theta = 0.0$ and $\theta = 0.9$. Bottom panel: $h = 0$; middle panel: $h = 0.3$; top panel: $h = 1.3$.

down ($\sigma = -1$), then each elementary triangle has two AF bonds and one F bond, which is the best we can do for the nearest neighbor triangular lattice Ising antiferromagnet. The energy of this configuration is given in part (b) above: $E = NJm^2 + 2NJmm_{\rm C} = -NJ$, since $m = 1$ and $m_{\rm C} = -1$. However, it is clear that at each site of the B sublattice, the choice of σ_i is arbitrary. This is because one third of all the links on the lattice are AC links, and they are already antiferromagnetically aligned. Now there are $\frac{1}{3}N$ sites on each of the sublattices, hence we have identified $2^{N/3}$ degenerate ground states. This set of ground state configurations is not complete, however. We could immediately double it simply by choosing to reverse spins on the A sublattice instead, leaving the B sublattice with $m_{\rm B} = 1$. But even this enumeration is not complete – we have simply identified a lower bound to the number of degenerate ground states. The ground state entropy per spin is then

$$\frac{S_0}{N} \geq \tfrac{1}{3} \ln 2 \approx 0.23105 \ .$$

The exact value, obtained by Wannier and by Houtappel in 1950, is $s_0 \approx 0.3231$ per spin. So there are exponentially (in the system size!) many more ground states than we have identified here.

And now, a disappointment. It turns out that at $h = 0$, the model is exactly solvable, and there is no phase transition at any temperature θ. The ground state at $\theta = 0$ has finite entropy per site, as we have discussed. For finite $h \in (0,1)$, there is a finite $\theta_c(h)$ which goes to zero as one approaches either endpoint. Thus, the actual phase diagram is quite different than that in Fig. 3. The boundary of the ordered phase does not intersect the θ axis at a finite value, but instead bends back and intersects the origin.

(3) Consider a spin-S magnet on a cubic lattice system with mixed ferromagnetic and antiferromagnetic interactions:

$$J_{ij} = \begin{cases} +J_1 > 0 & \text{6 nearest neighbors} \\ -J_2 < 0 & \text{12 next-nearest neighbors} \\ 0 & \text{otherwise .} \end{cases}$$

(a) Find $\hat{J}(\boldsymbol{q})$. Show that the ordering wavevector $\boldsymbol{Q}$ depends on the ratio $r = J_2/J_1$, with $\boldsymbol{Q} = 0$ for $r < r_c$ and $\boldsymbol{Q} \neq 0$ for $r > r_c$. Find r_c and $\boldsymbol{Q}$ in the latter regime. In general $\boldsymbol{Q}$ is incommensurate with the lattice. Such a system is called a *helimagnet*. *Hint : Assume* $\boldsymbol{Q} = Q(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$*, which is consistent with the cubic symmetry.*

(b) Find the critical temperature T_c where order sets in for the cases $r < r_c$ and $r > r_c$.

(c) Find the uniform susceptibility $\chi(T) \equiv \hat{\chi}(\boldsymbol{q} = 0, T)$. Over what range of r is it resembling that of a Curie-Weiss ferromagnet, *i.e.* with a positive T-axis intercept for $\chi^{-1}(T)$, and over what range is it resembling that of a Curie-Weiss antiferromagnet, *i.e.* with a negative T-axis intercept for $\chi^{-1}(T)$?

Solution :

(a) We have

$$\hat{J}(\boldsymbol{q}) = 2J_1\big[\cos(q_x a) + \cos(q_y a) + \cos(q_z a)\big]$$
$$- 4J_2\big[\cos(q_x a)\cos(q_y a) + \cos(q_x a)\cos(q_z a) + \cos(q_y a)\cos(q_z a)\big] .$$

Taking $\boldsymbol{q} \equiv q\,(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$, we define $c \equiv \cos(qa)$, in which case

$$\hat{J}(q) = 6J_1\big(c - 2rc^2\big) \quad ,$$

with $r \equiv J_2/J_1$. Differentiating to find the value $q = Q$ which maximizes $\hat{J}(\boldsymbol{q})$, we find $c = 1/4r$, which is only possible if $r > \frac{1}{4}$. If $r < \frac{1}{4}$, the maximum occurs at $c = 1$, *i.e.* $Q = 0$. Thus, the ordering wavevector is then

$$Qa = \begin{cases} 0 & \text{if } J_2 < \frac{1}{4}J_1 \\ \cos^{-1}(J_1/4J_2) & \text{if } J_2 > \frac{1}{4}J_1 \end{cases} .$$

(b) For $r > \frac{1}{4}$ the order is in general *incommensurate* with the lattice, meaning Qa is not any rational multiple of 2π. The maximum value of $\hat{J}(\boldsymbol{q})$ is

$$\hat{J}(\boldsymbol{Q}) = \begin{cases} 6(J_1 - 2J_2) & \text{if } J_2 < \frac{1}{4}J_1 \\ 3J_1^2/4J_2 & \text{if } J_2 > \frac{1}{4}J_1 \end{cases} ,$$

and therefore

$$\frac{k_{\mathrm{B}}T_{\mathrm{c}}}{6J_1} = \begin{cases} (1-2r) & \text{if } r < \frac{1}{4} \\ 1/8r & \text{if } r > \frac{1}{4} \end{cases} .$$

Note that $T_{\mathrm{c}}(J_1, r)$ is continuous at the transition to the incommensurate phase ($r = \frac{1}{4}$).

(c) The uniform susceptibility is

$$\chi(T) = \frac{1}{\chi^{-1}(T) - \hat{J}(0)} = \left[\frac{3k_{\mathrm{B}}T}{S(S+1)} - (6J_1 - 12J_2)\right]^{-1}$$
$$= \frac{S(S+1)/3k_{\mathrm{B}}}{T - (1-2r)\,T_1} ,$$

where $T_1 \equiv 2J_1/S(S+1)k_{\mathrm{B}}$. The intercept is at $T^* = (1-2r)T_1$. Thus, in the commensurate phase, where $r < \frac{1}{4}$, T^* is always positive, which is to say FM-like. In the incommensurate phase, for $r \in [\frac{1}{4}, \frac{1}{2})$, T^* remains positive, but switches sign to the AF-like case for $r > \frac{1}{2}$.