

**PHYSICS 140B W26 : STATISTICAL PHYSICS
FINAL EXAMINATION SOLUTIONS**

(1) Consider the 4-state clock model on a one-dimensional ring of N sites. The Hamiltonian is given by

$$\hat{H} = -J \sum_{j=1}^N \hat{\mathbf{n}}_j \cdot \hat{\mathbf{n}}_{j+1} - H \hat{\mathbf{x}} \cdot \sum_{j=1}^N \hat{\mathbf{n}}_j \quad .$$

Each unit vector $\hat{\mathbf{n}}_j$ can take one of four possible values: $\hat{\mathbf{n}}_j \in \{\hat{\mathbf{x}}, \hat{\mathbf{y}}, -\hat{\mathbf{x}}, -\hat{\mathbf{y}}\}$.

(a) Find an expression for the symmetric transfer matrix $T_{\hat{\mathbf{n}}, \hat{\mathbf{n}'}}$ and express it in matrix form. [10 points]

(b) Find all the eigenvalues of the transfer matrix when $H = 0$. [8 points]

Big Hint: For the matrix

$$T = \begin{pmatrix} r & 1 & r^{-1} & 1 \\ 1 & r & 1 & r^{-1} \\ r^{-1} & 1 & r & 1 \\ 1 & r^{-1} & 1 & r \end{pmatrix}$$

the four (unnormalized) eigenvectors may be taken to be

$$\psi_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad \psi_2 = \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \quad \psi_3 = \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, \quad \psi_4 = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} \quad .$$

(c) Find the free energy per site in the thermodynamic limit $N \rightarrow \infty$ when $H = 0$. Interpret the $T \rightarrow \infty$ limit of your result. [7 points]

Solution :

(a) The transfer matrix may be written symmetrically as

$$\begin{aligned} T_{\hat{\mathbf{n}}, \hat{\mathbf{n}'}} &= e^{\beta J \hat{\mathbf{n}} \cdot \hat{\mathbf{n}'}} e^{\beta H \hat{\mathbf{x}} \cdot \hat{\mathbf{n}}/2} e^{\beta H \hat{\mathbf{x}} \cdot \hat{\mathbf{n}'}/2} \\ &= \begin{pmatrix} e^{\beta J} e^{\beta H} & e^{\beta H/2} & e^{-\beta J} & e^{\beta H/2} \\ e^{\beta H/2} & e^{\beta J} & e^{-\beta H/2} & e^{-\beta J} \\ e^{-\beta J} & e^{-\beta H/2} & e^{\beta J} e^{-\beta H} & e^{-\beta H/2} \\ e^{\beta H/2} & e^{-\beta J} & e^{-\beta H/2} & e^{\beta J} \end{pmatrix} \quad , \end{aligned}$$

where the order of the row and column indices is $\{\hat{\mathbf{x}}, \hat{\mathbf{y}}, -\hat{\mathbf{x}}, -\hat{\mathbf{y}}\}$.

(b) When $H = 0$ the transfer matrix is identical to that given in the Big Hint, with $r = \exp(\beta J)$. To find the eigenvalues, we simply apply T to the Big Hint eigenvectors and we find

$$\lambda_1 = 2 \cosh(\beta J) + 2 \quad , \quad \lambda_2 = 2 \cosh(\beta J) - 2 \quad , \quad \lambda_3 = \lambda_4 = 2 \sinh(\beta J) \quad .$$

Note that $\text{Tr } T = \sum_{a=1}^4 \lambda_a = 4 \exp(\beta J) = 4r$, which is the sum of the diagonal elements.

(c) In the thermodynamic limit, $Z(T, N) = \lambda_1^N$, since λ_1 is the largest eigenvalue. Thus,

$$f(T) = -\frac{k_B T}{N} \log Z = -k_B T \log \lambda_1 = -k_B T \log (2 \cosh(J/k_B T) + 2) \quad .$$

As $T \rightarrow \infty$ we find $f(T) = -k_B T \log 4 = -Ts$, where $s = k_B \log 4$ is the high temperature entropy per site.

(2) Consider the modified van der Waals equation of state

$$\left(p + \frac{a}{(v+b)^2} \right) (v-b) = RT \quad ,$$

where $v = N_A V/N$ is the molar volume. Find the critical point (v_c, T_c, p_c) .

(a) Find v_c . [8 points]

(b) Find T_c . [8 points]

(c) Find p_c . [9 points]

Solution :

We have

$$p = \frac{RT}{v-b} - \frac{a}{(v+b)^2} \quad .$$

Differentiating with respect to v , we have

$$= \frac{1}{v \kappa_T} = \left(\frac{\partial p}{\partial v} \right)_T = -\frac{RT}{(v-b)^2} + \frac{2a}{(v+b)^3}$$

Setting this to zero, *i.e.* $\kappa_T = \infty$, we obtain

$$f(u) \equiv \frac{(u+1)^3}{(u-1)^2} = \frac{2a}{bRT} \quad ,$$

where $u \equiv v/b$. Clearly $f(u)$ diverges as $u \rightarrow 1^+$, *i.e.* $v \rightarrow b^+$, which is the dense packing limit. As $u \rightarrow \infty$ we have $f(u) \sim u$. The minimum of $f(u)$ occurs when $f'(u^*) = 0$. So we examine

$$f'(u) = \frac{3(u+1)^2(u-1) - 2(u+1)^3}{(u-1)^3} = \frac{(u+1)^2(u-5)}{(u-1)^3} \quad ,$$

hence we conclude $u^* = 5$ and $v_c = u^*b = 5b$. We then have $f(u^*) = 2a/bRT_c = \frac{27}{2}$, which is to say $T_c = 4a/27bR$. Sticking both these results into the equation of state yields p_c , and we then have

$$v_c = 5b \quad , \quad T_c = \frac{4a}{27bR} \quad , \quad p_c = \frac{a}{108b^2} \quad .$$

(3) The Blume-Capel Hamiltonian is

$$\hat{H} = -\frac{1}{2} \sum_{i,j=1}^N J_{ij} S_i S_j + \Delta \sum_{i=1}^N S_i^2 \quad .$$

The spin variables S_i range over the values $\{-1, 0, +1\}$, so this is an extension of the $S = 1$ Ising model. All the diagonal entries of the interaction matrix J are set to zero: $J_{ii} \equiv 0$.

(a) *In the first term only*, make the mean field Ansatz, writing $S_i = m + \delta S_i$ and derive the mean field Hamiltonian \hat{H}_{MF} . The term proportional to Δ enters \hat{H}_{MF} as it appears above. You may assume $J_{ij} = J(|\mathbf{R}_i - \mathbf{R}_j|)$ and write $\hat{J}(0) \equiv \sum_{\mathbf{R}} J(\mathbf{R})$ as we have done before, where \mathbf{R} is a lattice translation symmetry vector. (If the interactions are only between nearest-neighbor sites, then $\hat{J}(0) = zJ$ where z is the number of nearest neighbors.) Again, *only neglect fluctuations in the first term – you will treat the second term exactly*. [7 points]

(b) Derive the mean field free energy $F(m, T, \Delta, N)$. [6 points]

(c) Write the dimensionless mean field free energy per site $f(m, \theta, \delta) = F/N\hat{J}(0)$, where $\theta = k_{\text{B}}T/\hat{J}(0)$, $f = F/N\hat{J}(0)$, and $\delta = \Delta/\hat{J}(0)$. What is the self-consistent mean field equation? [6 points]

(d) If an external field term $-H \sum_{i=1}^N S_i$ is included in the Hamiltonian, what is the free energy $f(m, \theta, h, \delta)$, where $h = H/\hat{J}(0)$, and what is the mean field equation? [6 points]

Solution :

(a) The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \frac{1}{2} N \hat{J}(0) m^2 - \hat{J}(0) m \sum_{i=1}^N S_i + \Delta \sum_{i=1}^N S_i^2 \quad .$$

(b) The mean field free energy is

$$F(m, T, \Delta, N) = \frac{1}{2} N \hat{J}(0) m^2 - N k_{\text{B}} T \log \left[1 + 2 \exp(-\Delta/k_{\text{B}}T) \cosh \left(\frac{\hat{J}(0)m}{k_{\text{B}}T} \right) \right]$$

(c) The dimensionless free energy per site is then

$$f(m, \theta, \delta) = \frac{1}{2} m^2 - \theta \log \left(1 + 2 \exp(-\Delta/k_{\text{B}}T) \cosh(m/\theta) \right)$$

and the self-consistent mean-field equation is

$$\frac{\partial f}{\partial m} = 0 = m - \frac{2 \sinh(m/\theta)}{\exp(\delta/\theta) + 2 \cosh(m/\theta)} \quad .$$

(d) In the presence of an external magnetic field, we have

$$f(m, \theta, h, \delta) = \frac{1}{2}m^2 - \theta \log \left[1 + 2e^{-\delta/\theta} \cosh\left(\frac{m+h}{\theta}\right) \right]$$

and

$$m = \frac{2 \sinh((m+h)/\theta)}{\exp(\delta/\theta) + 2 \cosh((m+h)/\theta)} .$$

Note added :

Finding the slope of the RHS of the $h = 0$ mean field equation at $m = 0$ and setting it to unity gives at $\theta = \theta^*$ yields

$$\theta^*(\delta) = \frac{2}{\exp(\delta/\theta^*) + 2} .$$

This is an implicit equation for θ^* in terms of the vacancy energy δ . Equivalently, we can write

$$\delta^*(\theta) = \theta \log\left(\frac{2}{\theta} - 2\right) .$$

Is $\theta^*(\delta)$ the critical temperature? We need to investigate further.

Let's expand the free energy in terms of the magnetization m . We find, to fourth order,

$$\begin{aligned} f = & -\theta \log(1 + 2e^{-\delta/\theta}) + \frac{1}{2\theta} \left(\theta - \frac{2}{2 + \exp(\delta/\theta)} \right) m^2 \\ & + \frac{1}{12(2 + \exp(\delta/\theta))\theta^3} \left(\frac{6}{2 + \exp(\delta/\theta)} - 1 \right) m^4 + \dots \end{aligned}$$

Note that setting the coefficient of the m^2 term to zero yields the equation for $\theta^*(\delta)$. However, upon further examination, we see that the coefficient of the m^4 term can *also* vanish. As we have seen, when the coefficients of the m^2 and the m^4 terms vanish concomitantly, we have a *tricritical point*¹. Setting both coefficients to zero, we obtain

$$\theta_t = \frac{1}{3} \quad , \quad \delta_t = \frac{2}{3} \log 2 .$$

At $\theta = 0$, it is easy to see we have a first order transition at $\delta = \frac{1}{2}$, simply by comparing the energies of the paramagnetic ($S_i = 0$) and ferromagnetic ($S_i = +1$ or $S_i = -1$) states. We have

$$\frac{E_{\text{MF}}}{N\hat{J}(0)} = \begin{cases} 0 & \text{if } m = 0 \\ \frac{1}{2} - \delta & \text{if } m = \pm 1 \end{cases} .$$

These results are exact, and not only valid for the mean field theory. Mean field theory is approximate because it neglects fluctuations, but at zero temperature, there are no fluctuations to neglect!

¹We should really check that the coefficient of the sixth order term is positive, but that is left as an exercise to the eager student.

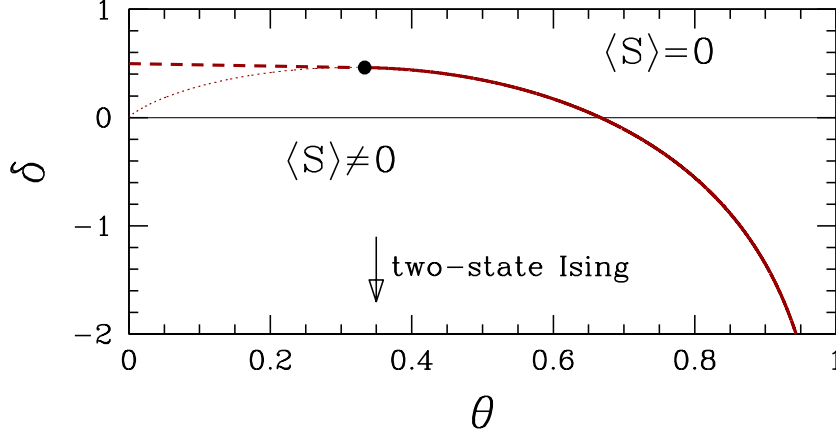


Figure 1: Mean field phase diagram for the Blume-Capel model. The black dot signifies a tricritical point, where the coefficients of m^2 and m^4 in the Landau free energy expansion both vanish. The dashed curve denotes a first order transition, and the solid curve a second order transition. The thin dotted line is the continuation of the $\delta^*(\theta)$ relation to zero temperature.

How about the first order line in the phase diagram? This requires that $\partial^2 f / \partial m^2 > 0$ for $m = 0$, with means $\delta > \delta^*(\theta)$. We then invoke the mean field equation eqn. ?? as well as the condition $f(m) = f(0)$. This latter condition is found to be

$$m^2 = 2\theta \log \left(\frac{1 + 2e^{-\delta/\theta} \cosh(m/\theta)}{1 + 2e^{-\delta/\theta}} \right) .$$

The simultaneous solution of this equation and the mean field equation yield the equation of the first order portion of the critical line $\delta_c(\theta)$, as well as the order parameter discontinuity $m^*(\theta)$ at the first order transition.. As $\theta \rightarrow \theta_t^-$, we have $\delta^*(\theta_t^-) = \delta_t = \frac{1}{3}$ and $m^*(\theta_t^-) = 0$.

The phase diagram is shown in fig. 1. Note that for δ large and negative, vacancies are strongly disfavored, hence the only allowed states on each site have $S_i = \pm 1$, which is our old friend the two-state Ising model. Accordingly, the phase boundary there approaches the vertical line $\theta_c = 1$, which is the mean field transition temperature for the two-state Ising model.

(4) Consider a monatomic ideal gas in the presence of a temperature gradient ∇T . Answer the following questions within the framework of the relaxation time approximation to the Boltzmann equation.

- (a) Compute the particle current j and show that it vanishes. [8 points]
- (b) Compute the 'energy squared' current,

$$j_{\epsilon^2} = \int d^3p \epsilon^2 \mathbf{v} f(\mathbf{r}, \mathbf{p}, t) .$$

Hints: Equilibrium averages of $\phi(\mathbf{v})$:

$$\int d^3p f^0(\mathbf{p}) \phi(\mathbf{v}) = n \int d^3v P(\mathbf{v}) \phi(\mathbf{v}) \quad , \quad P(\mathbf{v}) = \left(\frac{m}{2\pi k_B T} \right)^{3/2} \exp \left(-\frac{m\mathbf{v}^2}{2k_B T} \right)$$

For the Maxwell distribution of energies:

$$\langle \varepsilon^\alpha \rangle = \frac{2}{\sqrt{\pi}} \Gamma\left(\alpha + \frac{3}{2}\right) (k_B T)^\alpha \quad .$$

Recall $\Gamma(1/2) = \sqrt{\pi}$ and $z \Gamma(z) = \Gamma(z+1)$. [8 points]

(c) Compute the scalar momentum current,

$$\mathbf{j}_p = \int d^3p p \mathbf{v} f(\mathbf{r}, \mathbf{p}, t) \quad .$$

[9 points]

Solution:

(a) Under steady state conditions, the solution to the Boltzmann equation is $f = f^0 + \delta f$, where f^0 is the equilibrium distribution and

$$\delta f = -\frac{\tau f^0}{k_B T} \cdot \frac{\varepsilon - c_p T}{T} \mathbf{v} \cdot \nabla T \quad .$$

For the monatomic ideal gas, $c_p = \frac{5}{2} k_B$. The particle current is

$$\begin{aligned} j^\alpha &= \int d^3p v^\alpha \delta f \\ &= -\frac{\tau}{k_B T^2} \int d^3p f^0(\mathbf{p}) v^\alpha v^\beta (\varepsilon - \frac{5}{2} k_B T) \frac{\partial T}{\partial x^\beta} \\ &= -\frac{2n\tau}{3mk_B T^2} \frac{\partial T}{\partial x^\alpha} \langle \varepsilon (\varepsilon - \frac{5}{2} k_B T) \rangle \quad , \end{aligned}$$

where the average over momentum/velocity is converted into an average over the energy distribution,

$$\mathcal{P}(\varepsilon) = 4\pi v^2 \frac{dv}{d\varepsilon} P(v) = \frac{2}{\sqrt{\pi}} (k_B T)^{-3/2} \varepsilon^{1/2} e^{-\varepsilon/k_B T} \quad .$$

As discussed in the lecture notes, the average of a homogeneous function of ε under this distribution is given by

$$\langle \varepsilon^\alpha \rangle = \frac{2}{\sqrt{\pi}} \Gamma\left(\alpha + \frac{3}{2}\right) (k_B T)^\alpha \quad .$$

Thus,

$$\langle \varepsilon (\varepsilon - \frac{5}{2} k_B T) \rangle = \frac{2}{\sqrt{\pi}} (k_B T)^2 \left\{ \Gamma\left(\frac{7}{2}\right) - \frac{5}{2} \Gamma\left(\frac{5}{2}\right) \right\} = 0 \quad .$$

(b) Now we must compute

$$\begin{aligned} j_{\varepsilon^2}^\alpha &= \int d^3p v^\alpha \varepsilon^2 \delta f \\ &= -\frac{2n\tau}{3mk_B T^2} \frac{\partial T}{\partial x^\alpha} \langle \varepsilon^3 (\varepsilon - \frac{5}{2}k_B T) \rangle . \end{aligned}$$

We then have

$$\langle \varepsilon^3 (\varepsilon - \frac{5}{2}k_B T) \rangle = \frac{2}{\sqrt{\pi}} (k_B T)^4 \left\{ \Gamma\left(\frac{11}{2}\right) - \frac{5}{2} \Gamma\left(\frac{9}{2}\right) \right\} = \frac{105}{2} (k_B T)^4$$

and so

$$\mathbf{j}_{\varepsilon^2} = -\frac{35 n \tau k_B}{m} (k_B T)^2 \nabla T .$$

(c) Now we must compute

$$\begin{aligned} j_p^\alpha &= \int d^3p v^\alpha p \delta f \\ &= -\frac{\sqrt{8}n\tau}{3\sqrt{m}k_B T^2} \frac{\partial T}{\partial x^\alpha} \langle \varepsilon^{3/2} (\varepsilon - \frac{5}{2}k_B T) \rangle , \end{aligned}$$

where we have substituted $p = \sqrt{2m\varepsilon}$. We then have

$$\langle \varepsilon^{3/2} (\varepsilon - \frac{5}{2}k_B T) \rangle = \frac{2}{\sqrt{\pi}} (k_B T)^{5/2} \left\{ \Gamma(4) - \frac{5}{2} \Gamma(3) \right\} = \frac{2}{\sqrt{\pi}} (k_B T)^{5/2}$$

and so

$$\mathbf{j}_p = -\frac{4\sqrt{2}}{3\sqrt{\pi}} \left(\frac{n\tau k_B}{\sqrt{m}} \right) (k_B T)^{1/2} \nabla T .$$

Note added :

It is interesting to note that there is no particle current flowing in response to a temperature gradient when τ is energy-independent. This is a consequence of the fact that the pressure gradient ∇p vanishes. Newton's Second Law for the fluid says that $nm\dot{\mathbf{V}} + \nabla p = 0$, to lowest relevant order. With $\nabla p \neq 0$, the fluid will accelerate. In a pipe, for example, eventually a steady state is reached where the flow is determined by the fluid viscosity, which is one of the terms we just dropped. This is called *Poiseuille flow*. When p is constant, the local equilibrium distribution is

$$f^0(\mathbf{r}, \mathbf{p}) = \frac{p/k_B T}{(2\pi m k_B T)^{3/2}} e^{-\mathbf{p}^2/2mk_B T} ,$$

where $T = T(\mathbf{r})$. We then have

$$f(\mathbf{r}, \mathbf{p}) = f^0(\mathbf{r} - \mathbf{v}\tau, \mathbf{p}) ,$$

which says that no new collisions happen for a time τ after a given particle thermalizes. *I.e.* we evolve the streaming terms for a time τ . Expanding, we have

$$\begin{aligned} f &= f^0 - \frac{\tau \mathbf{p}}{m} \cdot \frac{\partial f^0}{\partial \mathbf{r}} + \dots \\ &= \left\{ 1 - \frac{\tau}{2k_B T^2} \left(\varepsilon(\mathbf{p}) - \frac{5}{2} k_B T \right) \frac{\mathbf{p}}{m} \cdot \nabla T + \dots \right\} f^0(\mathbf{r}, \mathbf{p}) \quad , \end{aligned}$$

which leads to $\mathbf{j} = 0$, assuming the relaxation time τ is energy-independent.

When the flow takes place in a restricted geometry, a dimensionless figure of merit emerges, known as the *Knudsen number*, $\text{Kn} = \ell/L$, where ℓ is the mean free path and L is the characteristic linear dimension associated with the geometry. For $\text{Kn} \ll 1$, our Boltzmann transport calculations of quantities like κ , η , and ζ hold, and we may apply the Navier-Stokes equations². In the opposite limit $\text{Kn} \gg 1$, the boundary conditions on the distribution are crucial. Consider, for example, the case $\ell = \infty$. Suppose we have ideal gas flow in a cylinder whose symmetry axis is \hat{x} . Particles with $v_x > 0$ enter from the left, and particles with $v_x < 0$ enter from the right. Their respective velocity distributions are

$$P_j(\mathbf{v}) = n_j \left(\frac{m}{2\pi k_B T_j} \right)^{3/2} e^{-m\mathbf{v}^2/2k_B T_j} \quad ,$$

where $j = \text{L}$ or R . The average current is then

$$\begin{aligned} j_x &= \int d^3v \left\{ n_L v_x P_L(\mathbf{v}) \Theta(v_x) + n_R v_x P_R(\mathbf{v}) \Theta(-v_x) \right\} \\ &= n_L \sqrt{\frac{2k_B T_L}{m}} - n_R \sqrt{\frac{2k_B T_R}{m}} \quad . \end{aligned}$$

²These equations may need to be supplemented by certain conditions which apply in the vicinity of solid boundaries.