PHYSICS 140B : STATISTICAL PHYSICS
FINAL EXAMINATION SOLUTIONS

(1) Provide clear, accurate, and substantial answers for each of the following:

(a) For a fermionic system of number density n and with single particle dispersion $\varepsilon(\boldsymbol{k})$, where $\boldsymbol{k}$ is the wavevector, what is the definition of the Fermi energy and the Fermi surface? `[5 points]`

(b) Write down the symmetric transfer matrix R for the one-dimensional spin-1 Ising Hamiltonian,

$$\hat{H} = -J \sum_n S_n S_{n+1} \quad ,$$

where each $S_n \in \{-1, 0, +1\}$. `[5 points]`

(c) For the cluster γ shown in Fig. 1, identify the symmetry factor s_γ, the lowest order virial coefficient B_j to which γ contributes, and write an expression for the cluster integral $b_\gamma(T)$ in terms of the Mayer function $f(r)$. `[5 points]`

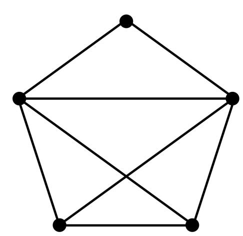

Figure 1: The connected cluster γ for problem 1c.

(d) Describe the physics of spinodal decomposition, phase separation, and the Maxwell construction. Include a sketch of $p(v,T)$ *versus* v to illustrate your description. `[5 points]`

(e) What does it mean to say that for the Landau free energy density (with $b > 0$)

$$f(m) = \tfrac{1}{2}am^2 - \tfrac{1}{3}ym^3 + \tfrac{1}{4}bm^4 \quad ,$$

that "a first order transition preempts the second order transition"? `[5 points]`

(a) The Fermi energy $\varepsilon_{\rm F}(n)$ is the the highest energy level achieved by occupying single particle states consecutively, subject to the Pauli principle. Thus,

$$n = \int\limits_{-\infty}^{\varepsilon_{\rm F}} d\varepsilon \; g(\varepsilon) \quad ,$$

where $g(\varepsilon)$ is the single particle density of states. The Fermi energy is also the value of the chemical potential at $T = 0$: $\mu(T = 0, n) = \varepsilon_{\rm F}(n)$. The Fermi surface is the locus of points in $\boldsymbol{k}$-space where $\varepsilon(\boldsymbol{k}) = \varepsilon_{\rm F}$.

(b) The transfer matrix is 3×3 and of the form

$$R_{SS'} = e^{JSS'/k_{\rm B}T} = \begin{pmatrix} e^{J/k_{\rm B}T} & 1 & e^{-J/k_{\rm B}T} \\ 1 & 1 & 1 \\ e^{-J/k_{\rm B}T} & 1 & e^{J/k_{\rm B}T} \end{pmatrix} \quad ,$$

with $\beta = 1/k_{\rm B}T$. The rows and columns consecutively correspond to $S = 1$, $S = 0$, and $S = -1$.

(c) The symmetry factor is $2! \cdot 2! = 4$, because, consulting the right panel of Fig. 2, vertices 2 and 5 can be exchanged, and vertices 3 and 4 can be exchanged. There are five vertices, hence the lowest order virial coefficient to which this cluster contributes is B_5. The cluster integral is

$$\begin{aligned} b_\gamma &= \frac{1}{4\,V} \int \! d^d\!x_1 \! \int \! d^d\!x_2 \! \int \! d^d\!x_3 \! \int \! d^d\!x_4 \! \int \! d^d\!x_5 \; f_{12}\, f_{15}\, f_{23}\, f_{23}\, f_{25}\, f_{34}\, f_{35}\, f_{45} \\ &= \frac{1}{4} \int \! d^d\!x_1 \! \int \! d^d\!x_2 \! \int \! d^d\!x_3 \! \int \! d^d\!x_4 \; f_{12}\, f_{15}\, f_{23}\, f_{23}\, f_{25}\, f_{34}\, f_{35}\, f_{45} \quad , \end{aligned}$$

where $f_{ij} = \exp\big[-u(r_{ij})/k_{\rm B}T\big] - 1$. See Fig. 2 for the labels.

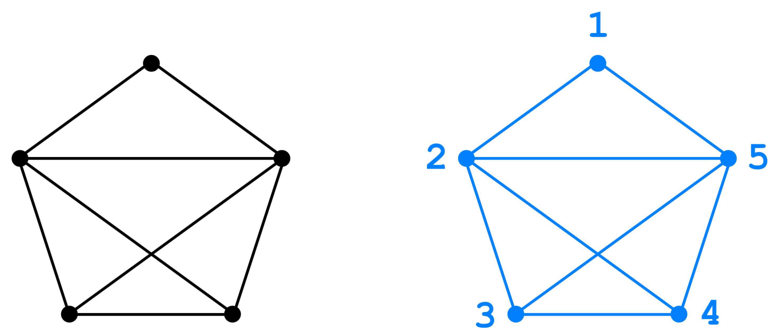

Figure 2: The connected cluster γ for problem 1b and its labeled version.

(d) The Maxwell construction is a fix for the van der Waals system and other related phenomenological equations of state $p = p(T,v)$ in which, throughout a region of temperature T, the pressure as a function of volume $p(v)$ is nonmonotonic. This is unphysical since the isothermal compressibility $\kappa_T = -v^{-1}(\partial v/\partial p)_T$ becomes negative, which signals an absolute thermal instability, known as *spinodal decomposition*. The regime of instability is even larger than this, however, because of the possibility of *phase separation* into regions of different bulk density. The situation is depicted in Fig. 3. To remedy these defects, one replaces the unstable part of the $p(v)$ curve with a flat line extending from $v = v_1$ to $v = v_2$ at each temperature T in the unstable region, such that the following two conditions hold:

$$\text{(i)}\ p(T,v_1) = p(T,v_2) \qquad , \qquad \text{(ii)} \int\limits_{v_1}^{v_2} \! dv\; p(T,v) = (v_2 - v_1)\, p(T,v_1) \quad .$$

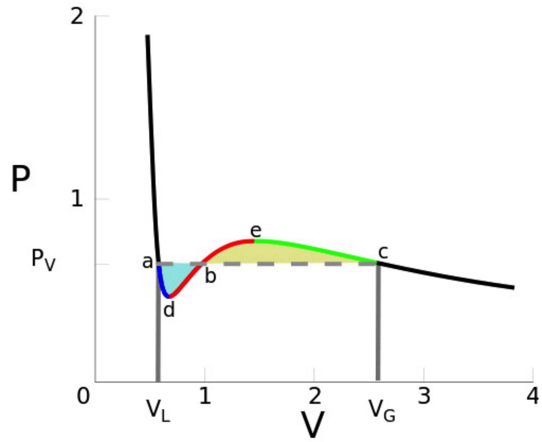

Figure 3: The Maxwell construction corrects a nonmonotonic $p(v)$ to include a flat section, known as the coexistence region, which guarantees that the Helmholtz free energy of the system is at a true minimum. The system is absolutely unstable between volumes v_d and v_e. For $v \in [v_\mathrm{a}, v_\mathrm{d}]$ of $v \in [v_\mathrm{e}, v_\mathrm{c}]$, the solution is unstable with respect to phase separation.

(e) Assuming $y > 0$, the minimum value of $f(m)$ lies below $f(0) = 0$ provided that $a < a_\mathrm{c} \equiv 2y^2/b$. At this critical value of $a \propto T - T_\mathrm{c}$, the location of the minimum discontinuously jumps from $m = 0$ at $a = a_\mathrm{c}^+$ to $m = 3a/y$ at $a = a_\mathrm{c}^-$. Thus the coefficient of the m^2 term remains positive at this transition. As a is lowered further below a_c, and eventually becomes negative, the location of the minimum evolves smoothly.

(2) Consider the equation of state

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

where v is the volume per mole.

(a) Find v_c. `[5 points]`

(b) Find T_c. `[5 points]`

(c) Find p_c. `[5 points]`

(d) Defining the dimensionless quantities $\bar{p} \equiv p/p_\mathrm{c}$, $\bar{T} \equiv T/T_\mathrm{c}$, and $\bar{v} \equiv v/v_\mathrm{c}$, write the equation of state $\bar{p} = \bar{p}(\bar{T}, \bar{v})$. Show that $\bar{p}(\bar{T} = 1, \bar{v} = 1) = 1$. `[10 points]`

(a) We examine $p(T,v)$ at fixed T and identify any temperature range where $(\partial p/\partial v)_T > 0$, which would indicate an absolute thermodynamic instability where $\kappa_T < 0$. It is convenient to compute

$$\frac{1}{p}\frac{\partial p}{\partial v} = \frac{\partial \ln p}{\partial v} = -\frac{1}{v-b} + \frac{2a}{RTv^3} \quad .$$

Setting the RHS to zero, and defining $v \equiv bu$, we obtain the equation

$$g(u) \equiv \frac{u^3}{u-1} = \frac{2a}{RTb^2} \quad .$$

Clearly $g(u)$ diverges as $u \to 1^+$ and as $u \to \infty$. Setting $g'(u) = 0$ we find a single minimum at $u^* = \frac{3}{2}$, where $g(\frac{3}{2})$. Thus, $v_c = u^* b = \frac{3}{2} b$.

(b) Since $g(u^*) = \frac{27}{4}$ is the minimum value, we identify T_c by setting

$$g(u^*) = \frac{27}{4} = \frac{2a}{RT_c\, b^2} \quad \Rightarrow \quad T_c = \frac{8a}{27R\, b^2} \quad .$$

(c) Now we plug v_c and T_c into the equation of state to obtain

$$p_c = p(T_c, v_c) = \frac{16a}{27b^3} \exp\big(-\tfrac{3}{2}\big) \quad .$$

(d) Writing $\bar{p} \equiv p/p_c$, $\bar{T} \equiv T/T_c$, and $\bar{v} \equiv v/v_c$, we have

$$\bar{p}(\bar{T}, \bar{v}) = \frac{\bar{T}}{3\bar{v} - 2} \exp\!\left(\frac{3}{2} - \frac{2}{2\bar{T}\bar{v}^2}\right) \quad .$$

Note that $\bar{p}(1,1) = 1$, which is equivalent to $p_c = p(T_c, v_c)$.

(3) Consider a system consisting of mobile ions of charge $+Ze > 0$ and electrons of charge $-e < 0$. Let the ion mass be m_+ and the electron mass be m_-. The average number density of ions is n_+.

(a) Let $z_\pm$ be the fugacities for the ions (+) and electrons (−). Within Debye-Hückel theory, what is the formula for the charge density $\rho(\boldsymbol{r})$? *Hint: Your formula should involve the local potential* $\phi(\boldsymbol{r})$. `[5 points]`

(b) Assuming overall charge neutrality, what is the number density n_- of electrons? What is the relation between the number densities $n_\pm$, the fugacities $z_\pm$, and the masses $m_\pm$ at temperature T? *Hint: At* $|\boldsymbol{r}| \to \infty$, *take* $\phi(\boldsymbol{r}) \to 0$. `[5 points]`

(c) What is the full nonlinear self-consistent equation for $\phi(\boldsymbol{r})$? `[5 points]`

(d) Assuming $|e\phi(\boldsymbol{r})| \ll k_B T$, the linearized self-consistent equation for $\phi(\boldsymbol{r})$ in the presence of an external charge distribution $\rho_{ext}(\boldsymbol{r}) = Q\,\delta(\boldsymbol{r})$ is

$$\nabla^2 \phi = \kappa_D^2\, \phi - 4\pi Q\, \delta(\boldsymbol{r}) \quad ,$$

where κ_D is the Debye screening wavevector. Find an expression for κ_D. `[5 points]`

(e) In $d = 3$ dimensions, again assuming $|e\phi(\boldsymbol{r})| \ll k_B T$, what is the total charge distribution $\rho_{tot}(\boldsymbol{r})$ in the presence of the external charge Q? `[5 points]`

(a) We have

$$\rho(\boldsymbol{r}) = Ze\, z_+\, \lambda_+^{-d} \exp\!\left(-\frac{Ze\phi(\boldsymbol{r})}{k_{\rm B}T}\right) - e\, z_-\, \lambda_-^{-d} \exp\!\left(\frac{e\phi(\boldsymbol{r})}{k_{\rm B}T}\right) \quad ,$$

where $\lambda_\pm = (2\pi\hbar^2/m_\pm k_{\rm B}T)^{1/2}$ and $z_\pm = \exp(\mu_\pm/k_{\rm B}T)$.

(b) Charge neutrality entails

$$Zen_+ - en_- = 0 \quad \Rightarrow \quad n_- = Zn_+ \quad .$$

The densities are $n_\pm = z_\pm\, \lambda_\pm^{-d}$. Thus, $Zz_+\lambda_+^{-d} = z_-\lambda_-^{-d}$.

(c) We have

$$\nabla^2\phi = -4\pi\rho = 4\pi Zen_+\left[\exp\!\left(\frac{e\phi(\boldsymbol{r})}{k_{\rm B}T}\right) - \exp\!\left(-\frac{Ze\phi(\boldsymbol{r})}{k_{\rm B}T}\right)\right] \quad ,$$

where we have used $n_- = Zn_+$.

(d) With $|e\phi| \ll k_{\rm B}T$, we expand the above nonlinear self-consistent Poisson equation, including the external charge, to obtain

$$\nabla^2\phi = \frac{4\pi Z(1+Z)n_+\, e^2}{k_{\rm B}T}\,\phi - 4\pi Q\,\delta(\boldsymbol{r}) \quad .$$

Thus we have

$$\kappa_{\rm D} = \left(\frac{4\pi Z(1+Z)n_+\, e^2}{k_{\rm B}T}\right)^{1/2} \quad .$$

(e) The potential is given by the Yukawa form,

$$\phi(\boldsymbol{r}) = \frac{Q}{r}\,\exp(-\kappa_{\rm D} r) \quad .$$

The total charge density is

$$\begin{aligned}\rho_{\rm tot}(\boldsymbol{r}) &= \rho_{\rm ext}(\boldsymbol{r}) + \rho(\boldsymbol{r}) \\ &= Q\,\delta(\boldsymbol{r}) - \frac{Q\kappa_{\rm D}^2\exp(-\kappa_{\rm D} r)}{4\pi r} \quad .\end{aligned}$$

Note that

$$\int\! d^3r\; \rho_{\rm tot}(\boldsymbol{r}) = 0 \quad ,$$

which says that the external charge is completely screened.

(4) Consider a four-state Ising model on a cubic lattice with Hamiltonian

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

where each spin variable S_i takes on one of four possible values: $S_i \in \{-2, -1, +1, +2\}$, and the first sum is over all nearest-neighbor pairs of the lattice (*i.e.* over all unique links). Note there is no $S_i = 0$ state.

(a) What is the mean field Hamiltonian $\hat{H}_{\rm MF}$? [5 points]

(b) Find the mean field free energy per site $f(\theta, h, m)$, where $m = \langle S_i \rangle$, $\theta = k_{\rm B}T/zJ$, $h = H/zJ$, and $f = F/NzJ$. Here z is the lattice coordination number. [5 points]

(c) Find the mean field equation relating m, θ, and h. [5 points]

(d) Expand f to fourth order in m, retaining terms only to first order in h, and working to lowest order in $\theta - \theta_{\rm c}$. What is $\theta_{\rm c}$? [5 points]

(e) If $J/k_{\rm B} = 100\,{\rm K}$, what is the critical temperature $T_{\rm c}$? [5 points]

(a) The mean field is $H_{\rm eff} = H + zJm$ where $m = \langle S_i \rangle$. The mean field Hamiltonian is

$$\hat{H}_{\rm MF} = \tfrac{1}{2} N z J m^2 - (H + zJm) \sum_i S_i \quad ,$$

where the square of the fluctuation terms on each site have been neglected.

(b) The partition function is $Z_{\rm MF} = {\rm Tr}\, \exp(-\hat{H}_{\rm MF}/k_{\rm B}T) \equiv \exp(-NzJf)$, with

$$\begin{aligned} f(\theta, h, m) &= \tfrac{1}{2} m^2 - \theta \ln \mathop{\rm Tr}_S \exp\big[-(m+h)S/\theta \big] \\ &= \tfrac{1}{2} m^2 - \theta \ln \left[2\cosh\left(\frac{m+h}{\theta}\right) + 2\cosh\left(\frac{2m+2h}{\theta}\right) \right] \quad . \end{aligned}$$

(c) Setting $f'(m) = 0$, we obtain the mean field equation:

$$m = \frac{\sinh\left(\frac{m+h}{\theta}\right) + 2\sinh\left(\frac{2m+2h}{\theta}\right)}{\cosh\left(\frac{m+h}{\theta}\right) + \cosh\left(\frac{2m+2h}{\theta}\right)} \quad .$$

(d) Isolating the contribution from the high temperature entropy, we have

$$f = \tfrac{1}{2} m^2 - \theta \ln \left[\tfrac{1}{2} \cosh\left(\frac{m+h}{\theta}\right) + \tfrac{1}{2}\cosh\left(\frac{2m+2h}{\theta}\right) \right] - \theta \ln 4$$

Now we expand using $\cosh u = 1 + \frac{1}{2}u^2 + \frac{1}{24}u^4 + \mathcal{O}(u^6)$ and $\ln(1+\varepsilon) = \varepsilon - \frac{1}{2}\varepsilon^2 + \mathcal{O}(\varepsilon^3)$, where both u and ε are small. This yields, with $u \equiv (m+h)/\theta$,

$$\begin{aligned}
f + \theta \ln 4 &= \tfrac{1}{2}m^2 - \theta \ln\Big[\tfrac{1}{2} + \tfrac{1}{4}u^2 + \tfrac{1}{48}u^4 + \ldots + \tfrac{1}{2} + \tfrac{1}{4}(2u)^2 + \tfrac{1}{48}(2u)^4 + \ldots\Big] \\
&= \tfrac{1}{2}m^2 - \theta \ln\Big[1 + \tfrac{5}{4}u^2 + \tfrac{17}{48}u^4 + \ldots\Big] \\
&= \tfrac{1}{2}m^2 - \theta\Big[\tfrac{5}{4}u^2 + \tfrac{17}{48}u^4 - \tfrac{1}{2}\big(\tfrac{5}{4}u^2\big)^2 + \ldots\Big] \\
&= \tfrac{1}{2}m^2 - \frac{5(m+h)^2}{4\theta} + \frac{41(m+h)^4}{96\,\theta^3} + \ldots \\
&= \left(\frac{1}{2} - \frac{5}{4\theta}\right) m^2 + \frac{41}{96\,\theta^3}m^4 - \frac{5}{2\theta}\,hm + \ldots \qquad .
\end{aligned}$$

From this we find $\theta_c = \frac{5}{2}$, and

$$f(\theta, h, m) = -\theta \ln 4 + \tfrac{1}{5}(\theta - \theta_c)\, m^2 + \tfrac{41}{1500}\, m^4 - hm \qquad .$$

(e) We have $k_B T_c = zJ\theta_c = 6 \times \frac{5}{2} \times 100\,\mathrm{K} = 1500\,\mathrm{K}$.