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 $\varepsilon(k)$, where $k$ 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,

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

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

(c) For the cluster $\gamma$ shown in Fig. 1, identify the symmetry factor $s_\gamma$, the lowest order virial coefficient $B_j$ to which $\gamma$ 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 $\gamma$ 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 $b > 0$)

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

that “a first order transition preempts the second order transition”? [5 points]

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

$$n = \int_{-\infty}^{\varepsilon_F} d\varepsilon g(\varepsilon),$$

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

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(b) The transfer matrix is $3 \times 3$ and of the form
\[
R_{SS'} = e^{JS'S'/k_B T} = \begin{pmatrix}
 e^{J/k_B T} & 1 & e^{-J/k_B T} \\
 1 & 1 & 1 \\
e^{-J/k_B T} & 1 & e^{J/k_B T}
\end{pmatrix},
\]
with $\beta = 1/k_B T$. 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
\[
b_\gamma = \frac{1}{4V} \int d^3x_1 \int d^3x_2 \int d^3x_3 \int d^3x_4 \int d^3x_5 f_{12} f_{15} f_{23} f_{25} f_{34} f_{35} f_{45},
\]
where $f_{ij} = \exp \left[ -u(r_{ij})/k_B T \right] - 1$. See Fig. 2 for the labels.

![Figure 2](image)

Figure 2: The connected cluster $\gamma$ 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 $\kappa_T = -\nu^{-1}(\partial v/\partial p)_T$ 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:

\begin{align*}
(i)\ p(T, v_1) = p(T, v_2) , \\
(ii)\ \int_{v_1}^{v_2} dv\ p(T, v) = (v_2 - v_1)\ p(T, v_1) .
\end{align*}
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 $v \in [v_a, v_d]$ of $v \in [v_e, v_c]$, 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 $a < a_c \equiv 2y^2/b$. At this critical value of $a \propto T - T_c$, the location of the minimum discontinuously jumps from $m = 0$ at $a = a_c^+$ to $m = 3a/y$ at $a = a_c^-$. 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

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

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 $\bar{p} \equiv p/p_c$, $\bar{T} \equiv T/T_c$, and $\bar{v} \equiv v/v_c$, 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

$$\frac{1}{p} \frac{\partial p}{\partial v} = \frac{\partial \ln p}{\partial v} = -\frac{1}{v - b} + \frac{2a}{RTv^3}. $$
Setting the RHS to zero, and defining \( v \equiv bu \), we obtain the equation

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

Clearly \( g(u) \) diverges as \( u \to 1^+ \) and as \( u \to \infty \). Setting \( g'(u) = 0 \) we find a single minimum at \( u^* = \frac{3}{7} \), where \( g\left(\frac{3}{7}\right) \). Thus, \( v_c = u^*b = \frac{3}{7}b \).

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

\[
g(u^*) = \frac{27}{4} = \frac{2a}{RT_c b^2} \quad \Rightarrow \quad T_c = \frac{8a}{27Rb^2}.
\]

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

\[
p_c = p(T_c, v_c) = \frac{16a}{27b^3} \exp\left(-\frac{3}{2}\right).
\]

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

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

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 \( \rho(r) \)? **Hint: Your formula should involve the local potential \( \phi(r) \).** [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 \( |r| \to \infty \), take \( \phi(r) \to 0 \).** [5 points]

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

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

\[
\nabla^2 \phi = \kappa_0^2 \phi - 4\pi Q \delta(r),
\]

where \( \kappa_0 \) is the Debye screening wavevector. Find an expression for \( \kappa_0 \). [5 points]

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

\[ \rho(r) = Ze z_+ \lambda^d - e z_- \lambda^{-d} \exp\left( \frac{Ze\phi(r)}{k_B T} \right) - e z_- \lambda^{-d} \exp\left( \frac{e\phi(r)}{k_B T} \right), \]

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

(b) Charge neutrality entails

\[ Z_{\pm} e n_+ - e n_- = 0 \implies n_- = Z n_+. \]

The densities are \( n_{\pm} = z_{\pm} \lambda^d \). Thus, \( Z z_+ \lambda^d = z_- \lambda^{-d} \).

(c) We have

\[ \nabla^2 \phi = -4\pi \rho = 4\pi Z e n_+ \left[ \exp\left( \frac{e\phi(r)}{k_B T} \right) - \exp\left( -\frac{Ze\phi(r)}{k_B T} \right) \right], \]

where we have used \( n_- = Z n_+ \).

(d) With \( |e\phi| \ll k_B T \), we expand the above nonlinear self-consistent Poisson equation, including the external charge, to obtain

\[ \nabla^2 \phi = \frac{4\pi Z(1 + Z)n_+ e^2}{k_B T} \phi - 4\pi Q \delta(r). \]

Thus we have

\[ \kappa_D = \left( \frac{4\pi Z(1 + Z)n_+ e^2}{k_B T} \right)^{1/2}. \]

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

\[ \phi(r) = \frac{Q}{r} \exp(-\kappa_D r). \]

The total charge density is

\[ \rho_{\text{tot}}(r) = \rho_{\text{ext}}(r) + \rho(r) = Q \delta(r) - \frac{Q \kappa_D^2 \exp(-\kappa_D r)}{4\pi r}. \]

Note that

\[ \int d^3 r \rho_{\text{tot}}(r) = 0, \]

which says that the external charge is completely screened.

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

\[ \hat{H} = -J \sum_{(ij)} S_i S_j - H \sum_i S_i, \]
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 $\hat{H}_{\text{MF}}$? [5 points]

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

(c) Find the mean field equation relating $m$, $\theta$, 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 $\theta - \theta_c$. What is $\theta_c$? [5 points]

(e) If $J/k_B = 100$ K, what is the critical temperature $T_c$? [5 points]

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(a) The mean field is $H_{\text{eff}} = H + zm$ where $m = \langle S_i \rangle$. The mean field Hamiltonian is
\[
\hat{H}_{\text{MF}} = \frac{1}{2}NzJm^2 - (H + zm) \sum_i S_i,
\]

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

(b) The partition function is $Z_{\text{MF}} = \text{Tr} \exp(-\hat{H}_{\text{MF}}/k_B T) \equiv \exp(-NZf)$, with
\[
f(\theta, h, m) = \frac{1}{2}m^2 - \theta \ln \text{Tr}_S \exp[-(m + h)S/\theta]
\]
\[
= \frac{1}{2}m^2 - \theta \ln \left[ 2 \cosh \left( \frac{m + h}{\theta} \right) + 2 \cosh \left( \frac{2m + 2h}{\theta} \right) \right].
\]

(c) Setting $f'(m) = 0$, we obtain the mean field equation:
\[
m = \frac{\sinh \left( \frac{m + h}{\theta} \right) + 2 \sinh \left( \frac{2m + 2h}{\theta} \right)}{\cosh \left( \frac{m + h}{\theta} \right) + \cosh \left( \frac{2m + 2h}{\theta} \right)}.
\]

(d) Isolating the contribution from the high temperature entropy, we have
\[
f = \frac{1}{2}m^2 - \theta \ln \left[ \frac{1}{2} \cosh \left( \frac{m + h}{\theta} \right) + \frac{1}{2} \cosh \left( \frac{2m + 2h}{\theta} \right) \right] - \theta \ln 4.
\]
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 \( \varepsilon \) are small. This yields, with \( u \equiv (m + h)/\theta \),

\[
f + \theta \ln 4 = \frac{1}{2}m^2 - \theta \ln \left[ \frac{1}{1} + \frac{1}{4}u^2 + \frac{1}{16}u^4 + \ldots + \frac{1}{2} + \frac{1}{4}(2u)^2 + \frac{1}{48}(2u)^4 + \ldots \right]
\]

\[
= \frac{1}{2}m^2 - \theta \ln \left[ 1 + \frac{5}{4}u^2 + \frac{17}{48}u^4 + \ldots \right]
\]

\[
= \frac{1}{2}m^2 - \theta \left[ \frac{5}{4}u^2 + \frac{17}{48}u^4 - \frac{1}{2} \left( \frac{5}{4}u^2 \right)^2 + \ldots \right]
\]

\[
= \frac{1}{2}m^2 - \frac{5(m + h)^2}{4\theta} + \frac{41(m + h)^4}{96\theta^3} + \ldots
\]

\[
= \left( \frac{1}{2} - \frac{5}{4\theta} \right)m^2 + \frac{41}{96\theta^3}m^4 - \frac{5}{2\theta}hm + \ldots
\]

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

\[
f(\theta, h, m) = -\theta \ln 4 + \frac{1}{5}(\theta - \theta_c)m^2 + \frac{41}{1500}m^4 - hm
\]

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