8.334 Statistical Mechanics II: Statistical Physics of Fields
Spring 2008

Review Problems

The test is 'closed book,' but if you wish you may bring a one-sided sheet of formulas. The intent of this sheet is as a reminder of important formulas and definitions, and not as a compact transcription of the answers provided here. If this privilege is abused, it will be revoked for future tests. The test will be composed entirely from a subset of the following problems. Thus if you are familiar and comfortable with these problems, there will be no surprises!

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1. *The binary alloy:* A binary alloy (as in β brass) consists of N_A atoms of type A, and N_B atoms of type B. The atoms form a simple cubic lattice, each interacting only with its six nearest neighbors. Assume an attractive energy of $-J$ $(J > 0)$ between like neighbors $A-A$ and $B-B$, but a repulsive energy of $+J$ for an $A-B$ pair.

(a) What is the minimum energy configuration, or the state of the system at zero temperature?

(b) Estimate the total interaction energy assuming that the atoms are randomly distributed among the N sites; i.e. each site is occupied independently with probabilities $p_A = N_A/N$ and $p_B = N_B/N$.

(c) Estimate the mixing entropy of the alloy with the same approximation. Assume $N_A, N_B \gg 1$.

(d) Using the above, obtain a free energy function $F(x)$, where $x = (N_A - N_B)/N$. Expand $F(x)$ to the fourth order in x, and show that the requirement of convexity of F breaks down below a critical temperature T_c. For the remainder of this problem use the expansion obtained in (d) in place of the full function $F(x)$.

(e) Sketch $F(x)$ for $T > T_c$, $T = T_c$, and $T < T_c$. For $T < T_c$ there is a range of compositions $x < |x_{sp}(T)|$ where $F(x)$ is not convex and hence the composition is locally unstable. Find $x_{sp}(T)$.

(f) The alloy globally minimizes its free energy by separating into A rich and B rich phases of compositions $\pm x_{eq}(T)$, where $x_{eq}(T)$ minimizes the function $F(x)$. Find $x_{eq}(T)$.

(g) In the (T, x) plane sketch the phase separation boundary $\pm x_{eq}(T)$; and the so called spinodal line $\pm x_{sp}(T)$. (The spinodal line indicates onset of metastability and hysteresis effects.)

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2. *The Ising model of magnetism:* The local environment of an electron in a crystal sometimes forces its spin to stay parallel or anti-parallel to a given lattice direction. As a model of magnetism in such materials we denote the direction of the spin by a single variable $\sigma_i = \pm 1$ (an Ising spin). The energy of a configuration $\{\sigma_i\}$ of spins is then given by

$$\mathcal{H} = \frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i \quad ;$$

where h is an external magnetic field, and J_{ij} is the interaction energy between spins at sites i and j.

(a) For N spins we make the drastic *approximation* that the interaction between all spins is the same, and $J_{ij} = -J/N$ (the equivalent neighbor model). Show that the energy can now be written as $E(M,h) = -N[Jm^2/2 + hm]$, with a magnetization $m = \sum_{i=1}^{N}\sigma_i/N = M/N$.

(b) Show that the partition function $Z(h,T) = \sum_{\{\sigma_i\}}\exp(-\beta\mathcal{H})$ can be re-written as $Z = \sum_M \exp[-\beta F(m,h)]$; with $F(m,h)$ easily calculated by analogy to problem (1). For the remainder of the problem work only with $F(m,h)$ expanded to 4th order in m.

(c) By saddle point integration show that the actual free energy $F(h,T) = -kT\ln Z(h,T)$ is given by $F(h,T) = \min[F(m,h)]_m$. When is the saddle point method valid? Note that $F(m,h)$ is an analytic function but not convex for $T < T_c$, while the true free energy $F(h,T)$ is convex but becomes non-analytic due to the minimization.

(d) For $h = 0$ find the critical temperature T_c below which spontaneous magnetization appears; and calculate the magnetization $\overline{m}(T)$ in the low temperature phase.

(e) Calculate the singular (non-analytic) behavior of the response functions

$$C = \left.\frac{\partial E}{\partial T}\right|_{h=0}, \quad \text{and} \quad \chi = \left.\frac{\partial \overline{m}}{\partial h}\right|_{h=0}.$$

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3. *The lattice–gas model:* Consider a gas of particles subject to a Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N}\frac{\vec{p_i}^{\,2}}{2m} + \frac{1}{2}\sum_{i,j}\mathcal{V}(\vec{r}_i - \vec{r}_j), \quad \text{in a volume } V.$$

(a) Show that the grand partition function Ξ can be written as

$$\Xi = \sum_{N=0}^{\infty}\frac{1}{N!}\left(\frac{e^{\beta\mu}}{\lambda^3}\right)^N \int\prod_{i=1}^{N} d^3\vec{r}_i \exp\left[-\frac{\beta}{2}\sum_{i,j}\mathcal{V}(\vec{r}_i - \vec{r}_j)\right].$$

(b) The volume V is now subdivided into $\mathcal{N} = V/a^3$ cells of volume a^3, with the spacing a chosen small enough so that each cell α is either empty or occupied by one particle; i.e. the cell occupation number n_α is restricted to 0 or 1 ($\alpha = 1, 2, \cdots, \mathcal{N}$). After approximating the integrals $\int d^3\vec{r}$ by sums $a^3 \sum_{\alpha=1}^{\mathcal{N}}$, show that

$$\Xi \approx \sum_{\{n_\alpha=0,1\}} \left(\frac{e^{\beta\mu}a^3}{\lambda^3}\right)^{\sum_\alpha n_\alpha} \exp\left[-\frac{\beta}{2}\sum_{\alpha,\beta=1}^{\mathcal{N}} n_\alpha n_\beta \mathcal{V}(\vec{r}_\alpha - \vec{r}_\beta)\right].$$

(c) By setting $n_\alpha = (1+\sigma_\alpha)/2$ and approximating the potential by $\mathcal{V}(\vec{r}_\alpha - \vec{r}_\beta) = -J/\mathcal{N}$, show that this model is identical to the one studied in problem (2). What does this imply about the behavior of this imperfect gas?

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4. *Surfactant condensation:* N surfactant molecules are added to the surface of water over an area A. They are subject to a Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}\sum_{i,j} \mathcal{V}(\vec{r}_i - \vec{r}_j),$$

where $\vec{r}_i$ and $\vec{p}_i$ are two dimensional vectors indicating the position and momentum of particle i.

(a) Write down the expression for the partition function $Z(N, T, A)$ in terms of integrals over $\vec{r}_i$ and $\vec{p}_i$, and perform the integrals over the momenta.

The inter–particle potential $\mathcal{V}(\vec{r})$ is infinite for separations $|\vec{r}| < a$, and attractive for $|\vec{r}| > a$ such that $\int_a^\infty 2\pi r dr \mathcal{V}(r) = -u_0$.

(b) Estimate the total non–excluded area available in the positional phase space of the system of N particles.

(c) Estimate the total *potential* energy of the system, *assuming a uniform density* $n = N/A$. Using this potential energy for all configurations allowed in the previous part, write down an approximation for Z.

(d) The surface tension of water without surfactants is σ_0, approximately independent of temperature. Calculate the surface tension $\sigma(n, T)$ in the presence of surfactants.

(e) Show that below a certain temperature, T_c, the expression for σ is manifestly incorrect. What do you think happens at low temperatures?

(f) Compute the heat capacities, C_A and write down an expression for C_σ without explicit evaluation, due to the surfactants.

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5. *Cubic invariants:* When the order parameter m, goes to zero discontinuously, the phase transition is said to be first order (discontinuous). A common example occurs in systems where symmetry considerations do not exclude a cubic term in the Landau free energy, as in

$$\beta\mathcal{H} = \int d^d\mathbf{x}\left[\frac{K}{2}(\nabla m)^2 + \frac{t}{2}m^2 + cm^3 + um^4\right] \qquad (K, c, u > 0).$$

(a) By plotting the energy density $\Psi(m)$, for uniform m at various values of t, show that as t is reduced there is a discontinuous jump to $\overline{m} \neq 0$ for a positive $\overline{t}$ in the saddle–point approximation.

(b) By writing down the two conditions that $\overline{m}$ and $\overline{t}$ must satisfy at the transition, solve for $\overline{m}$ and $\overline{t}$.

(c) Recall that the correlation length ξ is related to the curvature of $\Psi(m)$ at its minimum by $K\xi^{-2} = \partial^2\Psi/\partial m^2|_{eq.}$. Plot ξ as a function of t.

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6. *Tricritical point:* By tuning an additional parameter, a second order transition can be made first order. The special point separating the two types of transitions is known as a tricritical point, and can be studied by examining the Landau–Ginzburg Hamiltonian

$$\beta\mathcal{H} = \int d^d\mathbf{x}\left[\frac{K}{2}(\nabla m)^2 + \frac{t}{2}m^2 + um^4 + vm^6 - hm\right],$$

where u can be positive or negative. For $u < 0$, a positive v is necessary to ensure stability.

(a) By sketching the energy density $\Psi(m)$, for various t, show that in the saddle–point approximation there is a first-order transition for $u < 0$ and $h = 0$.

(b) Calculate $\overline{t}$ and the discontinuity $\overline{m}$ at this transition.

(c) For $h = 0$ and $v > 0$, plot the phase boundary in the (u, t) plane, identifying the phases, and order of the phase transitions.

(d) The special point $u = t = 0$, separating first– and second–order phase boundaries, is a *tricritical* point. For $u = 0$, calculate the tricritical exponents β, δ, γ, and α, governing the singularities in magnetization, susceptibility, and heat capacity. (Recall: $C \propto t^{-\alpha}$; $\overline{m}(h = 0) \propto t^{\beta}$; $\chi \propto t^{-\gamma}$; and $\overline{m}(t = 0) \propto h^{1/\delta}$.)

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7. *Transverse susceptibility:* An n–component magnetization field $\vec{m}(\mathbf{x})$ is coupled to an external field $\vec{h}$ through a term $-\int d^d\mathbf{x}\, \vec{h}\cdot\vec{m}(\mathbf{x})$ in the Hamiltonian $\beta\mathcal{H}$. If $\beta\mathcal{H}$ for $\vec{h} = 0$

is invariant under rotations of $\vec{m}(\mathbf{x})$; then the free energy density ($f = -\ln Z/V$) only depends on the absolute value of $\vec{h}$; i.e. $f(\vec{h}) = f(h)$, where $h = |\vec{h}|$.

(a) Show that $m_\alpha = \langle \int d^d\mathbf{x} m_\alpha(\mathbf{x})\rangle / V = -h_\alpha f'(h)/h$.

(b) Relate the susceptibility tensor $\chi_{\alpha\beta} = \partial m_\alpha / \partial h_\beta$, to $f''(h)$, $\vec{m}$, and $\vec{h}$.

(c) Show that the transverse and longitudinal susceptibilities are given by $\chi_t = m/h$ and $\chi_\ell = -f''(h)$; where m is the magnitude of $\vec{m}$.

(d) Conclude that χ_t diverges as $\vec{h} \to 0$, whenever there is a spontaneous magnetization. Is there any similar a priori reason for χ_ℓ to diverge?

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8. *Spin waves:* In the XY model of $n = 2$ magnetism, a unit vector $\vec{s} = (s_x, s_y)$ (with $s_x^2 + s_y^2 = 1$) is placed on each site of a d–dimensional lattice. There is an interaction that tends to keep nearest–neighbors parallel, i.e. a Hamiltonian

$$-\beta\mathcal{H} = K \sum_{<ij>} \vec{s}_i \cdot \vec{s}_j \qquad .$$

The notation $< ij >$ is conventionally used to indicate summing over all *nearest–neighbor* pairs (i, j).

(a) Rewrite the partition function $Z = \int \prod_i d\vec{s}_i \exp(-\beta\mathcal{H})$, as an integral over the set of angles $\{\theta_i\}$ between the spins $\{\vec{s}_i\}$ and some arbitrary axis.

(b) At low temperatures ($K \gg 1$), the angles $\{\theta_i\}$ vary slowly from site to site. In this case expand $-\beta\mathcal{H}$ to get a quadratic form in $\{\theta_i\}$.

(c) For $d = 1$, consider L sites with periodic boundary conditions (i.e. forming a closed chain). Find the normal modes θ_q that diagonalize the quadratic form (by Fourier transformation), and the corresponding eigenvalues $K(q)$. Pay careful attention to whether the modes are real or complex, and to the allowed values of q.

(d) Generalize the results from the previous part to a d–dimensional simple cubic lattice with periodic boundary conditions.

(e) Calculate the contribution of these modes to the free energy and heat capacity. (Evaluate the *classical* partition function, i.e. do not quantize the modes.)

(f) Find an expression for $\langle \vec{s}_0 \cdot \vec{s}_{\mathbf{x}} \rangle = \Re\langle \exp[i\theta_{\mathbf{x}} - i\theta_0]\rangle$ by adding contributions from different Fourier modes. Convince yourself that for $|\mathbf{x}| \to \infty$, only $\mathbf{q} \to \mathbf{0}$ modes contribute appreciably to this expression, and hence calculate the asymptotic limit.

(g) Calculate the transverse susceptibility from $\chi_t \propto \int d^d\mathbf{x} \langle \vec{s}_0 \cdot \vec{s}_{\mathbf{x}} \rangle_c$. How does it depend on the system size L?

(h) In $d = 2$, show that χ_t only diverges for K larger than a critical value $K_c = 1/(4\pi)$.

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9. *Capillary waves:* A reasonably flat surface in d–dimensions can be described by its height h, as a function of the remaining $(d-1)$ coordinates $\mathbf{x} = (x_1, ...x_{d-1})$. Convince yourself that the generalized "area" is given by $\mathcal{A} = \int d^{d-1}\mathbf{x}\sqrt{1+(\nabla h)^2}$. With a surface tension σ, the Hamiltonian is simply $\mathcal{H} = \sigma\mathcal{A}$.

(a) At sufficiently low temperatures, there are only slow variations in h. Expand the energy to quadratic order, and write down the partition function as a functional integral.

(b) Use Fourier transformation to diagonalize the quadratic Hamiltonian into its normal modes $\{h_{\mathbf{q}}\}$ (capillary waves).

(c) What symmetry breaking is responsible for these Goldstone modes?

(d) Calculate the height–height correlations $\langle \left(h(\mathbf{x}) - h(\mathbf{x}')\right)^2 \rangle$.

(e) Comment on the form of the result (d) in dimensions $d = 4$, 3, 2, and 1.

(f) By estimating typical values of ∇h, comment on when it is justified to ignore higher order terms in the expansion for $\mathcal{A}$.

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10. *Gauge fluctuations in superconductors:* The Landau–Ginzburg model of superconductivity describes a complex superconducting order parameter $\Psi(\mathbf{x}) = \Psi_1(\mathbf{x}) + i\Psi_2(\mathbf{x})$, and the electromagnetic vector potential $\vec{A}(\mathbf{x})$, which are subject to a Hamiltonian

$$\beta\mathcal{H} = \int d^3\mathbf{x}\left[\frac{t}{2}|\Psi|^2 + u|\Psi|^4 + \frac{K}{2}D_\mu\Psi D_\mu^*\Psi^* + \frac{L}{2}\left(\nabla\times A\right)^2\right].$$

The gauge-invariant derivative $D_\mu \equiv \partial_\mu - ieA_\mu(\mathbf{x})$, introduces the coupling between the two fields. (In terms of Cooper pair parameters, $e = e^*c/\hbar$, $K = \hbar^2/2m^*$.)

(a) Show that the above Hamiltonian is invariant under the *local gauge symmetry*:

$$\Psi(\mathbf{x}) \mapsto \Psi(x)\exp\left(i\theta(\mathbf{x})\right), \qquad \text{and} \qquad A_\mu(\mathbf{x}) \mapsto A_\mu(\mathbf{x}) + \frac{1}{e}\partial_\mu\theta.$$

(b) Show that there is a saddle point solution of the form $\Psi(\mathbf{x}) = \overline{\Psi}$, and $\vec{A}(\mathbf{x}) = 0$, and find $\overline{\Psi}$ for $t > 0$ and $t < 0$.

(c) For $t < 0$, calculate the cost of fluctuations by setting

$$\begin{cases} \Psi(\mathbf{x}) = \left(\overline{\Psi} + \phi(\mathbf{x})\right)\exp\left(i\theta(\mathbf{x})\right), \\ A_\mu(\mathbf{x}) = a_\mu(\mathbf{x}), \quad \text{(with } \partial_\mu a_\mu = 0 \text{ in the Coulomb gauge)} \end{cases}$$

and expanding $\beta\mathcal{H}$ to quadratic order in ϕ, θ, and $\vec{a}$.

(d) Perform a Fourier transformation, and calculate the expectation values of $\langle|\phi(\mathbf{q})|^2\rangle$, $\langle|\theta(\mathbf{q})|^2\rangle$, and $\langle|\vec{a}(\mathbf{q})|^2\rangle$.

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11. *Fluctuations around a tricritical point:* As shown in a previous problem, the Hamiltonian

$$\beta\mathcal{H} = \int d^d\mathbf{x}\left[\frac{K}{2}(\nabla m)^2 + \frac{t}{2}m^2 + um^4 + vm^6\right],$$

with $u = 0$ and $v > 0$ describes a tricritical point.

(a) Calculate the heat capacity singularity as $t \to 0$ by the saddle point approximation.

(b) Include both longitudinal and transverse fluctuations by setting

$$\vec{m}(\mathbf{x}) = \big(\overline{m} + \phi_\ell(\mathbf{x})\big)\hat{e}_\ell + \sum_{\alpha=2}^{n}\phi_t^\alpha(\mathbf{x})\hat{e}_\alpha,$$

and expanding $\beta\mathcal{H}$ to quadratic order in ϕ.

(c) Calculate the longitudinal and transverse correlation functions.

(d) Compute the first correction to the saddle point free energy from fluctuations.

(e) Find the fluctuation correction to the heat capacity.

(f) By comparing the results from parts (a) and (e) *for* $t < 0$ obtain a Ginzburg criterion, and the upper critical dimension for validity of mean–field theory at a tricritical point.

(g) A generalized multicritical point is described by replacing the term vm^6 with $u_{2n}m^{2n}$. Use simple power counting to find the upper critical dimension of this multicritical point.

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