PHYSICS 140B : STATISTICAL PHYSICS
HW ASSIGNMENT #5

(1) Consider a q-state Potts model on the body-centered cubic (BCC) lattice. The Hamiltonian is given by

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

where $\sigma_i \in \{1, \ldots, q\}$ on each site.

(a) Following the mean field treatment in §7.6.3 of the notes, write $x = \langle \delta_{\sigma_i\,,\,1} \rangle = q^{-1} + s$, and expand the free energy in powers of s through terms of order s^4. Neglecting all higher order terms in the free energy, find the critical temperature θ_c, where $\theta = k_B T / zJ$ as usual. Indicate whether the transition is first order or second order (this will depend on q).

(b) For second order transitions, the truncated Landau expansion is sufficient, since we care only about the sign of the quadratic term in the free energy. First order transitions involve a discontinuity in the order parameter, so any truncation of the free energy as a power series in the order parameter involves an approximation. Find a way to numerically determine $\theta_c(q)$ based on the full mean field (*i.e.* variational density matrix) free energy. Compare your results with what you found in part (a), and sketch both sets of results for several values of q.

(2) Consider the $\mathsf{U}(1)$ Ginsburg-Landau theory with

$$F = \int \! d^d\!\boldsymbol{r} \left[\tfrac{1}{2} a \, |\Psi|^2 + \tfrac{1}{4} b \, |\Psi|^4 + \tfrac{1}{2} \kappa \, |\boldsymbol{\nabla} \Psi|^2 \right] .$$

Here $\Psi(\boldsymbol{r})$ is a complex-valued field, and both b and κ are positive. This theory is appropriate for describing the transition to superfluidity. The order parameter is $\langle \Psi(\boldsymbol{r}) \rangle$. Note that the free energy is a functional of the two independent fields $\Psi(\boldsymbol{r})$ and $\Psi^*(\boldsymbol{r})$, where Ψ^* is the complex conjugate of Ψ. Alternatively, one can consider F a functional of the real and imaginary parts of Ψ.

(a) Show that one can rescale the field Ψ and the coordinates $\boldsymbol{r}$ so that the free energy can be written in the form

$$F = \varepsilon_0 \! \int \! d^d\!x \left[\pm \tfrac{1}{2} \, |\psi|^2 + \tfrac{1}{4} \, |\psi|^4 + \tfrac{1}{2} \, |\boldsymbol{\nabla} \psi|^2 \right] ,$$

where ψ and $\boldsymbol{x}$ are dimensionless, ε_0 has dimensions of energy, and where the sign on the first term on the RHS is $\mathsf{sgn}(a)$. Find ε_0 and the relations between Ψ and ψ and between $\boldsymbol{r}$ and $\boldsymbol{x}$.

(b) By extremizing the functional $F[\psi, \psi^*]$ with respect to ψ^*, find a partial differential equation describing the behavior of the order parameter field $\psi(\boldsymbol{x})$.

(c) Consider a two-dimensional system ($d = 2$) and let $a < 0$ (*i.e.* $T < T_c$). Consider the case where $\psi(\boldsymbol{x})$ describe a *vortex* configuration: $\psi(\boldsymbol{x}) = f(r)\, e^{i\phi}$, where (r, ϕ) are two-dimensional polar coordinates. Find the ordinary differential equation for $f(r)$ which extremizes F.

(d) Show that the free energy, up to a constant, may be written as

$$F = 2\pi\varepsilon_0 \int_0^R dr\, r \left[\tfrac{1}{2}(f')^2 + \frac{f^2}{2r^2} + \tfrac{1}{4}(1-f^2)^2 \right] ,$$

where R is the radius of the system, which we presume is confined to a disk. Consider a *trial solution* for $f(r)$ of the form

$$f(r) = \frac{r}{\sqrt{r^2+a^2}} ,$$

where a is the variational parameter. Compute $F(a,R)$ in the limit $R \to \infty$ and extremize with respect to a to find the optimum value of a within this variational class of functions.

(3) A system is described by the Hamiltonian

$$\hat{H} = -J \sum_{\langle ij \rangle} \mathcal{I}(\mu_i, \mu_j) - H \sum_i \delta_{\mu_i,\mathrm{A}} , \tag{1}$$

where on each site i there are four possible choices for μ_i : $\mu_i \in \{\mathrm{A},\mathrm{B},\mathrm{C},\mathrm{D}\}$. The interaction matrix $\mathcal{I}(\mu,\mu')$ is given in the following table:

$\mathcal{I}$	A	B	C	D
A	$+1$	-1	-1	0
B	-1	$+1$	0	-1
C	-1	0	$+1$	-1
D	0	-1	-1	$+1$

(a) Write a trial density matrix

$$\varrho(\mu_1,\ldots,\mu_N) = \prod_{i=1}^N \varrho_1(\mu_i)$$
$$\varrho_1(\mu) = x\,\delta_{\mu,\mathrm{A}} + y(\delta_{\mu,\mathrm{B}} + \delta_{\mu,\mathrm{C}} + \delta_{\mu,\mathrm{D}}) .$$

What is the relationship between x and y? Henceforth use this relationship to eliminate y in terms of x.

(b) What is the variational energy per site, $E(x,T,H)/N$?

(c) What is the variational entropy per site, $S(x,T,H)/N$?

(d) What is the mean field equation for x?

(e) What value x^* does x take when the system is disordered?

(f) Write $x = x^* + \frac{3}{4}\varepsilon$ and expand the free energy to fourth order in ε. (The factor $\frac{3}{4}$ should generate manageable coefficients in the Taylor series expansion.)

(g) Sketch ε as a function of T for $H = 0$ and find T_c. Is the transition first order or second order?

(4) The Blume-Capel model is a $S = 1$ Ising model described by the Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\sum_{i,j} J_{ij}\, S_i\, S_j + \Delta \sum_i S_i^2 \ ,$$

where $J_{ij} = J(\boldsymbol{R}_i - \boldsymbol{R}_j)$ and $S_i \in \{-1, 0, +1\}$. The mean field theory for this model is discussed in section 7.11 of the Lecture Notes, using the 'neglect of fluctuations' method. Consider instead a variational density matrix approach. Take $\varrho(S_1, \ldots, S_N) = \prod_i \tilde{\varrho}(S_i)$, where

$$\tilde{\varrho}(S) = \left(\frac{n+m}{2}\right)\delta_{S,+1} + (1-n)\,\delta_{S,0} + \left(\frac{n-m}{2}\right)\delta_{S,-1} \ .$$

(a) Find $\langle 1 \rangle$, $\langle S_i \rangle$, and $\langle S_i^2 \rangle$.

(b) Find $E = \mathsf{Tr}\,(\varrho H)$.

(c) Find $S = -k_B \mathsf{Tr}\,(\varrho \ln \varrho)$.

(d) Adimensionalizing by writing $\theta = k_B T/\hat{J}(0)$, $\delta = \Delta/\hat{J}(0)$, and $f = F/N\hat{J}(0)$, find the dimensionless free energy per site $f(m, n, \theta, \delta)$.

(e) Write down the mean field equations.

(f) Show that $m = 0$ always permits a solution to the mean field equations, and find $n(\theta, \delta)$ when $m = 0$.

(g) To find θ_c, set $m = 0$ but use both mean field equations. You should recover eqn. 7.322 of the Lecture Notes.

(h) Show that the equation for θ_c has two solutions for $\delta < \delta_*$ and no solutions for $\delta > \delta_*$, and find the value of δ_*.[1]

(i) Assume $m^2 \ll 1$ and solve for $n(m, \theta, \delta)$ using one of the mean field equations. Plug this into your result for part (d) and obtain an expansion of f in terms of powers of m^2 alone. Find the first order line. You may find it convenient to use `Mathematica` here.

[1]This problem has been corrected: (θ_*, δ_*) is not the tricritical point.