PHYSICS 210A : EQUILIBRIUM STATISTICAL PHYSICS
HW ASSIGNMENT #7 SOLUTIONS

(1) The Hamiltonian for the three state ($\mathbb{Z}_3$) clock model is written

$$\hat{H} = -J \sum_{\langle ij \rangle} \hat{\boldsymbol{n}}_i \cdot \hat{\boldsymbol{n}}_j \ ,$$

where each local unit vector $\hat{\boldsymbol{n}}_i$ can take one of three possible values:

$$\hat{\boldsymbol{n}} = \hat{\boldsymbol{x}} \quad , \quad \hat{\boldsymbol{n}} = -\tfrac{1}{2}\hat{\boldsymbol{x}} + \tfrac{\sqrt{3}}{2}\hat{\boldsymbol{y}} \quad , \quad \hat{\boldsymbol{n}} = -\tfrac{1}{2}\hat{\boldsymbol{x}} - \tfrac{\sqrt{3}}{2}\hat{\boldsymbol{y}} \ .$$

(a) Consider the $\mathbb{Z}_3$ clock model on a lattice of coordination number z. Make the mean field assumption $\langle \hat{\boldsymbol{n}}_i \rangle = m\hat{\boldsymbol{x}}$. Expanding the Hamiltonian to linear order in the fluctuations, derive the mean field Hamiltonian for this model $\hat{H}_{\text{MF}}$.

(b) Rescaling $\theta = k_{\text{B}}T/zJ$ and $f = F/NzJ$, where N is the number of sites, find $f(m,\theta)$.

(c) Find the mean field equation.

(d) Is the transition second order or first order?

(e) Show that this model is equivalent to the three state Potts model. Is the $\mathbb{Z}_4$ clock model equivalent to the four state Potts model? Why or why not?

Solution:

(a) The mean field Hamiltonian is

$$\hat{H}_{\text{MF}} = \tfrac{1}{2}NzJm^2 - zJm\,\hat{\boldsymbol{x}} \cdot \sum_i \hat{\boldsymbol{n}}_i \ .$$

(b) We have

$$\begin{aligned} f(m,\theta) &= \tfrac{1}{2}m^2 - \theta \ln \underset{\hat{\boldsymbol{n}}}{\mathsf{Tr}}\, e^{m\hat{\boldsymbol{x}}\cdot\hat{\boldsymbol{n}}/\theta} \\ &= \tfrac{1}{2}m^2 - \theta \ln\Big(\tfrac{1}{3}e^{m/\theta} + \tfrac{2}{3}e^{-m/2\theta}\Big) \\ &= \tfrac{1}{2}\Big(1 - \frac{1}{2\,\theta}\Big)m^2 - \frac{m^3}{24\,\theta^2} + \frac{m^4}{64\,\theta^3} + \mathcal{O}(m^5) \ . \end{aligned}$$

Here we have defined $\mathsf{Tr}_{\hat{\boldsymbol{n}}} = \frac{1}{3}\sum_{\hat{\boldsymbol{n}}}$ as the normalized trace. The last line is somewhat tedious to obtain, but is not necessary for this problem.

(c) The mean field equation is

$$0 = \frac{\partial f}{\partial m} = m - \frac{e^{m/\theta} - e^{-m/2\theta}}{e^{m/\theta} + 2\,e^{-m/2\theta}} \ .$$

$\varepsilon_{\sigma\sigma'}^{\text{clock}}$	$0°$	$120°$	$240°$
$0°$	$-J$	$\frac{1}{2}J$	$\frac{1}{2}J$
$120°$	$\frac{1}{2}J$	$-J$	$\frac{1}{2}J$
$240°$	$\frac{1}{2}J$	$\frac{1}{2}J$	$-J$

Table 1: $\mathbb{Z}_3$ clock model energy matrix.

$\varepsilon_{\sigma\sigma'}^{\text{Potts}}$	A	B	C
A	$-\tilde{J}$	0	0
B	0	$-\tilde{J}$	0
C	0	0	$-\tilde{J}$

Table 2: $q = 3$ Potts model energy matrix.

Expanding the RHS to lowest order in m and setting the slope to 1, we find $\theta_c = \frac{1}{2}$.

(d) Since $f(m, \theta) \neq f(-m, \theta)$, the Landau expansion of the free energy (other than constants) should include terms of all orders starting with $\mathcal{O}(m^2)$. This means that there will in general be a cubic term, hence we expect a first order transition.

(e) Let $\varepsilon(\hat{\boldsymbol{n}}, \hat{\boldsymbol{n}}') = -J\hat{\boldsymbol{n}} \cdot \hat{\boldsymbol{n}}'$ be the energy for a given link. The unit vectors $\hat{\boldsymbol{n}}$ and $\hat{\boldsymbol{n}}'$ can each point in any of three directions, which we can label as $0°$, $120°$, and $240°$. The matrix of possible bond energies is shown in Tab. 1.

Now consider the $q = 3$ Potts model, where the local states are labeled $|\,\text{A}\,\rangle$, $|\,\text{B}\,\rangle$, and $|\,\text{C}\,\rangle$. The Hamiltonian is

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

The interaction energy matrix for the Potts model is given in Tab. 2.

We can in each case label the three states by a local variable $\sigma \in \{1, 2, 3\}$, corresponding, respectively, to $0°$, $120°$, and $240°$ for the clock model and to A, B, and C for the Potts model. We then observe

$$\varepsilon_{\sigma\sigma'}^{\text{clock}}(J) = \varepsilon_{\sigma\sigma'}^{\text{Potts}}(\tfrac{3}{2}J) + \tfrac{1}{2}J \ .$$

Thus, the free energies satisfy

$$F^{\text{clock}}(J) = \tfrac{1}{4}NzJ + F^{\text{Potts}}(\tfrac{3}{2}J) \ ,$$

and the models are equivalent. However, the $\mathbb{Z}_q$ clock model and q-state Potts model are *not* equivalent for $q > 3$. Can you see why? *Hint: construct the corresponding energy matrices for* $q = 4$*.*

(2) 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 $\hat{H}_{\rm MF}$?

(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.

(c) Find the mean field equation relating m, θ, and h.

(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 $\theta_{\rm c}$?

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

Solution:

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

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

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 $u \equiv (m+h)/\theta$,

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

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

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

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

(3) Consider the free energy

$$f(\theta, m) = f_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 + \tfrac{1}{8}dm^8$$

with $d > 0$. Note there is an octic term but no sextic term. Derive results corresponding to those in fig. 7.16 of the lecture notes. Find the equation of the first order line in the $(a/d, b/d)$ plane. Also identify the region in parameter space where there exist metastable local minima in the free energy (curve E in fig. 7.16).

Solution:

We have

$$\begin{aligned}
f(m) &= f_0 + \tfrac{1}{2}am^2 + \tfrac{1}{4}bm^4 + \tfrac{1}{8}dm^8 \\
f'(m) &= am + bm^3 + dm^7 \\
f''(m) &= a + 3bm^2 + 7dm^6 \quad .
\end{aligned}$$

To find the first order line, we set $f(m) = f_0$ and $f'(m) = 0$ simultaneously. Dividing out by the root at $m = 0$ we obtain the simultaneous equations

$$\begin{aligned}
\tfrac{1}{2}a + \tfrac{1}{4}bm^2 + \tfrac{1}{8}dm^6 &= 0 \\
a + bm^2 + dm^6 &= 0 \quad .
\end{aligned}$$

Eliminating the m^6 terms, we obtain $m^2 = 3a/|b|$ (remember $a > 0$ and $b < 0$ for a first order transition). Inserting this back in either of the above equations yields the relation

$$a_c = \sqrt{\frac{2|b|^3}{27d}} \quad .$$

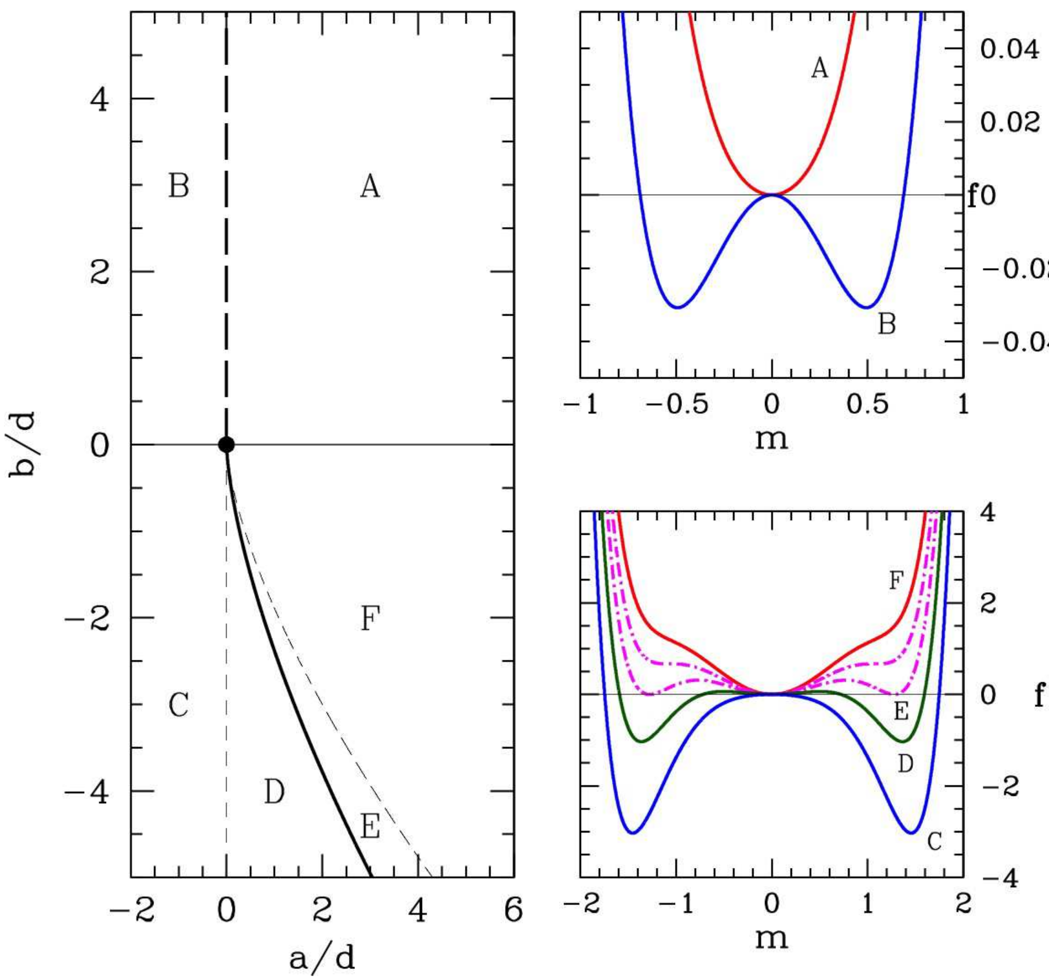

Figure 1: Regimes for the octic free energy in problem 5..

To obtain the condition for the saddle-node bifurcation, where the metastable $m \neq 0$ local minima in $f(m)$ first appear, we simultaneously solve $f'(m) = 0$ and $f''(m) = 0$, yielding the simultaneous equations

$$a + bm^2 + dm^6 = 0$$
$$a + 3bm^2 + 7dm^6 = 0 \quad .$$

Again we eliminate the m^6 term and solve for m^2, obtaining $m^2 = 3a/2|b|$. Inserting this back into either of the above equations yields the condition

$$a^* = \sqrt{\frac{4|b|^3}{27d}} \quad .$$

The results are plotted in fig. 1. Note $a^* > a_c$.

(4) Consider the 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

$$F = 2\pi\varepsilon_0 \int\limits_0^R dr \, r \left[\tfrac{1}{2} (f')^2 + \frac{f^2}{2r^2} + \tfrac{1}{4} (1 - f^2)^2 \right] ,$$

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.

Solution:

(a) Taking the ratio of the second and first terms in the free energy density, we learn that Ψ has units of $A \equiv \big(|a|/b\big)^{1/2}$. Taking the ratio of the third to the first terms yields a length scale $\xi = \big(\kappa/|a|\big)^{1/2}$. We therefore write $\Psi = A \, \psi$ and $\tilde{\boldsymbol{x}} = \xi x$ to obtain the desired form of the free energy, with

$$\varepsilon_0 = A^2 \, \xi^d \, |a| = |a|^{2 - \frac{1}{2}d} \, b^{-1} \, \kappa^{\frac{1}{2}d} \, .$$

(b) We extremize with respect to the field ψ^*. Writing $F = \varepsilon_0 \int d^3\!x\, \mathcal{F}$, with $\mathcal{F} = \pm\frac{1}{2}\,|\psi|^2 + \frac{1}{4}\,|\psi|^4 + \frac{1}{2}\,|\boldsymbol{\nabla}\psi|^2$,

$$\frac{\delta(F/\varepsilon_0)}{\delta\psi^*(\boldsymbol{x})} = \frac{\partial\mathcal{F}}{\partial\psi^*} - \boldsymbol{\nabla}\cdot\frac{\partial\mathcal{F}}{\partial\,\boldsymbol{\nabla}\psi^*} = \pm\tfrac{1}{2}\,\psi + \tfrac{1}{2}\,|\psi|^2\,\psi - \tfrac{1}{2}\,\nabla^2\psi\,.$$

Thus, the desired PDE is

$$-\nabla^2\psi \pm \psi + |\psi|^2\,\psi = 0\,,$$

which is known as the time-independent nonlinear Schrödinger equation.

(c) In two dimensions,

$$\boldsymbol{\nabla}^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\,\frac{\partial}{\partial r} + \frac{1}{r^2}\,\frac{\partial^2}{\partial\phi^2}\,.$$

Plugging in $\psi = f(r)\,e^{i\phi}$ into $\nabla^2\psi + \psi - |\psi|^2\psi = 0$, we obtain

$$\frac{d^2\!f}{dr^2} + \frac{1}{r}\,\frac{df}{dr} - \frac{f}{r^2} + f - f^3 = 0\,.$$

(d) Plugging $\boldsymbol{\nabla}\psi = \hat{\boldsymbol{r}}\,f'(r) + \frac{i}{r}\,f(r)\,\hat{\boldsymbol{\phi}}$ into our expression for F, we have

$$\begin{aligned}\mathcal{F} &= \tfrac{1}{2}\,|\boldsymbol{\nabla}\psi|^2 - \tfrac{1}{2}\,|\psi|^2 + \tfrac{1}{4}\,|\psi|^4\\ &= \tfrac{1}{2}\big(f'\big)^2 + \frac{f^2}{2r^2} + \tfrac{1}{4}\,\big(1-f^2\big)^2 - \tfrac{1}{4}\,,\end{aligned}$$

which, up to a constant, is the desired form of the free energy. It is a good exercise to show that the Euler-Lagrange equations,

$$\frac{\partial\,(r\mathcal{F})}{\partial f} - \frac{d}{dr}\bigg(\frac{\partial\,(r\mathcal{F})}{\partial f'}\bigg) = 0$$

results in the same ODE we obtained for f in part (c). We now insert the trial form for $f(r)$ into F. The resulting integrals are elementary, and we obtain

$$F(a,R) = \tfrac{1}{4}\pi\varepsilon_0\Bigg\{1 - \frac{a^4}{(R^2+a^2)^2} + 2\ln\!\bigg(\frac{R^2}{a^2}+1\bigg) + \frac{R^2\,a^2}{R^2+a^2}\Bigg\}\,.$$

Taking the limit $R\to\infty$, we have

$$F(a, R\to\infty) = 2\ln\!\bigg(\frac{R^2}{a^2}\bigg) + a^2\,.$$

We now extremize with respect to a, which yields $a = \sqrt{2}$. Note that the energy in the vortex state is logarithmically infinite. In order to have a finite total free energy (relative to the ground state), we need to introduce an *antivortex* somewhere in the system. An antivortex has a phase winding which is opposite to that of the vortex, *i.e.* $\psi = f\, e^{-i\phi}$. If the vortex and antivortex separation is r, the energy is

$$V(r) = \tfrac{1}{2}\pi\varepsilon_0 \ln\bigg(\frac{r^2}{a^2} + 1\bigg) \ .$$

This tends to $V(r) = \pi\varepsilon_0 \ln(d/a)$ for $d \gg a$ and smoothly approaches $V(0) = 0$, since when $r = 0$ the vortex and antivortex annihilate leaving the ground state condensate. Recall that two-dimensional point charges also interact via a logarithmic potential, according to Maxwell's equations. Indeed, there is a rather extensive analogy between the physics of two-dimensional models with $\mathsf{O}(2)$ symmetry and $(2+1)$-dimensional electrodynamics.