PHYSICS 140B W26 : STATISTICAL PHYSICS
HW ASSIGNMENT #6 SOLUTIONS

(1) 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

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

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

$$\begin{aligned} a + bm^2 + dm^6 &= 0 \\ a + 3bm^2 + 7dm^6 &= 0 \quad . \end{aligned}$$

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 $a^* > a_c$.

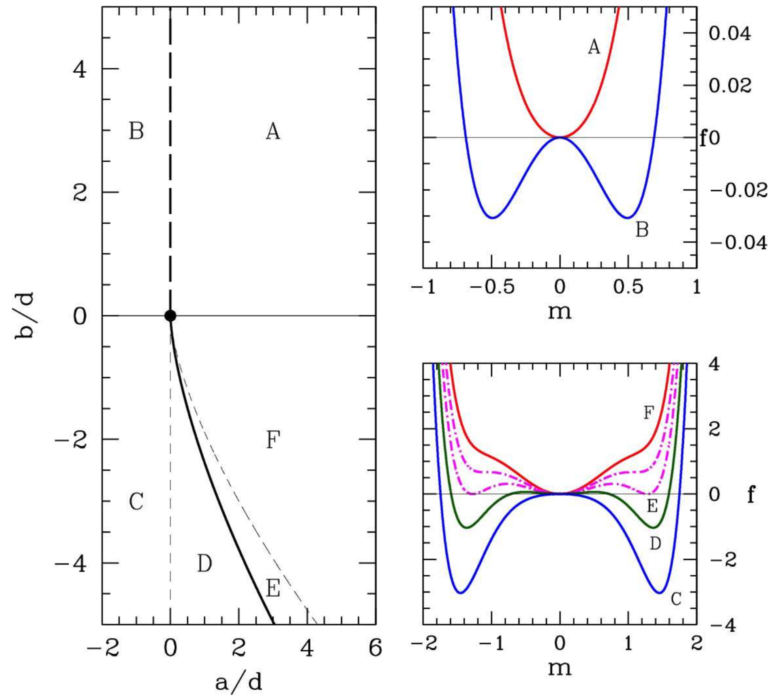

Figure 1: Regimes for the octic free energy in problem 1.

(2) Consider the four-state clock model,

$$\hat{H} = -\frac{1}{2}\sum_{i,j=1}^{N} J_{ij}\,\hat{\boldsymbol{n}}_i\cdot\hat{\boldsymbol{n}}_j - H\hat{\boldsymbol{x}}\cdot\sum_{i=1}^{N}\hat{\boldsymbol{n}}_i \quad ,$$

where at each site $\hat{\boldsymbol{n}}_i \in \{\pm\hat{\boldsymbol{x}}, \pm\hat{\boldsymbol{y}}\}$. Work out the variational density matrix mean field theory, taking $\varrho_{\mathsf{var}}(\hat{\boldsymbol{n}}_1,\ldots,\hat{\boldsymbol{n}}_N) = \prod_{i=1}^N \varrho(\hat{\boldsymbol{n}}_i)$ with the single site variational density matrix

$$\varrho(\hat{\boldsymbol{n}}) = \tfrac{1}{2}(1+u-v)\,\delta_{\hat{\boldsymbol{n}},\hat{\boldsymbol{x}}} + \tfrac{1}{2}(1-u-v)\,\delta_{\hat{\boldsymbol{n}},-\hat{\boldsymbol{x}}} + \tfrac{1}{2}\,v\,\delta_{\hat{\boldsymbol{n}},\hat{\boldsymbol{y}}} + \tfrac{1}{2}\,v\,\delta_{\hat{\boldsymbol{n}},-\hat{\boldsymbol{y}}} \quad .$$

(a) What is the global symmetry group for this Hamiltonian when $H=0$? (Give the name of the group, or express how the symmetry operations act in words/equations.)

(b) Evaluate $E = \mathsf{Tr}(\varrho_{\mathsf{var}}\,\hat{H})$.

(c) Evaluate $S = -k_{\rm B}\,\mathsf{Tr}(\varrho_{\mathsf{var}}\log\varrho_{\mathsf{var}})$.

(d) Adimensionalize by writing $\theta = k_{\rm B}T/\hat{J}(0)$ and $h = H/\hat{J}(0)$, where z is the lattice coordination number. Find $f(u,v,\theta,h) = F/N\hat{J}(0)$.

(e) Find all the mean field equations.

(f) Show that the solution to the mean field equations requires that $v=v(u)$ is a function of u alone and find $v(u)$

(g) Substituting $v(u)$, find $f(u, \theta, h) = f(u, v(u), \theta, h)$.

(h) Expand $f(u, \theta, h)$ as a power series in u up to order u^6 and identify the critical temperature θ_c and the order of the phase transition.

Solution:

(a) The global symmetry group is D_4, which has eight elements, $\{E, r, s, \bar{r}, h, v, d, \bar{d}\}$. These may be expressed as 2×2 matrices, *viz.*

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad r = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad , \quad s = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad \bar{r} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$
$$h = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \quad , \quad v = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad , \quad d = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \bar{d} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \quad .$$

Thus, E is the identity, r is the $90°$ counterclockwise rotation with $x' = -y$ and $y' = x$, $s = r^2$ and $\bar{r} = r^3$ are rotations through $180°$ and $270°$. Note that $\{E, r, s, \bar{r}\}$ are all *proper rotations*, each with determinant $+1$. The four *improper rotations* $\{h, v, d, \bar{d}\}$, each with determinant -1, are the horizontal, vertical, and two diagonal mirrors, with d reflecting in the line $y = x$ and $\bar{d}$ in the line $y = -x$. The (row $\times$ column) multiplication table, or *Cayley table*, for D_4 is

D_4	E	r	s	$\bar{r}$	h	v	d	$\bar{d}$
E	E	r	s	$\bar{r}$	h	v	d	$\bar{d}$
r	r	s	$\bar{r}$	E	$\bar{d}$	d	h	v
s	s	$\bar{r}$	E	r	v	h	$\bar{d}$	d
$\bar{r}$	$\bar{r}$	E	r	s	d	$\bar{d}$	v	h
h	h	d	v	$\bar{d}$	E	s	r	$\bar{r}$
v	v	$\bar{d}$	h	d	s	E	$\bar{r}$	r
d	d	v	$\bar{d}$	h	$\bar{r}$	r	E	s
$\bar{d}$	$\bar{d}$	h	d	v	r	$\bar{r}$	s	E

Table 1: Cayley table for D_4.

Note that D_4 is nonabelian. For example, $rv = d$ but $vr = \bar{d}$.

(b) We have

$$E = (\varrho_{\mathsf{var}}\, \hat{H}) = -\frac{1}{2} \sum_{i,j=1}^{N} J_{ij}\, \langle \hat{\boldsymbol{n}}_i \rangle \cdot \langle \hat{\boldsymbol{n}}_j \rangle - H \hat{\boldsymbol{x}} \cdot \sum_{i=1}^{N} \langle \hat{\boldsymbol{n}}_i \rangle \quad ,$$

where

$$\langle \hat{\boldsymbol{n}}_i \rangle = \mathsf{Tr}\left[\varrho(\hat{\boldsymbol{n}}_i)\, \hat{\boldsymbol{n}}_i\right] = u\hat{\boldsymbol{x}} \quad .$$

Thus,

$$E = -\tfrac{1}{2} N \hat{J}(0) u^2 - NHu \quad .$$

(c) The entropy is given by $S = Ns$, where

$$s = -k_{\rm B} \,\mathrm{Tr}\, \varrho \log \varrho = -k_{\rm B} \sum_{\hat{\boldsymbol{n}}} \varrho(\hat{\boldsymbol{n}}) \log \varrho(\hat{\boldsymbol{n}})$$

$$= -k_{\rm B} \Bigg\{ \bigg(\frac{1+u-v}{2}\bigg) \log\bigg(\frac{1+u-v}{2}\bigg) + \bigg(\frac{1-u-v}{2}\bigg) \log\bigg(\frac{1-u-v}{2}\bigg) + v \log\bigg(\frac{v}{2}\bigg) \Bigg\} \quad .$$

(d) We then have

$$f(u,v,\theta,h) = -\tfrac{1}{2}u^2 - hu + \theta \Bigg\{ \bigg(\frac{1+u-v}{2}\bigg) \log\bigg(\frac{1+u-v}{2}\bigg) + \bigg(\frac{1-u-v}{2}\bigg) \log\bigg(\frac{1-u-v}{2}\bigg) + v \log\bigg(\frac{v}{2}\bigg) \Bigg\} \quad .$$

(e) There are two mean field equations:

$$0 = \frac{\partial f}{\partial u} = -u - h + \tfrac{1}{2}\theta \, \log\bigg(\frac{1+u-v}{1-u-v}\bigg)$$

$$0 = \frac{\partial f}{\partial v} = \tfrac{1}{2} \log\bigg(\frac{v^2}{(1-v)^2 - u^2}\bigg) \quad .$$

(f) The solution to the second mean field equation is $v(u) = \frac{1}{2}(1-u^2)$.

(g) Substituting $v(u)$ into $f(u,v,\theta,h)$, we obtain, after a little work,

$$f(u,\theta,h) = -\tfrac{1}{2}u^2 - hu + \theta \left\{ \log(1-u^2) + u \log\bigg(\frac{1+u}{1-u}\bigg) \right\} - \theta \log 4$$

$$= -\theta \log 4 - hu + (\theta - \tfrac{1}{2})\, u^2 + \tfrac{1}{6}\theta\, u^4 + \tfrac{1}{15}\theta\, u^6 + \ldots \quad .$$

Thus h breaks $u \leftrightarrow -u$ symmetry of this free energy. For $n > 1$ the coefficient $a_2 n$ of the u^{2n} term is found to be $a_{2n} = \theta/[n(2n-1)]$. There is a second order transition when $a_2(\theta)$ vanishes, which is at $\theta_c = \frac{1}{2}$.