RG Methods in Statistical Field Theory: Problem Set 2 Solution

The ordered phase for the magnetic system we examined in class had a spatially uniform order parameter. Here we will look at a more general situation, with the possibility of a *modulated phase*, where the order parameter varies periodically in space. For simplicity, we consider an $n = 1$, $d = 1$ system along a line of length L, with a Hamiltonian functional given by:

$$\mathcal{H}[m(x)] = \int_0^L dx \left[\frac{r}{2} m^2(x) + u m^4(x) + \frac{c}{2}\left(\frac{\partial m}{\partial x}\right)^2 + \frac{D}{2}\left(\frac{\partial^2 m}{\partial x^2}\right)^2 \right]$$

Here r varies with temperature, and u, D, c are constants. We restrict u, $D > 0$, but we allow c to take on any value. When both $c > 0$ and $D > 0$, any spatial fluctuations in $m(x)$ cost energy, so we expect all phases to be uniform. On the other hand when $c < 0$ and $D > 0$, there is the possibility that the system can lower its free energy by going to a nonuniform phase. We will investigate this possibility by constructing the mean-field phase diagram in terms of r and c. We do this in several steps:

(a) Because we are dealing with the possibility of spatially fluctuating $m(x)$, it is reasonable to rewrite the Hamiltonian in terms of Fourier modes. We define the Fourier transforms:

$$m(x) = \frac{1}{L}\sum_{n=-\infty}^{\infty} m_n e^{iq_n x}\,, \qquad m_n = \int_0^L dx\, e^{-iq_n x} m(x)$$

where n is an integer and $q_n = 2\pi n/L$. The orthogonality and completeness properties for the Fourier modes $e^{iq_n x}$ are:

$$\int_0^L dx\, e^{i(q_n - q_{n'})x} = L\delta_{n,n'}\,, \qquad \sum_{n=-\infty}^{\infty} e^{-iq_n x} = L\delta(x)$$

Plug in the expansion for $m(x)$ into the Hamiltonian $\mathcal{H}$ and show that we can write:

$$\mathcal{H} = \frac{1}{2L}\sum_n K_n m_n m_{-n} + \frac{u}{L^3}\sum_{n,n',n''} m_n m_{n'} m_{n''} m_{-n-n'-n''}$$

where $K_n = r + cq_n^2 + Dq_n^4$.

<u>**Answer:**</u> Plugging the expansion term by term into the Hamiltonian:

$$\begin{aligned}
\int_0^L dx\, \frac{r}{2} m^2(x) &= \int_0^L dx\, \frac{r}{2L^2}\sum_{n,n'} m_n m_{n'} e^{i(q_n+q_{n'})x} \\
&= \frac{r}{2L^2}\sum_{n,n'} m_n m_{n'} L\delta_{n,-n'} = \frac{r}{2L}\sum_n m_n m_{-n} \\
\int_0^L dx\, \frac{c}{2}\left(\frac{\partial m}{\partial x}\right)^2 &= \int_0^L dx\, \frac{c}{2L^2}\sum_{n,n'} m_n m_{n'}(-q_n q_{n'}) e^{i(q_n+q_{n'})x} \\
&= \frac{c}{2L}\sum_n (-q_n q_{-n}) m_n m_{-n} = \frac{c}{2L}\sum_n q_n^2 m_n m_{-n}
\end{aligned}$$

$$\begin{aligned}
\int_0^L dx\, \frac{D}{2}\left(\frac{\partial^2 m}{\partial x^2}\right)^2 &= \int_0^L dx\, \frac{D}{2L^2}\sum_{n,n'} m_n m_{n'} q_n^2 q_{n'}^2 e^{i(q_n+q_{n'})x} \\
&= \frac{D}{2L}\sum_n q_n^2 q_{-n}^2 m_n m_{-n} = \frac{D}{2L}\sum_n q_n^4 m_n m_{-n} \\
\int_0^L dx\, u\, m^4(x) &= \int_0^L dx\, \frac{u}{L^4}\sum_{n,n',n'',n'''} m_n m_{n'} m_{n''} m_{n'''} e^{i(q_n+q_{n'}+q_{n''}+q_{n'''})x} \\
&= \frac{u}{L^4}\sum_{n,n',n'',n'''} m_n m_{n'} m_{n''} m_{n'''} L\delta_{n+n'+n'',-n'''} \\
&= \frac{u}{L^3}\sum_{n,n',n''} m_n m_{n'} m_{n''} m_{-n-n'-n''}
\end{aligned}$$

Putting all this together, we get the result for the Hamiltonian quoted above:

$$\mathcal{H} = \frac{1}{2L}\sum_n K_n m_n m_{-n} + \frac{u}{L^3}\sum_{n,n',n''} m_n m_{n'} m_{n''} m_{-n-n'-n''}$$

where $K_n = r + c q_n^2 + D q_n^4$. Note that $K_{-n} = K_n$.

(b) We solve this system using a mean-field approximation, writing the partition function $Z \approx \exp(-\beta\mathcal{H}[m_{\text{sad}}(x)])$, where $m_{\text{sad}}(x)$ minimizes $\mathcal{H}$. In terms of Fourier modes, the saddle point condition can be expressed as the series of coupled equations:

$$\frac{\partial \mathcal{H}}{\partial m_n} = 0 \quad \text{for all } n$$

Show that each of the following cases is a possible solution of the saddle point equations. In each case, also find the range of r and c for which the solution is possible. (Do not worry about the free energy of the solutions yet; we will look at this in the next part.)

Case I: $m_n = 0$ for all n. This case corresponds to an order parameter $m(x) = 0$ at every point.

Case II: $m_n = La_0\delta_{n,0}$ where $a_0 \neq 0$ is a real constant. This case corresponds to a uniform order parameter $m(x) = a_0$.

Case III: $m_n = La_k(\delta_{n,k} + \delta_{n,-k})$ for some positive integer $k \neq 0$ and real constant $a_k \neq 0$. This case corresponds to a spatially varying order parameter $m(x) = 2a_k\cos(2\pi kx/L)$.

Answer: The saddle point equations have two different forms, one for $n = 0$, and one for $n \neq 0$. The first form is:

$$0 = \frac{\partial \mathcal{H}}{\partial m_0} = \frac{K_0}{L}m_0 + \frac{4u}{L^3}\sum_{\substack{n',n'',n'''\neq 0\\ n'+n''+n'''=0}} m_{n'} m_{n''} m_{n'''} + \frac{12u}{L^3}\sum_{n'\neq 0} m_{n'} m_{-n'} m_0 + \frac{4u}{L^3}m_0^3$$

We derived this answer by considering every possible way in which m_0 could appear in $\mathcal{H}$. In particular, the u sum in $\mathcal{H}$ involves products like $m_n m_{n'} m_{n''} m_{n'''}$ where $n+n'+n''+n''' = 0$. The second term above comes from the derivative of the u sum where we have one m_0 component, and three components not equal to m_0. The third term comes from the derivative of the u sum where we have two m_0 components, and two components not equal to m_0. The last term comes from the derivative of the u sum where all four components are m_0.

Using a similar analysis, we can also derive the second form of the saddle point equations, when $n \neq 0$:

$$0 = \frac{\partial \mathcal{H}}{\partial m_n} = \frac{K_n}{L} m_{-n} + \frac{4u}{L^3} \sum_{\substack{n', n'', n''' \neq n \\ n'+n''+n'''=-n}} m_{n'} m_{n''} m_{n'''} + \frac{12u}{L^3} \sum_{\substack{n', n'' \neq n \\ n'+n''=-2n}} m_{n'} m_{n''} m_n + \frac{12u}{L^3} m_{-3n} m_n^2$$

Now let us consider each case in turn, and verify that the saddle point equations are satisfied:

Case I: When $m_n = 0$ for all n, all the saddle point equations are trivially satisfied. There are no restrictions on r and c.

Case II: Here $m_n = La_0 \delta_{n,0}$, where $a_0 \neq 0$ is a real constant. The $n \neq 0$ saddle point equations are satisfied, since each term involves at least one $m_{n'}$ where $n' \neq 0$, and these $m_{n'}$ are all zero. The $n = 0$ saddle point equation becomes:

$$0 = K_0 a_0 + 4ua_0^3$$

This is satisfied when $a_0 = \sqrt{-K_0/4u} = \sqrt{-r/4u}$. Thus we need to have $r < 0$ for this to be a possible solution, and c can be anything.

Case III: Here $m_n = La_k(\delta_{n,k} + \delta_{n,-k})$ for some positive integer $k \neq 0$ and real constant $a_k \neq 0$. The $n = 0$ saddle point equation is satisfied, since each term involves at least one $m_{n'}$ where $n' \neq \pm k$. The saddle point equations for $n \neq \pm k$ are also satisfied for the same reason. This leaves us with the saddle point equations for $n = k$ and $n = -k$, both of which give the same condition:

$$0 = K_k a_k + 12ua_k^3$$

This is satisfied when $a_k = \sqrt{-K_k/12u} = \sqrt{-(r + cq_k^2 + Dq_k^4)/12u}$. Thus we need to have $r < -cq_k^2 - Dq_k^4$ for this to be a possible solution.

c) We would now like to draw a phase diagram in terms of r and c, centered at the point $r = 0$, $c = 0$, and including regions of positive and negative r, and positive and negative c. For any given r and c, the phase at that point is determined by which of the three solutions in part (b) has the smallest free energy $A = -k_B T \ln Z \approx \mathcal{H}$. Case I corresponds to the paramagnetic phase, Case II to the ferromagnetic phase, and Case III to the modulated phase. Note that in Case III, for a given value of c, there will be a single value of k which gives the minimum free energy. You should find this k in terms of c and D, which tells you the wavevector of the order parameter in the modulated phase. When drawing the phase diagram, you should get exact equations for all transition curves in the diagram, and identify which transitions are first-order (discontinuous change of order parameter), and which transitions are second-order (continuous change of order parameter).

Answer: We start by plugging the three possible solutions into the Hamiltonian, to calculate their free energies. In the mean-field approximation $A \approx \mathcal{H}$ evaluated at the saddle point solution. For case I, the free energy is:

$$A_I = 0$$

For case II, the free energy is:

$$A_{II} = \frac{K_0 L}{2} a_0^2 + uLa_0^4 = -\frac{r^2 L}{8u} + \frac{r^2 L}{16u} = -\frac{r^2 L}{16u} \qquad \text{where } r < 0$$

For case III, the free energy is:

$$A_{III} = K_k L a_k^2 + 6uLa_k^4 = -\frac{(r + cq_k^2 + Dq_k^4)^2 L}{12u} + \frac{(r + cq_k^2 + Dq_k^4)^2 L}{24u}$$
$$= -\frac{(r + cq_k^2 + Dq_k^4)^2 L}{24u} \qquad \text{where } r < -cq_k^2 - Dq_k^4$$

The phase diagram can be divided into two regions, one for $c \geq 0$, and the other for $c < 0$:

$c \geq 0$ region: When $r > 0$ only case I is an allowed solution, so we get the paramagnetic phase. When $r < 0$ case I and II are allowed solutions, and if r is sufficiently negative, $r < -cq_k^2 - Dq_k^4$ for some $k \neq 0$, then case III is also a solution. Comparing the free energies, we find A_{II} is the lowest, so we get the ferromagnetic phase. The boundary between the paramagnetic and ferromagnetic phases is the line $r = 0$. As we decrease r below $r = 0$ the magnetization $a_0 = \sqrt{-r/4u}$ increases continuously from zero, so this phase transition is second-order.

$c < 0$ region: We note that for a given r, the only values of k which are allowed solutions in case III have to satisfy $-cq_k^2 - Dq_k^4 > r$. Of these possible k, the free energy A_{III} has a minimum at $k_{\min} = \frac{L}{2\pi}\sqrt{\frac{-c}{2D}}$, where

$$A_{III}(k_{\min}) = -\frac{(r - c^2/4D)^2 L}{24u}$$

For $r > 0$, case II is not a possible solution, so we only have to compare cases I and III. Case III only becomes possible for $r < c^2/4D$, and in this region $A_{III}(k_{\min})$ is smaller than $A_I = 0$, so the line $r = c^2/4D$ represents the phase transition between the paramagnetic and modulated phases. Since A_{III} below this line is always smallest for $k_{\min}$, the magnetization of the modulated phase has the form: $m(x) = 2a_{k_{\min}} \cos(2\pi k_{\min} x/L)$. The amplitude

$$2a_{k_{\min}} = 2\sqrt{\frac{-(r + cq_{k_{\min}}^2 + Dq_{k_{\min}}^4)}{12u}} = 2\sqrt{\frac{-(r - c^2/4D)}{12u}}$$

is zero on the line $r = c^2/4D$, and increases continuously as we decrease r below the line, so this phase transition is second-order.

For $r < 0$, all three cases are possible solutions, but A_{II} and $A_{III}(k_{\min})$ are both smaller than $A_I = 0$, so the competition is between the modulated and ferromagnetic phases. The phase transition between these two phases is on the curve $A_{II} = A_{III}(k_{\min})$, which can be written as follows:

$$-\frac{r^2 L}{16u} = -\frac{(r - c^2/4D)^2 L}{24u} \quad \Rightarrow \quad r = -\frac{c^2}{4D}(2 + \sqrt{6})$$

For r above this curve we have the modulated phase, for r below this curve we have the ferromagnetic phase. On the curve the magnetization of the ferromagnetic phase is:

$$a_0 = \sqrt{\frac{-r}{4u}} = \sqrt{\frac{c^2(2 + \sqrt{6})}{16uD}}$$

On the curve the amplitude of the magnetization in the modulated phase, $2a_{k_{\min}}$, is given by:

$$2a_{k_{\min}} = 2\sqrt{\frac{-(r - c^2/4D)}{12u}} = \sqrt{\frac{c^2(3 + \sqrt{6})}{12uD}}$$

Since there is a discontinuity in the magnetization crossing the phase boundary, the transition is first-order.

Below we plot the phase diagram for $D = 1$. The blue lines are second-order transitions, the red one first-order. The point at which the three transition lines meet is known as a *Lifshitz point*.