RG Methods in Statistical Field Theory: Problem Set 3 Solution

In class we discussed the spin wave fluctuations which occur when a continuous symmetry is broken. In this problem set, we will see that such fluctuations can actually *destroy* the ordered state completely under certain conditions. We will work in d dimensions, and concentrate on the case of an order parameter with $n = 2$ components (known as the XY model).

Let us start at the same place we did in class: by taking the mean-field solution and adding small fluctuations to it. Assume the mean-field solution has the form $\mathbf{m}(\mathbf{x}) = m\hat{\mathbf{e}}_1$, where m is independent of $\mathbf{x}$, and $\hat{\mathbf{e}}_1$ is a unit vector along the direction in which the system orders at low temperature. Instead of using the $\phi_\parallel$ and $\phi_\perp$ fluctuations we introduced in class, we choose to write the fluctuations in a different form, more convenient when the $\mathbf{m}(\mathbf{x})$ vector has only $n = 2$ components:

$$\mathbf{m}(\mathbf{x}) = m\cos\theta(\mathbf{x})\,\hat{\mathbf{e}}_1 + m\sin\theta(\mathbf{x})\,\hat{\mathbf{e}}_2$$

Here $\theta(\mathbf{x})$ is an angle that can vary with position. When there are no fluctuations, $\theta(\mathbf{x}) = 0$, and we get the mean-field solution with all the $\mathbf{m}(\mathbf{x})$ vectors pointing in the same direction. Let us now see what happens when we allow $\theta(\mathbf{x})$ to be nonzero.

(a) First, let us calculate the energy of the fluctuations. Plug the above form for $\mathbf{m}(\mathbf{x})$ into the Hamiltonian functional:

$$\mathcal{H}[\mathbf{m}(\mathbf{x})] = \int d^d\mathbf{x}\,\left[\frac{r}{2}m^2(\mathbf{x}) + um^4(\mathbf{x}) + \frac{c}{2}(\nabla\mathbf{m}(\mathbf{x}))^2\right]$$

Show that $\mathcal{H}$ can be written as:

$$\mathcal{H} = \mathcal{H}_0 + \frac{K}{2}\int d^d\mathbf{x}\,(\nabla\theta(\mathbf{x}))^2$$

where $\mathcal{H}_0 = V(\frac{r}{2}m^2 + um^4)$ is just the mean-field energy, and $K = cm^2$.

<u>Answer:</u> Let us plug $\mathbf{m}(\mathbf{x}) = m\cos\theta(\mathbf{x})\,\hat{\mathbf{e}}_1 + m\sin\theta(\mathbf{x})\,\hat{\mathbf{e}}_2$ into each term in the Hamiltonian:

$$\begin{aligned}
m^2(\mathbf{x}) &= \mathbf{m}(\mathbf{x})\cdot\mathbf{m}(\mathbf{x}) = m^2\cos^2\theta(\mathbf{x}) + m^2\sin^2\theta(\mathbf{x}) = m^2 \\
m^4(\mathbf{x}) &= (\mathbf{m}(\mathbf{x})\cdot\mathbf{m}(\mathbf{x}))^2 = m^4 \\
(\nabla\mathbf{m}(\mathbf{x}))^2 &= \sum_{i=1}^{2}\sum_{\alpha=1}^{d}\partial_\alpha m_i(\mathbf{x})\partial_\alpha m_i(\mathbf{x}) \\
&= m^2\sin^2\theta(\mathbf{x})\sum_\alpha(\partial_\alpha\theta(\mathbf{x}))^2 + m^2\cos^2\theta(\mathbf{x})\sum_\alpha(\partial_\alpha\theta(\mathbf{x}))^2 \\
&= m^2\sum_\alpha(\partial_\alpha\theta(\mathbf{x}))^2 \\
&= m^2(\nabla\theta(\mathbf{x}))^2
\end{aligned}$$

Putting everything together, we find:

$$\mathcal{H} = \int d^d\mathbf{x}\left[\frac{r}{2}m^2 + um^4 + \frac{cm^2}{2}(\nabla\theta(\mathbf{x}))^2\right]$$

$$
\begin{aligned}
&= V\left(\frac{r}{2}m^2 + um^4\right) + \int d^d\mathbf{x}\frac{cm^2}{2}(\nabla\theta(\mathbf{x}))^2 \\
&= \mathcal{H}_0 + \int d^d\mathbf{x}\frac{K}{2}(\nabla\theta(\mathbf{x}))^2
\end{aligned}
$$

(b) Now imagine the system is a box of volume $V = L^d$, and write $\theta(\mathbf{x})$ as a Fourier expansion:

$$
\theta(\mathbf{x}) = \frac{1}{V}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}\theta(\mathbf{q}), \qquad \theta(\mathbf{q}) = \int d^d\mathbf{x}\, e^{-i\mathbf{q}\cdot\mathbf{x}}\theta(\mathbf{x})
$$

where $\mathbf{q} = \frac{2\pi}{L}(n_1\hat{\mathbf{e}}_1 + n_2\hat{\mathbf{e}}_2 + \ldots n_d\hat{\mathbf{e}}_d)$ and the n_i are integers. The functions $e^{i\mathbf{q}\cdot\mathbf{x}}$ satisfy the orthogonality condition:

$$
\int d^d\mathbf{x}\, e^{i(\mathbf{q}-\mathbf{q}')\cdot\mathbf{x}} = V\delta_{\mathbf{q},\mathbf{q}'}
$$

Show that the Hamiltonian can be written as:

$$
\mathcal{H} = \mathcal{H}_0 + \frac{K}{2V}\sum_{\mathbf{q}} q^2\theta(\mathbf{q})\theta(-\mathbf{q})
$$

<u>**Answer:**</u>

$$
\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + \int d^d\mathbf{x}\frac{K}{2}(\nabla\theta(\mathbf{x}))^2 \\
&= \mathcal{H}_0 - \frac{K}{2V^2}\int d^d\mathbf{x}\sum_{\mathbf{q},\mathbf{q}'}\mathbf{q}\cdot\mathbf{q}' e^{i(\mathbf{q}+\mathbf{q}')\cdot\mathbf{x}}\theta(\mathbf{q})\theta(\mathbf{q}') \\
&= \mathcal{H}_0 - \frac{K}{2V^2}\sum_{\mathbf{q},\mathbf{q}'} V\delta_{\mathbf{q},-\mathbf{q}'}\mathbf{q}\cdot\mathbf{q}'\theta(\mathbf{q})\theta(\mathbf{q}') \\
&= \mathcal{H}_0 + \frac{K}{2V}\sum_{\mathbf{q}} q^2\theta(\mathbf{q})\theta(-\mathbf{q})
\end{aligned}
$$

(c) Use the fact that $\theta(\mathbf{x})$ is real to show that $\theta(-\mathbf{q}) = \theta^*(\mathbf{q})$. This means that $\theta(\mathbf{q})\theta(-\mathbf{q}) = \theta_R^2(\mathbf{q}) + \theta_I^2(\mathbf{q})$, where $\theta_R(\mathbf{q})$ and $\theta_I(\mathbf{q})$ are the real and imaginary parts of $\theta(\mathbf{q})$. Show that the Hamiltonian can be written as:

$$
\mathcal{H} = \mathcal{H}_0 + \frac{K}{V}\sum_{\mathbf{q}>0} q^2\left[\theta_R^2(\mathbf{q}) + \theta_I^2(\mathbf{q})\right]
$$

Here the sum over $\mathbf{q} > 0$ is shorthand notation that means we are summing over only half of the possible values of $\mathbf{q}$. (For example, we restrict one of the integers n_i to be positive.)

<u>**Answer:**</u>

$$
\theta^*(\mathbf{q}) = \int d^d\mathbf{x}\, e^{i\mathbf{q}\cdot\mathbf{x}}\theta(\mathbf{x}) = \theta(-\mathbf{q})
$$

Using $\theta(\mathbf{q})\theta(-\mathbf{q}) = \theta_R^2(\mathbf{q}) + \theta_I^2(\mathbf{q})$ we can write the Hamiltonian as:

$$
\mathcal{H} = \mathcal{H}_0 + \frac{K}{2V}\sum_{\mathbf{q}} q^2\left[\theta_R^2(\mathbf{q}) + \theta_I^2(\mathbf{q})\right]
$$

Note that $\theta_R(-\mathbf{q}) = \theta_R(\mathbf{q})$ and $\theta_I(-\mathbf{q}) = -\theta_I(\mathbf{q})$, so in the sum both $\mathbf{q}$ and $-\mathbf{q}$ contribute the same value $q^2\left[\theta_R^2(\mathbf{q}) + \theta_I^2(\mathbf{q})\right]$. Thus we can restrict the sum to half of $\mathbf{q}$ space, and multiply it by a factor of 2:

$$\mathcal{H} = \mathcal{H}_0 + \frac{K}{V}\sum_{\mathbf{q}>0} q^2\left[\theta_R^2(\mathbf{q}) + \theta_I^2(\mathbf{q})\right]$$

(d) The partition function involves integrating over all possible functions $\mathbf{m}(\mathbf{x})$. In terms of the Fourier-transformed Hamiltonian, this means integrating over all possible values of the Fourier components $\theta_R(\mathbf{q})$ and $\theta_I(\mathbf{q})$:

$$Z = \int_{-\infty}^{\infty}\prod_{\mathbf{q}>0} d\theta_R(\mathbf{q})d\theta_I(\mathbf{q})\, e^{-\beta\mathcal{H}}$$

We are interested in calculating the average of $\mathbf{m}(\mathbf{x})$ along the $\hat{\mathbf{e}}_1$ direction, which we can write as follows:

$$\langle m_1(\mathbf{x})\rangle = m\langle\cos\theta(\mathbf{x})\rangle = m\,\Re\langle e^{i\theta(\mathbf{x})}\rangle$$

where $\Re z$ denotes the real part of a complex number z. Thus to find $\langle m_1(\mathbf{x})\rangle$ we have to find the average:

$$\langle e^{i\theta(\mathbf{x})}\rangle = \frac{1}{Z}\int_{-\infty}^{\infty}\prod_{\mathbf{q}>0} d\theta_R(\mathbf{q})d\theta_I(\mathbf{q})\, e^{i\theta(\mathbf{x})}e^{-\beta\mathcal{H}}$$

Replace $\theta(\mathbf{x})$ by its Fourier expansion: it turns out that the integral above can be rewritten as a product over ordinary Gaussian integrals, which can be solved using the basic rule we showed in class:

$$\int_{-\infty}^{\infty} d\phi\, e^{-\frac{K}{2}\phi^2 + h\phi} = \sqrt{\frac{2\pi}{K}}e^{h^2/2K}$$

where K and h can be complex, with $\Re K > 0$. Show that:

$$\langle m_1(\mathbf{x})\rangle = me^{-W} \qquad \text{where} \qquad W = \frac{1}{\beta KV}\sum_{\mathbf{q}>0}\frac{1}{q^2}$$

<u>**Answer:**</u>

$$\begin{aligned}
\langle e^{i\theta(\mathbf{x})}\rangle &= \frac{1}{Z}\int_{-\infty}^{\infty}\prod_{\mathbf{q}>0} d\theta_R(\mathbf{q})d\theta_I(\mathbf{q})\, e^{i\theta(\mathbf{x})}e^{-\beta\mathcal{H}} \\
&= \frac{1}{Z}\int_{-\infty}^{\infty}\prod_{\mathbf{q}>0} d\theta_R(\mathbf{q})d\theta_I(\mathbf{q})\, e^{\frac{i}{V}\sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{x}}\theta(\mathbf{q})}e^{-\beta\mathcal{H}_0 - \frac{\beta K}{V}\sum_{\mathbf{q}>0} q^2\left[\theta_R^2(\mathbf{q})+\theta_I^2(\mathbf{q})\right]} \\
&= \frac{1}{Z}\int_{-\infty}^{\infty}\prod_{\mathbf{q}>0} d\theta_R(\mathbf{q})d\theta_I(\mathbf{q})\, e^{\frac{i}{V}\sum_{\mathbf{q}>0}\left(e^{i\mathbf{q}\cdot\mathbf{x}}\theta(\mathbf{q}) + e^{-i\mathbf{q}\cdot\mathbf{x}}\theta(-\mathbf{q})\right)}e^{-\beta\mathcal{H}_0 - \frac{\beta K}{V}\sum_{\mathbf{q}>0} q^2\left[\theta_R^2(\mathbf{q})+\theta_I^2(\mathbf{q})\right]} \\
&= \frac{e^{-\beta\mathcal{H}_0}}{Z}\prod_{\mathbf{q}>0}\int_{-\infty}^{\infty} d\theta_R(\mathbf{q})d\theta_I(\mathbf{q})\, e^{-\frac{\beta K}{V}q^2\left[\theta_R^2(\mathbf{q})+\theta_I^2(\mathbf{q})\right] + \frac{i}{V}\left(e^{i\mathbf{q}\cdot\mathbf{x}}\theta(\mathbf{q}) + e^{-i\mathbf{q}\cdot\mathbf{x}}\theta(-\mathbf{q})\right)} \\
&= \frac{e^{-\beta\mathcal{H}_0}}{Z}\prod_{\mathbf{q}>0}\int_{-\infty}^{\infty} d\theta_R(\mathbf{q})d\theta_I(\mathbf{q})\, e^{-\frac{\beta K}{V}q^2\left[\theta_R^2(\mathbf{q})+\theta_I^2(\mathbf{q})\right] + \frac{2i}{V}\left(\cos(\mathbf{q}\cdot\mathbf{x})\theta_R(\mathbf{q}) - \sin(\mathbf{q}\cdot\mathbf{x})\theta_I(\mathbf{q})\right)}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{e^{-\beta\mathcal{H}_0}}{Z} \prod_{\mathbf{q}>0} \sqrt{\frac{\pi V}{\beta K q^2}} e^{-\frac{\cos^2(\mathbf{q}\cdot\mathbf{x})}{V\beta K q^2}} \sqrt{\frac{\pi V}{\beta K q^2}} e^{-\frac{\sin^2(\mathbf{q}\cdot\mathbf{x})}{V\beta K q^2}} \\
&= \prod_{\mathbf{q}>0} e^{-1/(V\beta K q^2)} \\
&= e^{-\frac{1}{\beta K V}\sum_{\mathbf{q}>0}\frac{1}{q^2}} \equiv e^{-W}
\end{aligned}
$$

Clearly W is real. Thus:

$$\langle m_1(\mathbf{x})\rangle = m\,\Re\langle e^{i\theta(\mathbf{x})}\rangle = me^{-W}$$

(e) Mean-field theory tells us that the constant m will be nonzero below T_c. If $W < \infty$, then the result of part (d) shows us that we still have an ordered phase at low temperatures, though with an average magnetization $\langle m_1(\mathbf{x})\rangle = me^{-W}$ that is smaller than the mean-field solution because of the effects of fluctuations. However, if $W = \infty$, we get the interesting result that $\langle m_1(\mathbf{x})\rangle = 0$: the ordered phase has been destroyed by the fluctuations! Calculate W, and show that there is an ordered phase for dimensions $d > 2$. For $d \leq 2$ show that there is no order except at $T = 0$.

Hint: So how do we calculate the value of W? In the limit of large volume we can replace the sum over $\mathbf{q}$ by an integral:

$$W = \frac{1}{\beta K V}\sum_{\mathbf{q}>0}\frac{1}{q^2} \to \frac{1}{2\beta K}\int \frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{q^2}$$

where we add the factor of 1/2 because we make the integral go over all of $\mathbf{q}$-space, not just one-half. We have to be careful here: when we expanded $\theta(\mathbf{x})$ in terms of Fourier components, we did not specify any restrictions on $\mathbf{q}$. However it is unphysical to include fluctuations with such large $|\mathbf{q}|$ that the wavelengths $\lambda = 2\pi/|\mathbf{q}|$ are smaller than the microscopic lattice spacing of our system ℓ. Thus our integral should not really be over *all* $\mathbf{q}$-space, but rather within some cutoff $|\mathbf{q}| < \Lambda$, where $\Lambda \propto 1/\ell$. We are integrating inside a d-dimensional sphere of radius Λ, where Λ is large but not infinite. With this restriction in place, we can now calculate the integral. For $d > 1$ the infinitesimal d-dimensional volume $d^d\mathbf{q}$ can be written in radial coordinates as $d^d\mathbf{q} = q^{d-1}dq\,d\Omega_d$, where $d\Omega_d$ is a d-dimensional solid angle. The angular integration can be done using the fact that:

$$\int d\Omega_d = S_d \qquad \text{where} \qquad S_d = \frac{2\pi^{d/2}}{(d/2-1)!}$$

Here S_d is the area of a d-dimensional unit sphere.

<u>**Answer:**</u> Writing W as an integral:

$$
\begin{aligned}
W &= \frac{1}{2\beta K}\int \frac{d^d\mathbf{q}}{(2\pi)^d}\frac{1}{q^2} \\
&= \frac{k_B T S_d}{2K(2\pi)^d}\int_0^\Lambda dq\,\frac{q^{d-1}}{q^2} \\
&= \frac{k_B T S_d}{2K(2\pi)^d}\int_0^\Lambda dq\,q^{d-3}
\end{aligned}
$$

For $d \leq 2$ this integral blows up, so $W = \infty$ and there is no ordered phase for $T \neq 0$. When $d > 2$ the integral is convergent, and the expression for W becomes:

$$W = \frac{k_B T S_d \Lambda^{d-2}}{2K(2\pi)^d(d-2)}$$

Thus there is an ordered phase at low temperatures, with the magnetization suppressed by a factor of e^{-W} due to fluctuations.