P653 HW9

Due Nov 10, 2005

Problem 1. Susceptability of O(n) model

Consider a system of spins which sit in d-dimensional space and which can point in n dimensions, with Landau Free energy

$$F = \int d^d r (c/2)(\nabla_\mu S_i(r))(\nabla_\mu S_i(r)) + (a/2)S_i(r)S_i(r) + (b/4)(S_i(r)S_i(r))(S_j(r)S_j(r)) - h_i(r)S_i(r),$$

where Einstein summation is assumed with μ running from 1 to d and i, j running from 1 to n. We will flip between using integers and letters to denote the directions. For example if I say $\mathbf{h} = h\hat{x}$, that is equivalent to saying $h_j = \delta_{j1}h$.

In class we considered the case where $h = 0$, here we will consider $h \neq 0$.

1.1. First consider the case where $\mathbf{h}(r) = h_1\hat{x}$ is uniform and points in the $\hat{x}$ direction [ie $h_i = h\delta_{j1}$]. Minimize F, and show that $\mathbf{S} = S\hat{x}$, and S satisfied the cubic equation

$$aS + bS^3 - h = 0.$$

Solution 1.1. This equation is merely $\delta F/\delta S_1 = 0$. The derivatives with respect to other components $\delta F/\delta S_j$ give similar expressions but without h. The only way that all of these equations can be simultaneously satisfied is if $S_j = 0$ for all $j \neq 1$.

1.2. Fix $b > 0$, and find the boundary in the $h - a$ plane between where this equation has one and three solutions. For $h \neq 0$ this defines the spinodal.

Solution 1.2. At the spinodal, two of the extrema coincide. This means that $\partial^2 F/\partial S^2 = 0$, which yields

$$a + 3bS^2 = 0.$$

Eliminating S gives

$$-a = \frac{9}{4}bh^2.$$

1.3. Let $\mathbf{h} = h\hat{x} + \delta h_\| e^{ik\cdot r}\hat{x}$, and let $\mathbf{S} = S\hat{x} + \delta S e^{i\cdot r}\hat{x}$ minimize the free energy. Calculate δS to linear order in $\delta h_\|$. Your expression may contain S.

The longitudinal susceptability is defined as

$$\chi_\| = \frac{\delta S}{\delta h_\|}$$

Verify that when $h \to 0$ you recover the expression from class

$$\chi_{\|}\Big|_{h=0} = \frac{1}{ck^2 + 2|a|}.$$

Solution 1.3. To linear order one has

$$ck^2 \delta S + a\delta S + 3bS^2 \delta S - \delta h_{\|} = 0,$$

which yields

$$\delta S = \frac{\delta h_{\|}}{a + 3bS^2 + ck^2}.$$

When $h = 0$ this simplifies because $S^2 = -a/b$, yielding the result from class

$$\chi_{\|}\Big|_{h=0} = \frac{1}{ck^2 + 2|a|}.$$

1.4. What happens to the longitudinal susceptability in the metastable state at the spinodal? [ie. at the spinodal, one of the minima disapears. Evaluate the susceptability of that metastable state.]

Solution 1.4. At the spinodal, the metastable state satisfies

$$a + 3bS^2 = 0,$$

which tells us that

$$\chi_{\|} = \frac{1}{ck^2},$$

diverges as $k \to 0$.

1.5. Show that even in the presence of nonzero $\delta h_{\|}$ that $S_j = 0$ for all $j \neq 1$, and hence that

$$\chi_{yx} = \frac{\delta S_y}{\delta h_x} = 0,$$

where $h_x = h_{\|}$.

1.6. Now lets consider a transverse perturbation. Let $\mathbf{h} = h\hat{x} + \delta h_{\perp} e^{ik\cdot r}\hat{y}$, and let $\mathbf{S} = S\hat{x} + \delta S_y e^{i\cdot r}\hat{y}$ minimize the free energy. To linear order in $\delta h_{\perp}$, calculate δS_y. Show that as $h \to 0$ one recovers the result from class that

$$\chi_{\perp}|_{h=0} = \frac{1}{ck^2},$$

Solution 1.5. Linearizing the equation for the $\hat{y}$ component of $\mathbf{S}$ yields

$$ck^2 \delta S_y + a\delta S + bS^2 \delta S_y - \delta h_{\perp} = 0,$$

which gives

$$\delta S_y = \frac{\delta h_{\perp}}{h + ck^2},$$

where we have used the equation satisfied by the equilibrium S.

Problem 2. Continuum limit of x-y model Consider a microscopic x-y model on a square lattice in two dimensions,

$$H = -J \sum_{\langle i\langle j} \mathbf{S_i} \cdot \mathbf{S_j} = -JS^2 \sum_{\langle ij\rangle} \cos(\theta_i - \theta_j),$$

where S is the length of the spins, and θ defines their directions. We will derive a continuum version of this model, and evaluate the energy of some important quantities.

2.1. Suppose that θ_i varies slowly from one site to the next. Let $\theta(r)$ be a smooth function for which $\theta(r_i) = \theta_i$. Show that

$$H \approx \int d^2r \frac{-JS^2}{2} |\nabla\theta(r)|^2,$$

independent of the lattice spacing.

Solution 2.1. One approximates

$$\cos(\theta_i - \theta_j) \approx 1 - [\theta(r_i) - \theta(r_j)]^2/2 \approx 1 - \left[(\mathbf{r_i} - \mathbf{r_j}) \cdot nabla\theta(r_i)\right]^2/2.$$

Summing over nearest neighbors gives

$$\sum_{\text{neighbors}j} \cos(\theta_i - \theta_j) \approx 4 - a^2 \left|nabla\theta(r_i)\right|^2,$$

from which

$$\begin{aligned} H &\approx \text{const} + J\sum_i a^2 |\nabla\theta(r)|^2/2 \\ &\approx \text{const} + \int d^2r \frac{JS^2}{2} |\nabla\theta(r)|^2. \end{aligned}$$

Note the sign error in the posing of the question.

2.2. There can be spin configurations which are not smooth. An example is a vortex: $\theta(r) = \arctan(y/x) = \text{Im}\log(x + Iy)$. This configuration is smooth except for a region near $r = 0$. Let $\xi \sim a$ be a length for which $\theta(r)$ is smooth when $r > \xi$. If the size of the system is L, estimate the contribution to the energy of a vortex configuration from all spins at $r > \xi$. This is described as the region "outside the vortex core".

You should find that this energy diverges as $L \to \infty$.

Hint 1: The continuum approximation works in this region.

Hint 2: Take the sample to be circular in shape.

Solution 2.2.

$$E = 2\pi \int_\xi^L dr\, r \frac{JS^2}{2} \frac{1}{r^2} = \pi JS^2 \log(\xi/L)$$

2.3. Estimate the energy contributions from outside the vortex cores of a vortex-antivortex pair separated by a distance $d(\gg \xi)$: $\theta(r) = \mathrm{Im}\left[\log(x - d/2 + Iy) - \log(x + d/2 + Iy)\right]$.

Hint 1: Take the limit of an infinite system, this energy is finite in that limit.

Hint 2: Use Stoke's Theorem (ie integrate by parts):

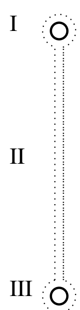
$$\int_\Omega d^2r|\nabla\theta|^2 = \int_{\partial\Omega} d\ell\cdot\theta\nabla\theta - \int_\Omega d^2r\theta\nabla^2\theta.$$

Note that $\nabla^2\theta = 0$. Look out for branch cuts.

Solution 2.3. Looks like a typo in the hint – sorry. The correct statement is

$$\int_\Omega d^2r|\nabla\theta|^2 = \int_{\partial\Omega} d\ell\hat{\mathbf{n}}\cdot\theta\nabla\theta - \int_\Omega d^2r\theta\nabla^2\theta,$$

where $\hat{n}$ is the outward normal. As stated in the hint, the second term on the right vanishes. In order to avoid branch-cuts we need to use a contour like the one shown below:



One can always choose the path so that $\nabla\theta$ is oriented purely aximuthal, there is no flow through the parts I and III of the contour, and one only gets a contribution from II. Along II, the flow is completely perpendicular to the contour so $\hat{n}\cdot\nabla\theta = |\nabla\theta| = 1/(d/2 - x) + 1/(d/2 + x)$. On the two sides of the contour θ differs by 2π, so

$$\begin{aligned} E &= \frac{JS^2}{2}2\pi\int_{-d/2+\xi}^{d/2-\xi} \frac{1}{d/2 - x} + \frac{1}{d/2 + x} \\ &= 2\pi JS^2 \log\left(\frac{d-\xi}{\xi}\right) \\ &\approx 2\pi JS^2 \log\left(\frac{d}{\xi}\right). \end{aligned}$$

Problem 3. Correlation functions in harmonic crystal

As a simple model of a crystal, consider a system of particles that want to for a square lattice in d dimensions, with lattice constant a. If we only consider the interaction between neighboring atoms one can approximate the Hamiltonian as

$$H = \sum_{\langle ij \rangle} V(\mathbf{r}_i - \mathbf{r}_j) + \sum_i \frac{\mathbf{p}_i^2}{2m},$$

where r_i is the position of the i'th particle and p_i is the momentum of that particle. We now assume that each particle stays near its equilibrium position, $r_i^{(0)}$, in which case $r_i = r_i^{(0)} + \delta_i$. Presumably V has a minimum at this point, so we can expand and get to an Einstein model,

$$H = \sum_{\langle ij \rangle} \frac{m\omega_0^2}{2}(\delta_i - \delta_j)^2 + \sum_i \frac{\mathbf{p}_i^2}{2m}.$$

3.1. Find the normal modes and their frequencies. What is the energy cost of exciting each of these modes with some given amplitude.

This is a system with a spontaneously broken continuous symmetry. How is Goldstone's theorem manifested in these modes?

Solution 3.1. Hamilton's equations give

$$\begin{aligned}\frac{\partial \delta_i}{\partial t} &= \frac{p_i}{m} \\ \frac{\partial p_i}{\partial t} &= -m\omega_0^2 \sum_j{}' (\delta_i - \delta_j),\end{aligned}$$

where the prime denotes only summing over neighbors of i. By symmetry, normal modes must be plane waves, so we substitute $\delta_i = Ae^{i(k\cdot r_i - \omega t)}$, which gives $p_i = -i\omega m A e^{i(k\cdot r_i - \omega t)}$, and

$$\begin{aligned}\omega^2 &= \omega_0^2 \sum_j{}' (1 - e^{ik\cdot(r_j - r_i)}) \\ &= 4\omega_0^2 \sum_{s=1}^{d} \sin^2(k_s a/2),\end{aligned}$$

where k_s is the s'th component of k. To get the energy of this excitation we need to plug this back into the Hamiltonian. Of course we need δ to be real, so we take $\delta = (\delta^+ + \delta^-)/\sqrt{2}$, with $\delta_i^\pm = Ae^{\pm i(k\cdot r_i - \omega t)}$, which gives

$$\begin{aligned}H &= H_0 + H_+ + H_- \\ H_0 &= A^2 \sum_i \left[\frac{m\omega_0^2}{4} \sum_j{}' (\delta_i^+ - \delta_j^+)(\delta_i^- - \delta_j^-) + \frac{m}{\omega^2} 2p_i^+ p_i^- \right] \\ H_+ &= A^2 \sum_i \left[\frac{m\omega_0^2}{8} (\delta_i^+ - \delta_j^+)^2 - \frac{m}{\omega^2} 4(p_i^+)^2 \right] \\ H_- &= H_+^*,\end{aligned}$$

where $H_\pm$ has time dependance $e^{2i\omega t}$. We know that the energy should be a constant of motion, so both of these terms must vanish. Although it is perfectly reasonable to assume this result, one can verify it by using the definition of ω to write

$$\begin{aligned}H_+ &= A^2 e^{2i\omega t} \frac{m\omega_0^2}{8} \sum_i \left[\sum_j{}' \left(e^{ik\cdot r_i} - e^{ik\cdot r_j}\right)^2 - 2\sum_j{}' \left(e^{ik\cdot r_i} - e^{ik\cdot r_j}\right) e^{ik\cdot r_i} \right] \\ &= A^2 e^{2i\omega t} \frac{m\omega_0^2}{8} \sum_i \left[\sum_j{}' \left(e^{ik\cdot r_i} - e^{ik\cdot r_j}\right)^2 - \sum_j{}' \left(e^{ik\cdot r_i} - e^{ik\cdot r_j}\right)^2 \right] = 0,\end{aligned}$$

where we used that i was a dummy variable to symmetrize the last term.
Similar manipulation of H_0 gives

$$H = NA^2 m\omega^2.$$

3.2. The equipartition theorem says that at finite temperature each degree of freedom should have an energy $kT/2$. Use the equipartition theorem and the normal modes to estimate $\langle |\delta_i|^2 \rangle$ as the system size becomes large.

What happens for $d = 1, 2$?

Hint 1: This result is independant of i, so you might as well take $r_i^0 = 0$.

Hint 2: Turn the sum into an integral. The integral is dominated by the modes of lowest energy. Approximate $\cos(x) \approx 1 - x^2/2$.

Solution 3.2. Associated with each k there are $2d$ independant modes – A has d components, each of which can be either cos or sin. Equipartition then says that

$$\langle A_k^2 \rangle = \frac{dk_BT}{Nm\omega_k^2},$$

and

$$\begin{aligned}
\langle |\delta_0|^2 &= \sum_k \frac{dk_BT}{Nm\omega_k^2} \\
&= \frac{dk_BT}{4Nm\omega_0^2} \frac{V}{(2\pi)^d} \int d^dk \, \frac{1}{\sum_{s=1}^d \sin^2(k_s a/2} \\
&\approx \frac{dk_BTa^d}{4m\omega_0^2} \frac{S_d}{(2\pi)^d} \int_{\pi/L}^{\pi/a} dk k^d \frac{1}{k^2a^2},
\end{aligned}$$

where we have used that $V/N = a^d$, and introduced S_d, the surface area of a unit sphere in d-dimensions. The resulting integral has an infrared cutoff at $k = \pi/L$ and an ultraviolet cutoff at $k \sim \pi/a$. For $d > 2$ one can ignore the ultraviolet cutoff. For $d = 2$,

$$\langle |\delta_0|^2 \propto \log(L/a)$$

and for $d = 1$

$$\langle |\delta_0|^2 \propto L.$$

In each case, the fluctuations diverge.

3.3. Use the same method to write down an integral for $g_{ij} = \langle \delta_i \delta_j \rangle$ as a function of the distance $r_i^{(0)} - r_j^{(0)}$. How does this integral behave in the infinite system as $r_i^{(0)} - r_j^{(0)} \to \infty$.

How is this related to the Mermin-Wagner theorem?

Solution 3.3. Here we have

$$\begin{aligned}
\langle|\delta_i\delta_j|^2 &= \sum_k \frac{dk_BT}{Nm\omega_k^2}\left[\cos(k\cdot r_i)\cos(k\cdot r_j)+\sin(k\cdot r_i)\sin(k\cdot r_j)\right] \\
&= \sum_k \frac{dk_BT}{Nm\omega_k^2} e^{ik\cdot(r_i-r_j)} \\
&\approx \frac{dk_BTa^d}{4m\omega_0^2}\frac{1}{(2\pi)^d}\int_{\pi/L}^{\pi/a} d^dk\,\frac{e^{ik\cdot(r_i-r_j)}}{k^2a^2},
\end{aligned}$$

We have done this integral before – its the Greens function for the Laplacian in d-dimensions. One carries out the asymptotics by scaling k, so that

$$I = \int_{\pi/L}^{\pi/a} d^dk\,\frac{e^{ik\cdot x}}{k^2}$$

$$= \quad |x|^{d-2}\int_{\pi|x|/L}^{\pi|x|/a} d^dk\,\frac{e^{ik_z}}{k^2},$$

where we have taken the $\hat{z}$ axis to be aligned with $\mathbf{x}$. For $d>2$ the integrand is well-behaved for small k and one can take the limit $L\to\infty$. There is no divergence at large k [due to the exponential] so one finds $I\propto|x|^{d-2}$.

For $d=2$, the infrared part of the integral contributes a $\log(L/|x|)$, and $I\propto\log(L/x)$. For $d=1$, the infrared part of the integral contributes L/x, and one finds $I\propto L$. In both cases the fluctuations diverge as one takes the locations to be far apart.

These divergent fluctuations means that there is no long-range crystaline order [a result given by the Mermin-Wagner theorem].