8.334: Statistical Mechanics II Problem Set # 7

XY model. Topological phase transition.

1. Topological quantities.

Consider continuous 2-component unit vector functions $\mathbf{n}(x)$ *on a circle* $0 < x \leq 2\pi$. *For any such function one can count the number of rotations of* $\mathbf{n}$ *upon a cyclic change of* x *from* 0 *to* 2π. *We would like to show that this integer number is a topological characteristic of the function, i.e. it does not change when the function is deformed in a continuous way.*

This problem can be analyzed using a complex number representation of 2-component unit vectors, $z(x) = n_1(x) + in_2(x)$, *and interpreting the functions as mappings from the unit circle parameterized by* x *to the unit circle* $|z| = 1$ *in the complex* z *plane.*

a) Define topological charge as

$$q = \frac{1}{2\pi i} \oint \frac{z'}{z}\, dx\,, \quad z' \equiv dz/dx. \tag{1}$$

Mathematically, this quantity is known as the degree of a mapping. Show that q *is an integer number. (Hint: In terms of the phase,* $z = e^{i\theta}$, *what is the meaning of the quantity* z'/z*?)*

For unit vector field $n(x) = (n_1, n_2)$ with $n_1 = \cos\theta$ and $n_2 = \sin\theta$, the quantity

$$q = \frac{1}{2\pi i} \oint \frac{z'}{z}\, dx = \frac{1}{2\pi} \int d(\arg z) = \frac{1}{2\pi} \int d\theta = \frac{1}{2\pi}(\theta(x = 2\pi) - \theta(x = 0)) \tag{2}$$

with $z = e^{i\theta}$ is an integer since $n(x)$ is continuous.

b) For any integer n *construct a function* $z(x)$ *with topological charge* $q = n$.

Consider $n(x) = (\cos(nx), \sin(nx))$. In this case $z(x) = e^{inx}$ and

$$q = \frac{1}{2\pi i} \int \frac{dz}{z} = \frac{2\pi n}{2\pi} = n \tag{3}$$

c) Show that q *does not change when the function* $z(x)$ *is replaced by* $z'(x)$ *such that* z' *is related to* z *by a small deformation:* $|z(x) - z'(x)| < \epsilon$, *where* ϵ *is a small positive number (e.g.* 10^{-2}*).*

Consider

$$q_z - q_{z'} = \int \frac{dz}{z} - \int \frac{dz'}{z'} = \int d\ln(z/z') = \ln(z/z')\Big|_0^{2\pi} \tag{4}$$

since $|z - z'| < \epsilon$, the RHS is also $O(\epsilon)$. On the other hand, it must be an integer. Therefore is must be zero.

2. Correlation function in the XY model.

Consider the XY model on a 2D square lattice:

$$\mathcal{H} = -J \sum_{|\mathbf{x}-\mathbf{x}'|=1} \mathbf{n}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}') = -J \sum_{|\mathbf{x}-\mathbf{x}'|=1} \cos(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'}) \tag{5}$$

where the angles $\theta_{\mathbf{x}}$ *are defined as in Problem 1,* $n_1 + in_2 = e^{i\theta}$, *or* $n_1 = \cos\theta$, $n_2 = \sin\theta$. *We are interested in the asymptotic behavior of the pair correlation function*

$$C_2(\mathbf{x} - \mathbf{y}) = \langle \mathbf{n}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{y}) \rangle \tag{6}$$

at large distances $|\mathbf{x}-\mathbf{y}|$.

a) At high temperature $T \gg J$*, the correlation between different phases is weak, and one can evaluate* $C_2(\mathbf{x}-\mathbf{y})$ *as*

$$\langle e^{i(\theta_{\mathbf{x}}-\theta_{\mathbf{y}})}\rangle = \langle e^{i(\theta_{\mathbf{x}}-\theta_{\mathbf{x}'})}e^{i(\theta_{\mathbf{x}'}-\theta_{\mathbf{x}''})}...e^{i(\theta_{\mathbf{x}^{(n)}}-\theta_{\mathbf{y}})}\rangle \approx \langle e^{i(\theta_{\mathbf{x}}-\theta_{\mathbf{x}'})}\rangle\langle e^{i(\theta_{\mathbf{x}'}-\theta_{\mathbf{x}''})}\rangle...\langle e^{i(\theta_{\mathbf{x}^{(n)}}-\theta_{\mathbf{y}})}\rangle \tag{7}$$

where the points $\mathbf{x}'$*,* $\mathbf{x}''$*, ...,* $\mathbf{x}^{(n)}$ *are taken on the shortest path connecting* $\mathbf{x}$ *and* $\mathbf{y}$*. Show that the correlation function, evaluated using (7), does not depend on the path between* $\mathbf{x}$ *and* $\mathbf{y}$*, and falls off exponentially with distance.*

At high temperature, $T \gg J$, the fluctuations of phases on different links are practically independent. For one link we estimate $\langle e^{i(\theta(x)-\theta(x'))}\rangle$ as

$$\frac{1}{Z}\int e^{i(\theta(x)-\theta(x'))}e^{K\cos(\theta(x)-\theta(x'))}\,d\theta = \frac{\int e^{i\theta+K\cos\theta}\,d\theta}{\int e^{K\cos\theta}\,d\theta} = \frac{J_1(K)}{J_0(K)} = \frac{1}{2}K + O(K^2) \tag{8}$$

with $K = \beta J$. For pair correlator $\langle e^{i(\theta(x)-\theta(x'))}\rangle$ at the points connected by a path of length n, the result is

$$\langle e^{i(\theta(x)-\theta(y))}\rangle = C_n\left(\frac{1}{2}K\right)^n \tag{9}$$

where C_n is the number of shortest paths connecting x and y. Since $C_n < 2^n$, obtain

$$\langle e^{i(\theta(x)-\theta(y))}\rangle = e^{-n\ln(T/J)} \tag{10}$$

b) At low temperature $T \ll J$*, the correlations are strong and the phase difference between neighboring sites is typically very small. This allows to expand cosine in the hamiltonian (5) and rewrite it as*

$$\mathcal{H}_{sw} = \sum_{|\mathbf{x}-\mathbf{x}'|=1}\frac{1}{2}J\left(\theta_{\mathbf{x}}-\theta_{\mathbf{x}'}\right)^2 \tag{11}$$

(we dropped constant term as well as the terms higher order in $\theta_{\mathbf{x}}-\theta_{\mathbf{x}'}$*). Expanding the XY hamiltonian in small phase difference is called a spin wave approximation. To evaluate the correlation function (6), one can perform a gaussian averaging with the distribution* $e^{-\beta\mathcal{H}_{sw}}$*.*

Find the asymptotic behavior of the correlation function at large distances. (Hint: How does the hamiltonian (6) look in Fourier representation?)

$$C_2(x-y) = \langle e^{i\theta_x}e^{-i\theta_y}\rangle = \exp\left(-\frac{1}{2}\langle(\theta_x-\theta_y)^2\rangle\right) = \exp\left(-\frac{1}{2}\left(2\langle\theta_x^2\rangle - 2\langle\theta_x\theta_y\rangle\right)\right) = \\ = \exp\left(-\left(G(0)-G(x-y)\right)\right) \tag{12}$$

where

$$G(x) = \sum_{-\pi<q_{1,2}<\pi}\frac{e^{iqx}}{K\left(2-\cos q_1-\cos q_2\right)} \tag{13}$$

at $|x| \gg 1$, obtain

$$G(x) = \int\frac{e^{iqx}}{Kq^2}\frac{d^2q}{(2\pi)^2} = \frac{1}{2\pi K}\ln\frac{L}{|x|} \tag{14}$$

where L is the system size. Since

$$G(0) - G(x) = \frac{1}{2\pi K} \ln \frac{|x|}{a},$$

the correlation function is

$$C_2(x-y) = \left(\frac{a}{|x-y|} \right)^{\alpha}, \qquad \alpha = \frac{1}{2\pi K} \tag{15}$$

c) To characterize the high and low temperature phases, define topological charge of a finite domain $\mathcal{D}$ as a sum of topological charges of the plaquettes p within the domain:

$$Q(\mathcal{D}) = \sum_{p_j \in \mathcal{D}} q(p_j)\,, \quad q(p_j) = \frac{1}{2\pi} \sum_{n=1,\ldots,4} \arg w^j_{n,n+1}\,, \quad w^j_{n,n+1} = e^{i(\theta_{\mathbf{x}^j_n} - \theta_{\mathbf{x}^j_{n+1}})} \tag{16}$$

with the sum over n taken over four square plaquette corner sites x^j_1, x^j_2, x^j_3, x^j_4, and the argument function taking values $-\pi < \arg w \le \pi$.

In the high temperature phase the fluctuations are strong, and typical values of $Q(\mathcal{D})$ with domain size. Show that $\langle Q(\mathcal{D}) \rangle = 0$ and estimate $\langle Q^2(\mathcal{D}) \rangle$ for a large domain of area A. Compare to the low temperature phase.

(i) In the high temperature phase, when vortices are unbound, there is total $O(\sqrt{A})$ of topological charge in a region of area A. The churges have random signs, therefore $\langle q \rangle = 0$, $\langle q^2 \rangle \propto A$.

(ii) In the low temperature phase, with vortices bound in pairs, the total topological charge of a region is $q \propto O(\sqrt{L})$, where L is the perimeter. It arises due to vortex pairs near the boundary, one of the vortices being inside the region and one outside. Thus $\langle q \rangle = 0$ and $\langle q^2 \rangle \propto L$

3. Vortex confinement.

Consider the XY model (5) perturbed by a term $\lambda \sin^2 \theta$, which introduces a weak anisotropy with respect to spin rotation. It is interesting to find out how the anisotropy changes the phase diagram. Let us study the ground states, vortices, and vortex-vortex interaction. At low temperature, the problem can be treated in the spin wave approximation:

$$\mathcal{H}_{sw} = \sum_{|\mathbf{x}-\mathbf{x}'|=1} \frac{1}{2} J \left(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'} \right)^2 + \sum_{\mathbf{x}} \lambda \sin^2 \theta_{\mathbf{x}} \tag{17}$$

The perturbation removes the degeneracy due to rotational symmetry: at $T = 0$ there are 2 ground states, $\theta = 0, \pi$.

a) Consider a spin distribution uniform within two domains: $\theta(x,y) \to 0$ at large negative x, and $\theta(x,y) \to \pi$ at large positive x. To find $\theta(\mathbf{x})$ at the domain interface, make a gradient expansion of the first term in (17) and, assuming that θ is a function of x only, look for a variational solution of the energy functional

$$\mathcal{H} = \int \frac{1}{2} J (d\theta/dx)^2 + \lambda \sin^2 \theta_x \tag{18}$$

with asymptotic values 0 and π at $x = \pm\infty$. Show that the width of the domain wall is of the order of $(J/\lambda)^{1/2}$ (which justifies using gradient expansion at small λ). Find the surface tension of the wall, i.e. the energy per unit length.

Look for a varational solution of

$$H = \int \left(\frac{K}{2} (\partial_x \theta)^2 + \lambda \sin^2 \theta \right) dx \tag{19}$$

with asymptotic values of *theta* equal to $0, \pi$ at $x = \pm\infty$.

$$\delta H = \int \left(-K \partial_x^2 \theta \delta\theta + 2\lambda \sin\theta \cos\theta \delta\theta \right) dx = 0 \tag{20}$$

Thus obtain equation

$$K\theta'' = \lambda \sin 2\theta. \tag{21}$$

To solve it, multiply both sides by θ':

$$K\theta''\theta' - \lambda \sin 2\theta\theta' = \left(\frac{K}{2} (\theta')^2 - \lambda \sin^2 \theta \right)' = 0 \tag{22}$$

which gives

$$\frac{K}{2} (\theta')^2 = \lambda \sin^2 \theta + C. \tag{23}$$

Using asymptotic values of θ, conclude that $C = 0$. Then $\theta' = \sqrt{2\lambda/K} \sin\theta$ and the solution is

$$\int \frac{d\theta}{\sin\theta} = (x - x_0)/w, \qquad w = (2\lambda/K)^{-1/2}. \tag{24}$$

Define $u = \cos\theta$. Then

$$\frac{x - x_0}{w} = -\int \frac{du}{1 - u^2} = -\frac{1}{2} \int \left(\frac{1}{1-u} + \frac{1}{1+u} \right) du = -\frac{1}{2} \ln \frac{1+u}{1-u}. \tag{25}$$

Therefore

$$\frac{1+u}{1-u} = e^{2(x-x_0)/w} \tag{26}$$

and

$$u = \tanh \frac{x - x_0}{w}. \tag{27}$$

Finally,

$$\theta(x) = \arccos \left(\tanh \frac{x - x_0}{w} \right). \tag{28}$$

Domain wall energy per unit length is

$$E_0 = \int_{-\infty}^{+\infty} \left((\frac{K}{2} (\theta')^2 + \lambda \sin^2 \theta \right) dx = \int 2\lambda \sin^2 \theta \, dx = 2\lambda \int \left(1 - \tanh^2 \frac{x - x_0}{w} \right) dx = \tag{29}$$

$$= 2\lambda \int \frac{dx}{\cosh^2((x - x_0)/w)} = 2\lambda w \tanh \frac{x - x_0}{w} \Big|_{-\infty}^{+\infty} = 4\lambda w = 2(2\lambda K)^{1/2}$$

b) Show that the spin distribution far away from a vortex with $q = \frac{1}{2\pi} \oint \nabla\theta dl = 1$ *can be described by 2 sectors, each being a domain with constant* $\theta = 0, \pi$. *The sector regions are separated by the*

domain walls similar to the one described in part a). The distortion field $\nabla\theta$ is nearly zero in the domains and is mainly concentrated in the walls. Estimate vortex energy in a system of size L.

c) Consider a vortex and an anti-vortex a large distance L apart. Describe spin distribution in the plane. How does the energy of their interaction vary asymptotically at large L?

Far away from a 2π vortex, around it, there will be two domains with $\theta = 0, \pi$. The domain wall has structure discussed in part a). In a vortex pair, these domain walls will connect the vortex and antivortex , as a pair of strings . The interaction potential of a pair is linear in vortex separation :

$$V(r) = 2E_0 r = 4(2\lambda K)^{1/2} r \tag{30}$$

d) Consider the system (17) at finite temperature. Using the above results for vortex interaction, discuss the possibility of a topological transition due to vortex pairs unbinding and vortices proliferation.