Problem set 6 for "Topology in condensed matter"

To be discussed in exercise class on February 13, 2024

1 Berezinskii-Kosterlitz-Thouless transition

In this problem we will analyze the behavior of the *classical* XY model. Consider two-dimensional square lattice, with each site $i \in \mathbb{Z}^2$ hosting a two-dimensional classical spin described by a unit vector $\mathbf{S}_i \in S^1$ parametrized by an angle $\varphi \in [0, 2\pi)$ as $\mathbf{S}_i = (\cos \varphi_i, \sin \varphi_j)$. Spins interact with the usual ferromagnetic interaction as follows:

$$H[\mathbf{S}] = -\sum_{\langle ij\rangle} J_{ij} \mathbf{S}_i \mathbf{S}_j = -\sum_{\langle ij\rangle} J_{ij} \cos(\varphi_i - \varphi_j), \quad J_{ij} = J$$
(1)

where the summation is performed over all links of the lattice. The system is in thermodynamic equilibrium described by the temperature T, thus its state is random and is described by the classical Boltzmann distribution $P[\mathbf{S}] = \exp(-\beta H[\mathbf{S}])/Z$, with $\beta = 1/T$ and Z being the partition function. We will analyze the behavior of the spin correlation function

$$\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_n \rangle = \left(\prod_k \int_0^{2\pi} \frac{d\varphi_k}{2\pi}\right) \cos(\varphi_m - \varphi_n) P[\boldsymbol{S}]$$
(2)

and argue that in this model there is a special phase transition, which is not associated with the appearance of the order parameter $\langle S_i \rangle$ (as happens in conventional second order phase transitions with spontaneous symmetry breaking), but instead manifests itself in the behavior of such correlation functions.

1.1 High-temperature expansion

1. We will start with the high-temperature expansion $\beta J \ll 1$, within which the Boltzmann weight can be expanded as

$$P[\mathbf{S}] = \frac{1}{Z} \prod_{\langle ij \rangle} \exp\left(\beta J \cos(\varphi_i - \varphi_j)\right) \approx \frac{1}{Z} \prod_{\langle ij \rangle} \left(1 + \beta J \cos(\varphi_i - \varphi_j)\right)$$
(3)

Show that further expansion of the product can be respresented as an expansion over all possible subgraphs \mathcal{G} of the original lattice, with each graph having the statistical weight $(\beta J)^{|E(\mathcal{G})|}$ (with $E(\mathcal{G})$ being set of links belonging to graph \mathcal{G} and $|E(\mathcal{G})|$ being number of such links):

$$P[\mathbf{S}] \approx \frac{1}{Z} \sum_{\mathcal{G}} \left((\beta J)^{|E(\mathcal{G})|} \prod_{\langle ij \rangle \in E(\mathcal{G})} \cos(\varphi_i - \varphi_j) \right)$$
(4)

Thus for small $\beta J \ll 1$, we are interested in graphs with the minimal number of links.

2. For the purposes of calculation of the spin correlation function, it will be sufficient to consider only trivial graph with no edges at all for the partition function and approximate $Z \approx 1$. Prove that only graphs that have non-zero contribution to the spin correlation function (2) should have following property: number of neighbors of each site (except nodes m and n) is even, whereas number of neighbors of sites m and n should be odd.

Hint: consider integral over arbitrary φ_i and argue how it changes upon shift $\varphi_i \mapsto \varphi_i + \pi$.

3. Therefore the minimal graph that gives non-zero contribution to the correlation function has a form of a single path connecting sites m and n. Consider the simplest case with site m having lattice coordinates $\mathbf{R}_n = (na, 0)$

and site n having coordinates $\mathbf{R}_m = (ma, 0)$ with $n, m \in \mathbb{Z}$, and a being lattice spacing. Calculate the integral corresponding to such minimal path and show that it gives the result:

$$\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_n \rangle \approx \left(\frac{\beta J}{2}\right)^{|n-m|} \equiv \exp\left(-R_{mn}/\xi\right)$$
 (5)

with $R_{nm} = a \cdot |n - m|$ being distance between sites a and b, and $\xi = a / \ln \frac{J}{T}$ being (small) correlation length. *Hint:* with the following property, the integral can be calculated iteratively:

$$\int_{0}^{2\pi} \frac{dy}{2\pi} \cos(x-y) \cos(y-z) = \frac{1}{2} \cos(x-z)$$
(6)

This calculation illustrates that at high temperatures, the system has a finite correlation length and all the correlation functions decay exponentially. This is the main property of the *high-temperature phase* in the BKT transition.

1.2 Low-temperature limit

At low temperatures it is natural to expect the fluctuations of the phase to be small, allowing one to describe the state of the system with a smoothly varying in space function $\{\varphi_i\} \mapsto \varphi(\mathbf{r})$ and expand:

$$\cos(\varphi_i - \varphi_j) \approx 1 - \frac{1}{2}(\varphi_i - \varphi_j)^2 \approx 1 - \frac{1}{2}(\boldsymbol{r}_i - \boldsymbol{r}_j) \cdot \nabla\varphi(\boldsymbol{r})$$
(7)

arriving at a *continuous* XY model:

$$H[\varphi] \approx \text{const} + \frac{J}{2} \int d^2 \boldsymbol{r} (\nabla \varphi(\boldsymbol{r}))^2,$$
(8)

using which the correlation function of interest can be expressed via the path integral:

$$\langle \boldsymbol{S}_{m} \cdot \boldsymbol{S}_{n} \rangle = \int \mathcal{D}\varphi(\boldsymbol{r}) \cdot \cos(\varphi(\boldsymbol{R}_{m}) - \varphi(\boldsymbol{R}_{n})) \cdot e^{-\beta H[\varphi]}$$
⁽⁹⁾

Although the target manifold of the original spin variables $S(\mathbf{r})$ is 1D sphere S^1 (i.e. $\varphi(\mathbf{r}) = \varphi_0$ and $\varphi(\mathbf{r}) = \varphi_0 + 2\pi$ are exactly same point), for now we will neglect it and return to it in the next section.

1. Calculate the Greens function of this Gaussian field theory and show that

$$\langle \varphi(\boldsymbol{r})\varphi(\boldsymbol{r}')\rangle = \int \frac{d^2\boldsymbol{q}}{(2\pi)^2} \frac{T/J}{q^2} e^{i\boldsymbol{q}(\boldsymbol{r}-\boldsymbol{r}')} \approx \frac{T}{2\pi J} \ln \frac{L}{|\boldsymbol{r}-\boldsymbol{r}'|}$$
(10)

where we have introduced an infrared cutoff $q_{\min} \sim 1/L$ related to the inverse system size because the integral is logarithmically divergent at small momenta q. Furthermore, phase fluctuations at a single site are also ultraviolet divergent and can be estimated as:

$$\left\langle \varphi^2(\boldsymbol{r}) \right\rangle \approx \frac{T}{2\pi J} \ln \frac{L}{a}$$
 (11)

where $q_{\rm max} \sim 1/a$ denotes ultraviolet cutoff of the order of inverse unit lattice cell size.

2. Let's assume there is a long-range order in the system, i.e. all spins point at some direction $\varphi(\mathbf{r}) = \varphi_0$. Calculate the average magnetization taking into account the statistical fluctuations of this phase and show that:

$$\langle S(\boldsymbol{r})\rangle = \begin{pmatrix} \langle \cos(\varphi_0 + \varphi(\boldsymbol{r}))\rangle \\ \langle \sin(\varphi_0 + \varphi(\boldsymbol{r}))\rangle \end{pmatrix} = \begin{pmatrix} \cos\varphi_0 \\ \sin\varphi_0 \end{pmatrix} \cdot \left(\frac{a}{L}\right)^{T/4\pi J}$$
(12)

i.e. at any finite temperature T, in the thermodynamic limit $L \to \infty$ the spontaneous magnetization is destroyed by the fluctuations of phase $\langle S(\mathbf{r}) \rangle \to 0$ and our initial assumption breaks down. This is manifestation of the *Mermin-Wagner theorem*: a continuous symmetry (S¹ in our case) cannot be spontaneously broken in 2D, and conventional second order phase transition is impossible.

Hint: calculation of averages of exponentials (and trigonometric functions) of Gaussian fields can be performed utilizing the following nice property: if variable A has the Gaussian distribution, then it follows that $\langle \exp(\alpha A) \rangle = \exp(\alpha^2 \langle A^2 \rangle / 2)$ with arbitrary $\alpha \in \mathbb{C}$. 3. Finally, show that infrared divergence cancels in (9) and the correlation function within this approximation is given by:

$$\langle \boldsymbol{S}_m \cdot \boldsymbol{S}_n \rangle \approx \left(\frac{a}{R_{mn}}\right)^{T/2\pi J}$$
(13)

i.e. they fall off at large distances only as a power law (with temperature-dependent power) and the correlation length is infinite. This is the main property of the *low-temperature phase* of the BKT transition, which has to be contrasted with an exponential decay at high temperatures obtained earlier.

The only way for the behavior of the correlation function to change so drastically is via the phase transition, which is precisely the BKT transition: there exists a transition temperature T_c , at which the correlation length appears. Below this temperature, the correlations follow power-law behavior (13), and above it they decay exponentially as in (5).

1.3Vortices

In the previous low-temperature analysis we have completely neglected the fact that $\varphi(\mathbf{r})$ is an angle defined modulo 2π , i.e. the fact that the symmetry of the problem is $S^1 \simeq U(1)$. Recall that the fundamental homotopy group $\pi_1(S^1) = \mathbb{Z}$, and thus that apart from conventional long-wavelength fluctuations of a phase, the system can also host point-like topological excitations — vortices, with an integer topological charge $n \in \mathbb{Z}$ — the winding number of a phase along a loop enclosing the vortex. Vortices play crucial role in the BKT transition.

- 1. Find classical configuration $\varphi(\mathbf{r})$ which corresponds to a single vortex with charge n. Show that its energy is logarithmically divergent as $E_n \ln \frac{L^2}{a^2}$. Show that $E_{n_1+n_2} > E_{n_1} + E_{n_2}$, i.e. unit charge vortices are energetically favorable.
- 2. Consider two vortices of charge n_1 and n_2 placed at r_1 and r_2 , and calculate their interaction energy. Show that the energy of the "charge-neutral" configuration (e.g. vortex-antivortex pair), does not diverge at $L \to \infty$.
- 3. An isolated vortex center be placed at any node in the system, thus there is also logarithmically divergent configurational entropy associated with each vortex $S = \ln N = \ln \frac{L^2}{a^2}$. Therefore at sufficiently high temperatures $T > T_c$, the free energy of an isolated vortex F = E TS becomes negative, i.e. vortices can spontaneously appear in the system. The associated temperature is the BKT transition temperature, and it follows that the high-temperature phase corresponds to a two-dimensional plasma of individual vortices, which interact according to the "Coulomb" law (the system is two-dimensional, so the Coulomb interaction is logarithmic). On the other hand, at lower temperatures isolated vortices are unlikely to exist, while bound vortex-antivortex pair still can appear. The BKT transition can then be thought of vortex-antivortex pair unbinding transition.

2 Double-layer FQHE — Halperin state

Consider fractional quantum hall state (FQHE) in double-layer system with N_1 electrons in the first layer and N_2 electrons in the second one. Such state, can be described by the following form proposed by Halperin:

$$\Psi_{q_1q_2n}(\{z_i\},\{w_j\}) = \prod_{i(14)$$

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where $\{z_i\}_{i=1}^{N_1}$ correspond to coordinates of electrons from the first layer, and $\{w_j\}_{j=1}^{N_2}$ are electron coordinates in the second layer. Here q_1 and q_2 are odd integers, and n is an integer. Particles in two layers are considered as distinguishable.

1. Express the highest power of arbitrary z_k and w_k , denoted as M_1 and M_2 , via the number of electrons in corresponding layers. They correspond to maximal angular momenta of single-electron states, and are related to the radius of electron "droplet" as $\pi R_{1,2}^2 = 2\pi l_0^2 \cdot M_{1,2}$. At which ratio N_1/N_2 , the disks have coinciding radius, i.e. $M_1 = M_2 = M$? Calculate the filling factor of each layer $\nu_{1,2} = N_{1,2}/M$.

2. Consider now a quasihole excitation in the first layer, described by the following wavefunction:

$$\Psi_1^h(\xi_1) = \prod_i (\xi_1 - z_i) \Psi_{q_1 q_2 n}(\{z_i\}, \{w_j\}), \tag{15}$$

Such quasihole increases M_1 by unity, thus from the plasma analogy electrons from both layers will adjust introducing additional charges $\Delta N_{1,2}$ to compensate for the charge of quasihole and maintain electroneutrality. Calculate the quasihole charge based on this argument, and generalize the result to the quasihole in the second layer. Show that the charge coincides with the filling factors obtained earlier.

3. Within the plasma analogy, the square of the wavefunction can be expressed as:

$$|\Psi_{q_1q_2n}(\{z_i\},\{w_j\})|^2 = \exp\left(-\frac{1}{2}\sum_{\alpha,\beta}\int d^2z d^2z' \rho_\alpha(z) K_{\alpha\beta} \ln\frac{1}{|z-z'|^2}\rho_\beta(z') - \sum_{\alpha}\int d^2z \rho_\alpha(z) \cdot \frac{|z|^2}{2l_0}\right) \equiv e^{-\beta V[\rho]}$$
(16)

where $\rho_1(z) = \sum_i \delta(z - z_i), \ \rho_2(w) = \sum_j \delta(w - w_j)$, and the interaction matrix has the following form:

$$K_{\alpha\beta} = \begin{pmatrix} q_1 & n \\ n & q_2 \end{pmatrix} \tag{17}$$

(strictly speaking, the expansion has also unphysical "self-action" term where two delta-functions coincide; such term can be made finite by introducing short-distance regularization of the logarithmic interaction, then it simply becomes constant and thus is not important).

Now consider a plasma with additional "test charges" $\delta \rho_{\alpha}(z) = \sum_{\beta} m_{\alpha\beta} \delta(z - \xi_{\beta})$. Show that for matrix $\hat{m} = \hat{K}^{-1}$, the corresponding "plasma potential" acquires following form:

$$e^{-\beta V[\rho+\delta\rho]} \equiv |\xi_1 - \xi_2|^{2p} \exp\left(-\frac{\nu_1 |\xi_1|^2 + \nu_2 |\xi_2|^2}{2l_0^2}\right) \left|\Psi_{12}^{hh}(\xi_1, \xi_2)\right|^2 \tag{18}$$

where $\nu_{1,2}$ exactly correspond to quasihole charges obtained earlier, and where we have introduced the nonnormalized wavefunction with two quasihole excitations, one in the first layer and another in the second:

$$\Psi_{12}^{hh}(\xi_1,\xi_2) = \prod_i (\xi_1 - z_i) \prod_j (\xi_2 - w_j) \Psi_{q_1 q_2 n}(\{z_i\},\{w_j\})$$
(19)

What is the value of p?

4. Based on the calculation from the lecture, show that p is related to the *mutual statistics* of two quasiholes: if one adiabatically moves one quasihole around another (note: particles in different layers are considered as distinguishable, so the complete loop should be made!), the acquired Berry phases consists of standard Aharonov-Bohm phase (taking into account the quasiparticle charge), and $\theta_{12} = -2\pi p$.