Advanced Statistical Physics

TD5: Renormalization group approach for the XY model

October 2021

The Kosterlitz-Thouless transition is a peculiar transition occurring in $2d$ systems in which topological defects play a crucial role. We will study it in the formulation of the XY model, which consists of two-dimensional vector (classical) spins placed at the vertices $\mathbf{r}$ of a two-dimensional square lattice of N sites and of size L ($N = (L/a)^2$, where a is the lattice spacing), and interacting ferromagnetically:

$$\mathcal{H} = -J \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \mathbf{S}_\mathbf{r} \cdot \mathbf{S}_{\mathbf{r}'} \,.$$

The correlation function decays as a power-law at low temperature and become short-ranged above a certain temperature. While the nature of the correlations changes drastically between the high and the low temperature regime, there is nonetheless no genuine ordering transition. The purpose of this exercise is to analyze the predictions of the renormalization group approach in the scale invariant regime in the Coulomb gas approximation.

(A) **Low temperature expansion: The spin-wave regime**

Each spin $\mathbf{S}_\mathbf{r}$ can be simply characterized by an orientation $\theta_\mathbf{r} \in [0,2\pi)$ (with respect to any arbitrarily chosen axes).

1. What is the ground state of $\mathcal{H}$?
2. Why is $\mathcal{H}_{\rm sw} = \frac{J}{2} \sum_{\langle \mathbf{r},\mathbf{r}' \rangle} \left(\theta_\mathbf{r} - \theta_{\mathbf{r}'}\right)^2$ a good approximation of $\mathcal{H}$ at low temperature?
3. We define the discretized version of the derivative operator along the x axis as:

$$\frac{\partial f}{\partial x} = \frac{f(x+a/2) - f(x-a/2)}{a} \,.$$

Show that the discretized version of the Laplace operator in two dimension is:

$$\nabla^2 f(x,y) = \frac{f(\mathbf{r}+a\mathbf{e}_x) + f(\mathbf{r}-a\mathbf{e}_x) + f(\mathbf{r}+a\mathbf{e}_y) + f(\mathbf{r}-a\mathbf{e}_y) - 4f(\mathbf{r})}{a^2} \,.$$

We also introduce the Green's function of ($-a^2$ times) the two-dimensional Laplacian on the square lattice (i.e. the $2d$ Coulomb potential) defined as:

$$-a^2 \nabla^2 G_\mathbf{r} = \delta_{\mathbf{r},\mathbf{0}} \,.$$

The properties of G are given in the Appendix. We call $Z_{\rm sw}$ the partition function of the system in this temperature regime and we define $K=\beta J$. Show that $Z_{\rm sw}$ can be written as:

$$Z_{\rm sw}=\int \mathcal{D}\theta\, e^{-\frac{K}{2}\sum_{\mathbf{r}}\theta_{\mathbf{r}}(-a^2\nabla^2)\theta_{\mathbf{r}}}\,,$$

and give the expression of the correlations $\langle\theta_{\mathbf{r}}\theta_{\mathbf{r}'}\rangle$ in terms of the Green's function of the Laplacian operator.

4. How does the spin spin correlation function $C(|\mathbf{r}-\mathbf{r}'|)=\langle\mathbf{S}_{\mathbf{r}}\cdot\mathbf{S}_{\mathbf{r}'}\rangle$ behaves in this low temperature regime? Is there any spontaneous magnetization?

(B) **The high temperature expansion**

1. Let $\mathcal{N}(\mathbf{r})$ the number of shortest paths connecting an arbitrary site $\mathbf{r}=(x,y)$ to the origin. Express $\mathcal{N}(\mathbf{r})$ as a function of $|x|$ and $|y|$. The combination $|x|+|y|$ is called the Manhattan distance $||\mathbf{r}||_1$ between the origin and $\mathbf{r}$. Argue that $\mathcal{N}(\mathbf{r})$ is bounded by $2^{||\mathbf{r}||_1}$.
2. Show that

$$\int \mathrm{d}\theta_2\cos(\theta_1-\theta_2)\cos(\theta_2-\theta_3)=\pi\cos(\theta_1-\theta_3)\,.$$

3. Justify that in the high temperature regime, to the leading order in an expansion in powers of K one has:

$$C(|\mathbf{r}-\mathbf{r}'|)\sim\mathcal{N}(\mathbf{r}-\mathbf{r}')\,(\pi K)^{||\mathbf{r}-\mathbf{r}'||_1}\,.$$

Give an estimation of the correlation length ξ in terms of K.

(C) **The Coulomb gas formulation within the Villain approximation**

The aim of this part of the excercise is to establish a connection between the XY model and a system of charges interacting via a Coulomb potential in two dimensions. The charges can be seen as *vortices* in the local magnetization field.

1. The Bessel functions of imaginary argument $I_n=\int_0^{2\pi}\frac{\mathrm{d}\theta}{2\pi}e^{x\cos\theta+in\theta}$ allows us to writhe the Fourier series of $e^{K\cos\theta}$ as

$$e^{K\cos\theta}=\sum_{n=-\infty}^{\infty}e^{in\theta}I_n(K)\,.$$

In which regime we can approximate $I_n(K)\simeq\frac{1}{\sqrt{2\pi K}}e^{K-n^2/2K}$?

2. In the following we will use

$$e^{K\cos\theta}\simeq\frac{e^K}{\sqrt{2\pi K}}\sum_{n=-\infty}^{\infty}e^{in\theta-n^2/2K}\,.$$

Which physical symmetry of the model is preserved by this approximation and *not* by the spin-wave approximation treated above $e^{K\cos\theta}\approx e^{K-K\theta^2/2}$?

3. Using the definition of the discretized version of the derivative $\partial_\mu \theta_{\mathbf{r}} = \theta_{\mathbf{r}+a\mathbf{e}_\mu} - \theta_{\mathbf{r}}$, with $\mu = x{,}y$, show that:

$$Z \approx \left(\frac{e^K}{\sqrt{2\pi K}}\right)^N \sum_{\{\mathbf{n}(\mathbf{r})\in\mathbb{Z}\}} \int \mathcal{D}\theta \prod_{\mathbf{r}} e^{-i\sum_\mu \partial_\mu n_\mu(\mathbf{r})\theta_{\mathbf{r}} - n^2(\mathbf{r})/2K} ,$$

   where $\mathbf{n}(\mathbf{r})$ is an integer two-dimensional vector field.
4. Henceforth the K-dependent prefactor will be omitted (it only contributes to the free-energy but not to the correlation function). Show that integrating over each $\theta_{\mathbf{r}}$ yields a zero divergence condition for the $\mathbf{n}(\mathbf{r})$ field.
5. Recall that a field with zero divergence can be written in the form of a curl: $\mathbf{n}(\mathbf{r}) = \nabla \times \mathbf{A}(\mathbf{r})$, where $\mathbf{A}(\mathbf{r}) = p(\mathbf{r})\mathbf{e}_z$, i.e. $n_x = \partial_y p$ and $n_y = -\partial_x p$. Show that the partition function can be recast as a summation over configurations of the field $p(\mathbf{r})$ (given the linear relation between p and $\mathbf{n}$, any possible Jacobian associated to this change of variable would be a constant).
6. We now recall the Poisson summation formula, which states that for an arbitrary function f one has that:

$$\sum_{p=-\infty}^{\infty} f(p) = \sum_{m=-\infty}^{\infty} \int_{-\infty}^{+\infty} \mathrm{d}\phi f(\phi) e^{i2\pi m\phi} .$$

   Apply this formula to the partition function by introducing an integer field $m(\mathbf{r})$ and a Gaussian field $\phi(\mathbf{r})$ for any point of the lattice.
7. Integrate out explicitly the Gaussian field $\phi(\mathbf{r})$ and write the resulting partition function in terms of Z_{sw} and the Green's function of the Laplacian operator. In the following, without any loss of description of the large-scale physics, we replace the Green's function by its large-distance asymptotic behavior: $G_{|\mathbf{r}|\gg a} - G_{\mathbf{0}} \simeq -\frac{1}{2\pi}\log\frac{|\mathbf{r}|}{a} - c$. Justify that in the large L limit only *neutral* configurations such that $\sum_{\mathbf{r}} m(\mathbf{r}) = 0$ survive.

(D) **Real space renormalization**

The partition function $Z_{\mathrm{v}} = Z/Z_{\mathrm{sw}}$ is the partition function of a two-dimensional Coulomb gas at temperature T of $2\pi\sqrt{J}m(\mathbf{r})$ charges sitting at the nodes of a $2d$ square lattice whose density is controlled by the fugacity $z = e^{-2\pi^2 Kc}$. Physically, the field $m(\mathbf{r})$ represents the circulation of the local magnetization field around some specific point $\mathbf{r}$, and can be then seen as a vorticity field. Vortices at distance r in $2d$ interact via a $\log r$ potential. As z is increased, more and more charges (vorices) appear, while for $z \to 0$ the number of charges (vortices) vanishes and they stop interacting with each other. In the high temperature regime vortices proliferate and correlations decay exponentially fast. In the low temperature regime a quasi long-range order sets in, characterized by power-law correlations. In the following we attempt a $z \to 0$ expansion of Z_{v}.

1. Consider the case where at most two non-zero opposite charges are present and justify that:

$$Z_{\mathrm{v}} \approx 1 + \frac{z^2}{a^4}\int_{|\mathbf{r}-\mathbf{r}'|>a} \mathrm{d}^2\mathbf{r}\,\mathrm{d}^2\mathbf{r}' \left|\frac{a}{\mathbf{r}-\mathbf{r}'}\right|^{2\pi K} .$$

2. We now introduce the coarse-graining parameter $b = e^\ell$ (with $\ell = \log b \ll 1$) and split the integrals in the right hand side as $\int_a^\infty \mathrm{d}r \cdots = \int_a^{ba} \mathrm{d}r \cdots + \int_{ba}^\infty \mathrm{d}r \cdots$. Rescale the large-$r$ integration variables so that the integrals again run from a to ∞. The rescaling can be absorbed into the definition of a renormalized fugacity. Determine the differential equation governing the evolution of the fugacity under rescaling.
3. In order to get the renormalization of K one has to study the spin spin correlation function $C(|\mathbf{r}-\mathbf{r}'|) = \langle S_{\mathbf{0}} \cdot S_{\mathbf{r}} \rangle$ and compute how the exponent of the power-law decay is modified. We use the result of the paper José, Kadanoff, Kirckpatrick, and Nelson, Phys. Rev. B **16**, 1217 (1997), where it is shown that the expansion of C in powers of z yields (equation (5.1))

$$C(|\mathbf{r}-\mathbf{r}'|) \propto |\mathbf{r}-\mathbf{r}'|^{-\frac{1}{2\pi K_{\text{eff}}}} \,, \qquad \frac{1}{K_{\text{eff}}} = \frac{1}{K} + 4\pi^3 z^2 \int_a^L \frac{\mathrm{d}r}{a} \left(\frac{r}{a}\right)^{3-2\pi K} .$$

Below which value of K the perturbative expansion breaks down? Split the integrals in the right hand side as $\int_a^\infty \mathrm{d}r \cdots = \int_a^{ba} \mathrm{d}r \cdots + \int_{ba}^\infty \mathrm{d}r \cdots$. Rescale the large-$r$ integration variables so that the integrals again run from a to ∞, and find the renormalized bare coupling constant K' and its evolution equation upon rescaling.
4. Recall the relationship between z and K at the microscopic level before any sort of renormalization. Plot the $z(K)$ line in the (K,z) plane. This is the so-called line of initial conditions.
5. The RG flow is then made up by two equations:

$$\frac{\mathrm{d}z}{\mathrm{d}\ell} = z(2-\pi K) \,, \qquad \frac{\mathrm{d}K}{\mathrm{d}\ell} = -4\pi^3 z^2 K^2 \,.$$

What are the fixed points of these equations? Locate them on the (K,y) plane.
6. Show that, for K in the vicinity of $K_\star = 2/\pi$ one has that:

$$16\pi^2 z^2 + (2-\pi K)^2 = \text{cst} \,.$$

Draw on the phase diagram the asymptotes of the resulting hyperboles describing the flow lines.
7. We want now to exploit the RG flow to predict the temperature dependence of the correlation length in the high-temperature phase. What is the correlation length in the low temperature phase? How would you define T_c?
8. Let us now consider the regime close to the critical point, $T \to T_c^+$. Find $K(\ell)$ by direct integration of the flow equations between 0 and ℓ. How would you define the correlation length ξ? Determine how it diverges when T_c is approached from above.

APPENDIX: Green's function of the two-dimensional Laplacian on the square lattice

We define the Fourier transform as:

$$\hat{G}_{\mathbf{q}} = \sum_{\mathbf{r}} e^{i\mathbf{q}\cdot\mathbf{r}} G_{\mathbf{r}} \,, \qquad G_{\mathbf{r}} = \frac{1}{N} \sum_{\mathbf{q}\neq\mathbf{0}} e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{G}_{\mathbf{q}} \,,$$

where the wave vectors are $\mathbf{q} = \frac{2\pi}{L}(n_x,n_y)$, and (n_x,n_y) are integers varying between $-L/(2a)$ and $L/(2a)$. Inserting the last expression into the definition of the Green's function we have that:

$$\begin{aligned}
-a^2\nabla^2 G_{\mathbf{r}} &= 4G_{\mathbf{r}} - G_{\mathbf{r}+a\mathbf{e}_x} - G_{\mathbf{r}-a\mathbf{e}_x} - G_{\mathbf{r}+a\mathbf{e}_y} - G_{\mathbf{r}-a\mathbf{e}_y} \\
&= \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} e^{i\mathbf{q}\cdot\mathbf{r}}\hat{G}_{\mathbf{q}}\left[4 - 2\cos(aq_x) - 2\cos(aq_y)\right] = \delta_{\mathbf{r},\mathbf{0}}\,.
\end{aligned}$$

We than obtain that:

$$\hat{G}_{\mathbf{q}} = \frac{1}{4 - 2\cos(aq_x) - 2\cos(aq_y)} \qquad\qquad G_{\mathbf{r}} = \frac{1}{N}\sum_{\mathbf{q}\neq\mathbf{0}} \frac{e^{-i\mathbf{q}\cdot\mathbf{r}}}{4 - 2\cos(aq_x) - 2\cos(aq_y)}\,.$$

We will use the following properties of the Green's function (without proving them):

$$G_{\mathbf{0}} \simeq \frac{1}{2\pi}\log\frac{L}{a}\,, \qquad G_{|\mathbf{r}|\gg a} - G_{\mathbf{0}} \simeq -\frac{1}{2\pi}\log\frac{|\mathbf{r}|}{a} - c + o(1)\,,$$

where $c = \frac{1}{2\pi}(\gamma + \frac{3}{2}\log(2)) \approx \frac{1}{4}$.