Advanced Statistical Physics

TD — Renormalization group approach for the Berezinski-Kosterlitz-Thouless transition in the XY model

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The Berezinski-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:

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

We have seen in the TD2 that the correlation function behaves in a drastically different way at high at low temperatures: It decays as a power-law at low temperature and become short-ranged at high temperature.

$$C(|\mathbf{r}|) = \langle \mathbf{S_0} \cdot \mathbf{S_r} \rangle \simeq \begin{cases} \left(\frac{a}{|\mathbf{r}|}\right)^{\eta(T)} & \eta = \frac{T}{2\pi J} \qquad \text{for } T \ll J \, , \\ e^{-|\mathbf{r}|/\xi} & \xi \simeq -\frac{1}{\ln\left(\frac{J}{2T}\right)} \qquad \text{for } T \gg J \, . \end{cases}$$

This indicates that there exists a phase transition, called the BKT transition, between a high-temperature phase characterized by exponential decay of correlations and a low-temperature phase characterized by algebraic decay of correlations. The goal of this tutorial is to provide a quantitative study of this transition using a real-space renormalization group approach (exercise C). To this purpose, we need to reformulate the XY Hamiltonian as a $2d$ Coulombg gas. We will first do this by means of the phenomenological arguments given by Kosterlitz and Thouless in their theory of phenomenological defects (exercise A), and then more formally using the so-called Villain approximation (optional exercise B). More details can be found in M. Kardar, *Statistical physics of fields*, Cambridge University Press (2007).

A) Phenomenological analysis

In this part of the exercise we will follow J. M. Kosterlitz, D. J. Thouless, *Ordering, metastability and phase transitions in two-dimensional systems*, J. Phys. C: Solid State Phys. **6**, 1181 (1973). In the continuum limit the XY Hamiltonian can be approximated as:

$$\mathcal{H} = \text{cst} + \frac{J}{2}\int \mathrm{d}^2\mathbf{r}\,(\nabla\theta(\mathbf{r}))^2 \ .$$

1. Write the condition that gives stable configurations of the field $\theta(\mathbf{r})$ that dominates the Gibbs measure at very low temperature.
2. Note that $\theta(\mathbf{r})$ is not physical, contrary to $\mathbf{S}$; There are multiple choices of $\theta(\mathbf{r})$ which can lead to the same spin configuration. The equation $\Delta\theta = 0$ is the subject of harmonic theory. Liouville theorem states that if $\theta(\mathbf{r})$ has no singularity, then it is a constant; Therefore, non-trivial solutions must have singular points, or *defects*. Then, Stokes theorem tells us that the integrals of $\mathrm{d}\theta$ on different contours containing the singularity are all equal to $2\pi n$ for some $n \in \mathbb{Z}$. Hence, the non trivial stable configurations of the field, such that $\theta(\mathbf{r}$ is not constant, must satisfy

$$\oint \mathrm{d}\theta = 2\pi n\,, \qquad\qquad n \in \mathbb{Z}\,.$$

   The integer n is a characteristic of the defect, often called "charge". Show that the general solution of the equation $\Delta\theta = 0$ can be written as $\theta(\mathbf{r}) = n\phi + \theta_0$, where ϕ is the polar coordinate of the point $\mathbf{r}$. Draw the configuration of the spins for $n = \pm 1$ and $\theta_0 = 0, \pi/2$.
3. Compute the energy of a defect of charge n (the integration over $\mathrm{d}^2\mathbf{r}$ varies between $a \leq |\mathbf{r}| \leq L$).
4. The defects have several interesting properties: Only one of them is enough to destroy long-range ferromagnetic order; A finite density of defects even kills algebraic correlations; Defects are topologically stable (this means that there is no continuous transformation of the field allowing to change their charge n); Defects with the same charge are topologically equivalent (it is possible to deform the θ field from $\theta(\mathbf{r}) = \phi$ to $\theta(\mathbf{r}) = \phi + \pi/2$ in a smooth manner); Finally, show that these topological defects are energetically stable. To do this, determine how much energy it would cost to destroy one of the defects.
5. Applying the Peierl's argument, and using the answer to question 3, compute the free-energy cost for creating a defect, and estimate the critical temperature T_c at which topological defects start to form. For $T < T_c$ there are no defects and, according to the spin-waves analysis, the system is characterized by algebraic correlations. For $T > T_c$ topological defects proliferate and correlations decay exponentially. Estimate the correlation length as a function of the density of defects.

It is possible to show that topological defects behave as Coulomb electric charges in $2d$: two defects of charge n_1 and n_2 interact as

$$E_{\text{int}} = A\, n_1 n_2 \ln\left(\frac{a}{|\mathbf{r}_1 - \mathbf{r}_2|}\right)\,,$$

i.e., two defects of opposite charge attract each other.

In the next part of the tutorial (optional), we will determine more formally the effective model describing these topological defects.

B) **Optional exercise: 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 *defects* or *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.

C) **Real space renormalization**

Using the Villain approximation we have seen that the partition function of the model can be rewritten as:

$$Z = e^{2NJ}\, Z_{\rm sw}\, Z_v\,,$$

$$Z_v = \sum_{\substack{\{m(\mathbf{r})\}\in\mathbb{Z}^N \\ \sum_{\mathbf{r}} m(\mathbf{r})=0}} e^{\pi K \sum_{\mathbf{r}_1\neq\mathbf{r}_2} m(\mathbf{r}_1)\, m(\mathbf{r}_2)\ln\left(\frac{|\mathbf{r}_1-\mathbf{r}_2|}{a}\right)}\, e^{-\frac{\pi^2 K}{2}\sum_{\mathbf{r}} m^2(\mathbf{r})}\,.$$

1. The partition function Z_v is the (grand-canonical) partition function of of a two-dimensional Coulomb gas of charges sitting at the nodes of a $2d$ square lattice (with a neutrality condition). Give the physical interpretation of the different terms. Which parameter control the density of charges?
2. Consider the case where at most two non-zero opposite charges are present and justify that:
$$Z_{\rm v} \approx 1 + \frac{z^2}{a^4}\int_{|\mathbf{r}-\mathbf{r}'|>a} \mathrm{d}^2\mathbf{r}\,\mathrm{d}^2\mathbf{r}' \left|\frac{a}{\mathbf{r}-\mathbf{r}'}\right|^{2\pi K}\,.$$
3. 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.
4. 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 J. V. José, L. P. Kadanoff, S. Kirckpatrick, and D. R. Nelson, *Renormalization, vortices, and symmetry-breaking perturbations in the two-dimensional planar model*, Phys. Rev. B **16**, 1217 (1997), where it is shown that the expansion of C in powers of z yields (equation (5.1))
$$C(|\mathbf{r}-\mathbf{r}'|) \propto |\mathbf{r}-\mathbf{r}'|^{-\frac{1}{2\pi K_{\rm eff}}}\,, \qquad \frac{1}{K_{\rm eff}} = \frac{1}{K} + 4\pi^3 z^2 \int_a^L \frac{\mathrm{d}r}{a}\left(\frac{r}{a}\right)^{3-2\pi K}\,.$$
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.
5. 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.

6. 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,z) plane.
7. Show that, for K in the vicinity of $K_\star = 2/\pi$ one has that:

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

   Draw on the phase diagram the asymptotes of the resulting hyperboles describing the flow lines.
8. 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?
9. 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 $c = \frac{1}{2\pi}(\gamma + \frac{3}{2}\log(2)) \approx \frac{1}{4}$.