Advanced Statistical Physics

TD2: The XY model and the spin-wave regime

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The Kosterlitz-Thouless (KT) transition is a peculiar phase transition occurring in two-dimensional systems, in which topological defects play a crucial role. We will study it in the framework of the XY model, which is defined by two-dimensional (classical) vector spins located at the vertices \mathbf{r} of a square lattice of N sites and linear size L ($N = (L/a)^2$, where a is the lattice spacing). The spins interact ferromagnetically according to the Hamiltonian

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

The model is considered in canonical equilibrium with a thermal bath at temperature T.

At low temperatures, the spin–spin correlation function decays algebraically as a power law, whereas above a certain temperature it becomes short-ranged. Although the nature of correlations changes dramatically between the low- and high-temperature regimes, there is no conventional symmetry-breaking phase transition.

The goal of this exercise is to analyze the XY model using both low- and high-temperature expansions.

A) Phenomenological analysis

- 1. Which kind of order is favored by the exchange J?
- 2. At which temperatures do you expect to see this kind of order?
- 3. Which kind of configurations do you expect to find at high temperatures?

B) Low temperature expansion: The spin-wave regime

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

- 1. What is the ground state of \mathcal{H} in terms of the angles?
- 2. Why is

$$\mathcal{H}_{\mathrm{sw}} = \frac{J}{2} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})^2$$

a good approximation of \mathcal{H} at low temperature?

3. We define the discretized derivative along x as

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

Show that the discretized Laplacian in 2d is

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

4. We introduce the Green's function of $(-a^2 \text{ times})$ the 2d Laplacian on the square lattice:

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

The properties of G are given in the Appendix. Show that the partition function under this approximation is

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

with $K = \beta J$ and $\mathcal{D}\theta = \prod_{\mathbf{r}} d\theta_{\mathbf{r}}$, and express the correlation $\langle \theta_{\mathbf{r}} \theta_{\mathbf{r}'} \rangle$ in terms of in terms of the Green's function of the discrete Laplacian operator.

- 5. What is the average angle $\langle \theta_{\mathbf{r}} \rangle$? Is there any spontaneous magnetization $\langle S_{\mathbf{r}} \rangle \neq 0$?
- 6. How does the spin-spin correlation $C(\mathbf{r},\mathbf{r}') = \langle \mathbf{S}_{\mathbf{r}} \cdot \mathbf{S}_{\mathbf{r}'} \rangle$ behave?
- 7. What is the correlation length ξ ?
- 8. What is the linear magnetic susceptibility?

C) The high temperature expansion

- 1. Let $\mathcal{N}(\mathbf{r})$ be the number of shortest paths connecting $\mathbf{r} = (x,y)$ to the origin. Express $\mathcal{N}(\mathbf{r})$ as a function of |x|,|y|. Argue that $\mathcal{N}(\mathbf{r}) \leq 2^{\|\mathbf{r}\|_1}$ with $\|\mathbf{r}\|_1 = |x| + |y|$ (called the "Manhattan distance").
- 2. Show that

$$\int d\theta_2 \cos(\theta_1 - \theta_2) \cos(\theta_2 - \theta_3) = \pi \cos(\theta_1 - \theta_3).$$

3. Justify that in the high-T regime, to leading order in K,

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

Give an estimate of ξ in terms of K.

Appendix: Green's function of the 2d Laplacian on a square lattice

We define the Fourier transform as

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

with $\mathbf{q} = \frac{2\pi}{L}(n_x,n_y)$ and integers $n_x,n_y \in [-L/(2a),L/(2a)]$. Inserting into the definition gives

$$\hat{G}_{\mathbf{q}} = \frac{1}{4 - 2\cos(aq_x) - 2\cos(aq_y)}.$$

Hence

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

Useful properties:

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

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