Advanced Statistical Physics
TD3 First analysis of the $2d$ XY model
Spin-waves and high temperature expansion

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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 vectors (classical) spins $\mathbf{S} = (S_x, S_y)$, placed at the vertices $\mathbf{r}$ of a two-dimensional lattice and interacting ferromagnetically:

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

$J > 0$. For a square lattice and neglecting possible boundary effects there are $N = (L/a)^2$ spins in the sample, where L is the linear size and a is the spacing of the lattice. The sites of the lattice, and hence the spins, are labeled by $\mathbf{r}$.

The models is considered to be in canonical equilibrium with a thermal bath at temperature T.

Phenomenological analysis

1. Which kind of order favours 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?

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 axis.

1. What is the ground state of $\mathcal{H}$ in terms of the angles?
2. Why is $\mathcal{H}_{\text{sw}} = \frac{J}{2} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} (\theta_{\mathbf{r}} - \theta_{\mathbf{r}'})^2$ a good approximation of $\mathcal{H}$ at low temperature?
3. We define the discretized 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:

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

4. We 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 $\mathcal{Z}_{\rm sw}$ the partition function of the system under this "low-temperature approximation" and we define $K = \beta J$. Show that $\mathcal{Z}_{\rm sw}$ can be written as:

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

with $\mathcal{D}\theta = \prod_{\mathbf{r}} d\theta$ and give the expression of the correlations

$$\langle\theta_{\mathbf{r}}\theta_{\mathbf{r}'}\rangle = \frac{1}{\mathcal{Z}_{\rm sw}}\int \mathcal{D}\theta\;\theta_{\mathbf{r}}\theta_{\mathbf{r}'}\; e^{-\frac{K}{2}\sum_{\mathbf{r}}\theta_{\mathbf{r}}(-a^2\nabla^2)\theta_{\mathbf{r}}}$$

in terms of the Green's function of the Laplacian operator.

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

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.

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

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

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