ICFP M2 - Statistical physics 1 – TD n^{o} 8
$2d$-XY Model and the Kosterlitz-Thouless transition

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In this tutorial we study the XY model defined by the Hamiltonian

$$\beta H_{\rm XY} = -K \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \mathbf{S_i}\cdot\mathbf{S_j} = -K \sum_{\langle \mathbf{i},\mathbf{j}\rangle} \cos(\theta_{\mathbf{i}}-\theta_{\mathbf{j}}) \tag{1}$$

on a two-dimensional square lattice of linear size L, with lattice spacing a and periodic boundary conditions. In Eq. (1) $\mathbf{i}$ and $\mathbf{j}$ are $2d$ vectors of the square lattice $\mathbb{Z}^2$, $\langle \mathbf{i},\mathbf{j}\rangle$ denotes nearest neighbours on this square lattice, while $\theta_{\mathbf{i}}$ is the angle between the spin at site $\mathbf{i}$, $\mathbf{S}_{\rm i} \in \mathbb{R}^2$ with $\mathbf{S_i}^2 = 1$, and the x-axis.

During the lectures, you have seen that the spin-spin correlation function

$$C(\mathbf{r}) = \langle \mathbf{S_0}\cdot\mathbf{S_r}\rangle = \langle \cos(\theta_{\mathbf{0}}-\theta_{\mathbf{r}})\rangle \tag{2}$$

between the spin at the origin $\mathbf{S_0}$ and the spin at site $\mathbf{r}$, $\mathbf{S_r}$ behaves quite differently at high and low temperature. At high temperature (i.e. small K), it decays exponentially

$$C(\mathbf{r}) \underset{r\gg a}{\approx} \exp\left(-\frac{r}{\xi(K)}\right) \;,\; \xi(K) \approx -\frac{1}{\ln(K/2)} \;, \tag{3}$$

with $r = |\mathbf{r}|$. In the other low temperature limit, $K \gg 1$, the correlation function decays algebraically

$$C(\mathbf{r}) \underset{r\gg a}{\approx} \left(\frac{a}{r}\right)^{\eta(K)} \tag{4}$$

with $\eta(K) \approx 1/(2\pi K)$ at large K.

The comparison of correlations at low temperature in Eq. (4) and at high-temperature in Eq. (3) indicates that there exists a transition, the so-called Kosterlitz-Thouless transition [1], where the algebraic decay (4) transforms into an exponential decay (3). The goal of this tutorial is to provide a quantitative study of this transition using a renormalisation group (RG) analysis. To this purpose, we will first reformulate the $2d$-XY model as a $2d$-Coulomb gas – through the so-called Villain approximation – and then present a real space renormalisation group (RG) analysis of this Coulomb gas.

1 From the XY model to the Coulomb gas via the Villain approximation

We would like to provide a renormalisation group description of this KT transition. This is however very hard to do directly on the XY Hamiltonian (1) where the spin-waves and the vortices are coupled. That is why we will construct an *approximate* (though reliable for large K, i.e. small temperature), description of the XY model in terms of $2d$-Coulomb gas. This can be conveniently achieved using the Villain approximation.

It is useful to start with the following Fourier decomposition

$$e^{K\cos u} = \sum_{n\in\mathbb{Z}} e^{inu} I_n(K) \;,\; I_n(x) = \int_0^{2\pi} \frac{d\theta}{2\pi} e^{x\cos\theta + in\theta} \;, \tag{5}$$

where $I_n(x)$ is a (modified) Bessel function.

1. Justify the large K asymptotic behavior

$$I_n(K) \approx \frac{1}{\sqrt{2\pi K}} e^{K-n^2/(2K)} \ . \tag{6}$$

We will use this asymptotic behavior (6) to rewrite the partition function of the XY model (1)

$$Z_{\rm XY} = \prod_{\mathbf{i}} \int_0^{2\pi} d\theta_{\mathbf{i}} \, e^{K \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \cos(\theta_{\mathbf{i}} - \theta_{\mathbf{j}})} \ . \tag{7}$$

2. Show, using (6), that $Z_{\rm XY}$ can be rewritten, for $K \gg 1$, as

$$Z_{\rm XY} \approx \prod_{\mathbf{i}} \int_0^{2\pi} d\theta_{\mathbf{i}} \left(\frac{e^K}{\sqrt{2\pi K}} \right)^{2N} \prod_{\mathbf{i},\mu=x,y} \sum_{n_{\mathbf{i},\mu} \in \mathbb{Z}} \exp\left[i n_{\mathbf{i},\mu} \partial_\mu \theta_{\mathbf{i}} - n_{\mathbf{i},\mu}^2/(2K) \right] , \tag{8}$$

where $n_{\mathbf{i},\mu}$ with $\mu = x, y$ is a $2d$-vector with integer component, associated to each site $\mathbf{i}$ and $N = (L/a)^2$ is the total number of spins. In (8) we have introduced the notation

$$\partial_\mu \theta_{\mathbf{i}} = \theta_{\mathbf{i}+\mathbf{e}_\mu} - \theta_{\mathbf{i}} \ , \tag{9}$$

where $\mathbf{e}_x$ and $\mathbf{e}_y$ are the two unit vectors along the x and y directions.

Under this form (8), we can now perform the integral over the angles $\theta_{\mathbf{i}}$'s.

3. Show that the integral over $\theta_{\mathbf{i}}$'s imposes the constraint, for each site $\mathbf{i}$ of the lattice,

$$n_{\mathbf{i},x} - n_{\mathbf{i}-\mathbf{e}_x,x} + n_{\mathbf{i},y} - n_{\mathbf{i}-\mathbf{e}_y,y} = 0 \ , \tag{10}$$

which can be re-written as a discrete divergence-free condition, i.e. $\sum_{\mu=x,y} \partial_\mu n_{\mathbf{i},\mu} = 0$. As is the case of continuum valued vectors, the vector $\mathbf{n}_{\mathbf{i}} = (n_{\mathbf{i},x}, n_{\mathbf{i},y})$ can thus be expressed as the discrete curl of an integer valued scalar field, i.e. $n_{\mathbf{i},x} = \partial_y p_{\mathbf{i}}$ and $n_{\mathbf{i},y} = -\partial_x p_{\mathbf{i}}$ [with the notation defined in (9)]. Therefore the partition function in (8) can be rewritten – up to irrelevant numerical prefactors – as

$$Z_{\rm XY} \propto \sum_{p_{\mathbf{i}} \in \mathbb{Z}} e^{-\frac{1}{2K} \sum_{\mathbf{i},\mu=x,y} (\partial_\mu p_{\mathbf{i}})^2} \ . \tag{11}$$

Note that this can also be interpreted as the partition function of a $2d$ discrete height model.

4. Use the Poisson summation formula

$$\sum_{n \in \mathbb{Z}} g(n) = \sum_{m \in \mathbb{Z}} \int_{-\infty}^{\infty} d\varphi \, g(\varphi) \, e^{2i\pi m \varphi} \tag{12}$$

to re-write the partition function in (11) as

$$Z_{\rm XY} \propto Z_{\rm sw} \sum_{m_{\mathbf{i}} \in \mathbb{Z}} e^{-2\pi^2 K \sum_{\mathbf{i},\mathbf{j}} m_{\mathbf{i}} \, G(\mathbf{i}-\mathbf{j}) \, m_{\mathbf{j}}} \ , \tag{13}$$

where $G(\mathbf{r})$ is the following Green's function

$$G(\mathbf{r}) = \left(\frac{a}{L} \right)^2 \sum_{\mathbf{q} \neq \mathbf{0}} \frac{e^{i \, \mathbf{q} \cdot \mathbf{r}}}{4 - 2\cos(q_x \, a) - 2\cos(q_y \, a)} \ , \tag{14}$$

where $\mathbf{q} = \frac{2\pi}{L}(n_x, n_y)$ where n_x, n_y are integers with $n_x, n_y = -\frac{L}{2a}, -\frac{L}{2a}+1, \cdots, \frac{L}{2a}$ (we assume, for simplicity, that $\frac{L}{2a}$ is an integer). In Eq. (13), $Z_{\rm sw}$ is the partition function corresponding to the spin-wave excitations, i.e. $Z_{\rm sw} = \prod_{\mathbf{i}} \int_{-\infty}^{\infty} d\varphi_{\mathbf{i}} \, e^{-\frac{1}{2K} \sum_{\langle \mathbf{i},\mathbf{j} \rangle} (\varphi_{\mathbf{i}} - \varphi_{\mathbf{j}})^2}$.

It is useful to introduce a regularised Green's function defined as

$$\overline{G}(\mathbf{r}) = G(\mathbf{r}) - G(\mathbf{0}) \ . \tag{15}$$

In the following we will use the following asymptotic behaviors (see also the tutorial n$^{\underline{o}}$ 7)

$$G(\mathbf{0}) \underset{L\gg a}{\approx} \frac{1}{2\pi} \ln\left(\frac{L}{a}\right) \ , \ \overline{G}(\mathbf{r}) \underset{r\gg a}{\approx} -\frac{1}{2\pi} \ln\left(\frac{r}{a}\right) - c \tag{16}$$

where $r = |\mathbf{r}|$ and c is a constant, $c = \frac{1}{2\pi}(\gamma_E + \frac{3}{2}\ln 2) = 0.257\ldots \approx \frac{1}{4}$ (we recall that $\gamma_E = 0.577\ldots$ is the Euler constant).

5. Finally, working with the regularised propagator $\overline{G}(\mathbf{r})$ in Eq. (16) instead of $G(\mathbf{r})$, show that the partition function $Z_{\rm XY}$ in (13) can finally be written as

$$Z_{\rm XY} \propto Z_{\rm sw} Z_{\rm v} \ , \ Z_{\rm v} = \sum_{m_{\mathbf{i}}\in\mathbb{Z}}{}' \, y^{\sum_{\mathbf{i}} m_{\mathbf{i}}^2} e^{\pi K \sum_{\mathbf{i},\mathbf{j}} m_{\mathbf{i}} \ln(|\mathbf{i}-\mathbf{j}|/a) m_{\mathbf{j}}} \tag{17}$$

where $\sum_{m_{\mathbf{i}}\in\mathbb{Z}}{}'$ indicates a constrained sum such that $\sum_{\mathbf{i}} m_{\mathbf{i}} = 0$ and $y = e^{-\pi^2 K/2}$. What is the physical interpretation of the different terms in (17)?

2 Renormalisation group flow

Thanks to the Villain approximation, the spin-waves and and the vortices are now decoupled in Eq. (17). The spin-wave part is a simple Gaussian theory and the corresponding partition function $Z_{\rm sw}$ can be evaluated exactly. The second part, describing the vortices, $Z_{\rm v}$ is much harder but it can be understood perturbatively in the limit $y \to 0$. In particular, under this form (17), it is possible to compute the correlation function in Eq. (2), in perturbation, for small y (the computation is a bit cumbersome and we refer the interested reader to the original paper Ref. [2] or to the more recent textbook [3] for details)

$$C(\mathbf{r}) \underset{r\gg a}{\approx} \left(\frac{r}{a}\right)^{-\frac{1}{2\pi K_{\rm eff}}} \ , \ \frac{1}{K_{\rm eff}} = \frac{1}{K} + 4\pi^3 y^2 \int_a^L \frac{dr}{a} \left(\frac{r}{a}\right)^{3-2\pi K} \ . \tag{18}$$

1. Argue that this perturbation theory is well defined for $K > K_c = 2/\pi$. What is the physical origin of this critical temperature K_c?

   To make sense of this perturbation theory for $K \geq K_c$ requires a renormalisation group (RG) analysis which is conveniently performed in real space as follows.

2. We introduce $b > 1$ and split the integral in the right hand side of (18) as $\int_a^L dr \ldots = \int_a^{ba} dr \ldots + \int_{ba}^L dr \ldots$. We thus define $K' \equiv K(ba)$ as

$$K'^{-1} = K^{-1} + 4\pi^3 y^2 \int_a^{ba} \frac{dr}{a} \left(\frac{r}{a}\right)^{3-2\pi K} \ . \tag{19}$$

   Show that if we define $y' \equiv y(ba)$ as

$$y' = b^{2-\pi K} y \tag{20}$$

   then the relation in Eq. (18) can be written (to lowest order in y) as

$$\frac{1}{K_{\rm eff}} = \frac{1}{K'} + 4\pi^3 y'^2 \int_{\tilde{a}}^L \frac{dr}{\tilde{a}} \left(\frac{r}{\tilde{a}}\right)^{3-2\pi K'} \ , \ \tilde{a} = ba \ . \tag{21}$$

   Therefore, K' in (19) and y' in (20) appear as the effective parameters of the theory with an effective lattice spacing $\tilde{a} = ba > a$ (where "high-energy modes" have been integrated out).

3. We now consider an infinitesimal RG transformation where $b = 1 + \delta l$, with $\delta l \ll 1$. Show that the running couplings $K \equiv K(l)$ and $y \equiv y(l)$ satisfy the RG equations (to lowest order in y)

$$\frac{d}{dl} K^{-1} = 4\pi^3 y^2 \ , \ \frac{d}{dl} y = (2 - \pi K) y \ . \tag{22}$$

4. What are the fixed points of this RG flow (22) in the (K^{-1}, y) plane? Discuss their stability.

5. We now study the RG flow in the vicinity of $K_c = 2/\pi$ and set $K^{-1} = \pi/2 + x$, with $x \ll 1$. Show that, to lowest order in x and y, the RG equations (22) read

$$\frac{dx}{dl} = 4\pi^3 y^2 \ , \ \frac{dy}{dl} = \frac{4}{\pi} x y \ . \tag{23}$$

6. Deduce from (22) that the RG trajectories in (K^{-1}, y) plane, in the vicinity of $(K^{-1} = \pi/2, y = 0)$, are hyperbolas of equations

$$x^2 - \pi^4 y^2 = \kappa \ , \tag{24}$$

where κ is a real constant (positive or negative). Plot a few trajectories, as well as the curve corresponding to the "initial" physical XY Hamiltonian, corresponding to $y(0) = e^{-\pi^2 K(0)/2}$. Explain graphically when the phase transition occurs.

References

[1] J. M. Kosterlitz, D. J Thouless, *Ordering, metastability and phase transitions in two-dimensional systems*, J. Phys. C: Solid State Phys. **6**, 1181 (1973).

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[3] M. Kardar, *Statistical physics of fields*, Cambridge University Press (2007).