Notes on the KosterlitzThouless transition

W. Zhu[1]

[1] *Westlake Institute of Advanced Study,*

Westlake University, Hangzhou, P. C. China

Contents

Copyright by Wei Zhu

The XY model is described through a classical hamiltonian

$$H = -J \sum_{<i,j>} \mathbf{S}_i \cdot \mathbf{S}_j = -J \sum_{<i,j>} \cos\left[\theta_i - \theta_j\right] , \tag{1}$$

where the sum is over all pairs of nearest neighbors, *i.e.* bonds on the square lattice. In the second form of the hamiltonian, we took advantage of the $O(2)$ symmetry (hence the XY name - spins lie in the XY plane), such that $\mathbf{S}_i = (\cos\theta_i, \sin\theta_i)$. Owing to the ferromagnetic interaction J, at $T = 0$, the system would be in an ordered state where $\theta_i = \theta_0$ for all i. What is the fate of such a state in the presence of thermal fluctuations?

The Mermin-Wagner theorem states that ”in $d \leq 2$, no stable ordered phase at finite temperature can exist if the system is invariant under a continuous symmetry”. So, there is no long-range order in the 2D XY model. This is probably disappointing, as in the Ising model in 2D, where spins can only take the discrete values $\sigma_i = \pm 1$, an exact solution by Onsager shows that there is a critical temperature $T_c = 2J/\log(1+\sqrt{2})$. Below this temperature there is long-range order.

The feat of Berezinskii, Kosterlitz and Thouless in the late 1970s was to show that XY model instead shows quasi-long-range order, and to point out directly the mechanism by which this ordered phase sets in. This transition is peculiar - it does not fall in any second or first order universality class. Instead, it is referred as an infinite-order phase transition.

Copyright by Wei Zhu

ALGEBRAIC ORDER IN THE 2D XY MODEL

In a low-temperature expansion, the angle difference between two spins will be small: $|\theta_i - \theta_j| \ll 2\pi$. In this small fluctuation regime, we can approximate the cosine term in the hamiltonian to extract the long-range behavior.

$$\begin{aligned} H &= -J \sum_{<i,j>} \cos\left(\theta_i - \theta_j\right) \\ &= -JN + \frac{J}{2} \sum_{<i,j>} \left(\theta_i - \theta_j\right)^2 \\ &= E_0 + \frac{J}{4} \sum_{\mathbf{r},\mathbf{a}} (\theta(\mathbf{r}+\mathbf{a}) - \theta(\mathbf{r}))^2 \\ &\simeq E_0 + \frac{J}{2} \int d^2r (\nabla\theta(\mathbf{r})^2 \ . \end{aligned} \tag{2}$$

In the last line, we have taken the continuum limit, and replaced the field θ_i by a continuous one, $\theta(\mathbf{r})$, as slowly varying function of $\mathbf{r}$. From this, we can extract a lot of information about the magnetization and correlation functions.

Average magnetization

We calculate the average magnetization in the x direction for the 2D XY model (y is identical). We have:

$$\langle S_x \rangle =< \cos\theta(\mathbf{r}) >=< \cos\theta(0) > \tag{3}$$
$$= \frac{Tr_{\{\theta_i\}} \cos\theta(0) e^{-\beta H}}{Tr_{\{\theta_i\}} e^{-\beta H}} \tag{4}$$
$$= Re\left(\frac{1}{\mathcal{Z}} \int \mathcal{D}[\theta_i] e^{-\beta H + i\theta(0)}\right) \tag{5}$$

where $\mathcal{Z}$ is the partition function $Tr_{\{\theta_i\}} e^{-\beta H}$, and in the first line, we took advantage of translation invariance to set the spin at site $\mathbf{r} = 0$. In order to calculate that expression, we Fourier transform the θ variable, with periodic boundary conditions. We then have

$$\theta(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \theta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \ , \tag{6}$$
$$\theta(\mathbf{r} = 0) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \theta_{\mathbf{k}} \tag{7}$$

This leads to, after Gaussian integral:

$$< S_x >= \exp\left(-\frac{T}{2J} I_d(L)\right) \ , \tag{8}$$

with $I_d(L)$ a geometric factor written as

$$I_d(L) = S_d \int_{\pi/L}^{\pi/a} dk k^{d-3} = \begin{cases} L^{2-d}, d < 2 \\ \ln\left(\frac{L}{a}\right), d = 2 \\ \frac{1}{d-2}\left(\frac{\pi}{a}\right)^{d-2}, d > 2 \end{cases} \tag{9}$$

Therefore,

$$\langle S_x \rangle = \begin{cases} 0, d \le 2 \\ \exp(-\frac{S_d}{2Ja^{2-d}} AT), d > 2 \end{cases} \tag{10}$$

Copyright by Wei Zhu

Then, for any $T \neq 0$ and d=2, the logarithmic divergence of this geometric factor will force $< S_x >= 0$. This is directly the statement of the Mermin-Wagner theorem. Hence there can be no ordered low-temperature phase (in the conventional long-range order) in the 2D XY model.

Correlation functions

We now set on the same path, but for the spin-spin correlation function:

$$g(r) =< \exp\{i(\theta(\mathbf{r}) - \theta(0))\} >=< \frac{Tr_{\{\theta_i\}}e^{i(\theta(\mathbf{r})-\theta(0))}e^{-\beta H}}{Tr_{\{\theta_i\}}e^{-\beta H}} > \tag{11}$$

$$= e^{-\frac{1}{2}<[\theta(\mathbf{r})-\theta(0)]^2>} = e^{-<\theta^2(0)-\theta(\mathbf{r})\theta(0)>} \tag{12}$$

and

$$< \theta^2(0) - \theta(\mathbf{r})\theta(0) > = \int \frac{d^2k_1}{(2\pi)^2} \int \frac{d^2k_2}{(2\pi)^2} < \theta(k_1)\theta(k_2) > (1 - e^{i\mathbf{k_1}\cdot\mathbf{r}}) \tag{13}$$

$$= T \int_0^\Lambda \frac{1 - e^{i\mathbf{k_1}\cdot\mathbf{r}}}{k^2} \tag{14}$$

$$= T\frac{1}{4\pi^2} \int_0^{2\pi} d\phi \int_0^\Lambda dk \frac{1}{k}(1 - e^{ikr\cos\phi}) = T\frac{1}{2\pi} \int_0^\Lambda dk \frac{1 - J_0(kr)}{k} \tag{15}$$

$$\approx \frac{T}{2\pi} \ln\frac{r}{a} \tag{16}$$

So

$$g(r) = e^{-\frac{T}{2\pi}\ln\frac{r}{a}} = (\frac{r}{a})^{-\eta(T)}, \eta = \frac{T}{2\pi} \tag{17}$$

and we can conclude from this that, at low-temperatures, the XY model has an quasi-long-range correlations with index η temperature dependent. This means that, at all low-temperatures, the system is critical.

Vortices and entropic argument

Vortices are topological defects of the field $\theta(\mathbf{r})$, satisfying the Laplace equation $\nabla^2\theta(\mathbf{r}) = 0$. Apart from the trivial solution to this equation ($\theta(\mathbf{r}) = 0$, the ferromagnetic ground state), there are solutions called vortices. For a single vortex situated at $\mathbf{r}_0$, the circulation loop integral around it needs to be quantized:

Copyright by Wei Zhu

$$\oint_{\mathbf{r}_0} \nabla\theta(\mathbf{r}) \cdot d\mathbf{l} = 2\pi n, \tag{18}$$

with $n < 0$ corresponding to clockwise winding vortices, and $n > 0$ to anticlockwise. Such configurations are illustrated in Fig. **??**.

Can the proliferation of these objects be the culprit for the loss of quasi-long-range order? To estimate this, we consider the cost to the free energy $\Delta F = \Delta E - T\Delta S$ of adding a free vortex a system with no vortex in it. In order to estimate the energy generated by the presence of an isolated vortex, we must first estimate $\nabla\theta$. We use our equation 18, from which we estimate that, if there is one vortex on the lattice, then $\nabla\theta = \frac{n}{r}\hat{\theta}$. Therefore, the energy difference associated with this isolated vortex is

$$\Delta E = \frac{J}{2} \int d^2r (\nabla\theta(\mathbf{r}))^2 = \pi J n^2 \int_a^L \frac{dr}{r} = \pi J n^2 \ln \frac{L}{a} \ , \tag{19}$$

with L being the linear dimension of the system. We note that is a truly continuous system, we would have to start the integral at 0. However, our integral would then be divergent. It is therefore important here to consider the fact that all of this truly takes place on a lattice, where we have a lower spatial bound to this integral, the lattice constant a.

We then calculate the entropic cost to the creation of a vortex. We have that $\Delta S = k_B \ln\Omega$, with Ω being the number of microstates that can be occupied with one vortex. Since we work on a lattice of size L^2 with a lattice constant a, this means there are $(L/a)^2$ ways to put this one vortex on the lattice. Hence, we have:

$$\Delta S = k_B \ln (L/a)^2 = 2k_B \ln L/a \ . \tag{20}$$

Hence, the cost in free energy to the creation of an isolated vortex is, in this heuristic approximation,

$$\Delta F = \Delta E - T\Delta S = (\pi J n^2 - 2k_B T) \ln \frac{L}{a} \ . \tag{21}$$

We can clearly see the following two regimes:

- For $k_B T < \pi J/2$, $\Delta F > 0$, and then isolated vortices are unfavourable. If they exist at all in the system, it will be in neutral pairs, where their effect at long distance is negated;

Copyright by Wei Zhu

- For $k_BT > \pi J/2$, $\Delta F < 0$, and then isolated vortices are favourable and proliferate.

This provides us with our first crude estimate for the KT transition: $k_BT_c = \pi J/2$. We can now say that it is the unchecked proliferation of free vortices that kills the quasi-long-range order and leads to disorder. This remarkably simple argument from Kosterlitz and Thouless is not too far from the truth; one has to include the effect of the screening of ambient vortex pairs in the system to the interaction strength J to get a faithful and complete picture. To further probe this mechanism, we need to map the spin model to that of the 2D Coulomb gas and proceed with a renormalization group analysis.

Copyright by Wei Zhu

RENORMALIZATION-GROUP ANALYSIS

Let $\mu = x, y$ label the unit vectors along the nearest-neighbor bonds on the square lattice. The partition function can be written as

$$Z = \int \prod_i \frac{d\theta_i}{2\pi} e^{\frac{J}{T}\sum_{i,\mu}\cos(\theta_i - \theta_{i+\mu})} = \int \prod_i \frac{d\theta_i}{2\pi} e^{\frac{J}{T}\sum_{i,\mu}\cos(\Delta_\mu \theta_i)} \tag{22}$$

Next we would like to introduce a Fourier transformation:

$$F(m_{i\mu}) = \frac{1}{2\pi}\int_0^{2\pi} d(\Delta_\mu\theta_i) e^{-im_{i\mu}\Delta_\mu\theta_i} e^{\frac{J}{T}\cos(\Delta_\mu\theta_i)} = I_{m_{i\mu}}(\frac{J}{T}) \tag{23}$$

where $I_\nu(x)$ is modified Bessel function. And we assume the temperature is low, $J/T \gg 1$, so we take asymphobic form: $I_\nu(x) \approx \frac{1}{\sqrt{2\pi x}} e^{-\frac{\nu^2}{2x}}$. Plugging in this form into partition function,

$$e^{\frac{J}{T}\cos(\Delta_\mu\theta_i)} \approx \sqrt{\frac{T}{2\pi J}} e^{\frac{J}{T}} \sum_{m_{i\mu=-\infty}}^{+\infty} e^{im_{i\mu}\Delta_\mu\theta_i - \frac{Tm_{i\mu}^2}{2J}} \tag{24}$$

$$Z = \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \sum_{m_{i\mu}} e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2 + i\sum_{i\mu} m_{i\mu}\Delta_\mu\theta_i} \tag{25}$$

$$= \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \sum_{m_{i\mu}} e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2 + i\sum_{i\mu} m_{i\mu}(\theta_{i+\mu} - \theta_i)} \tag{26}$$

$$= \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \sum_{m_{i\mu}} e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2 + i\sum_{i\mu}(m_{i\mu} - m_{i-\mu,\mu})\theta_i} \tag{27}$$

$$= \sum_{m_{i\mu}} \delta(\vec{\Delta}\cdot\vec{m}_i) e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2} \tag{28}$$

At the last line, we integral θ_i and give a constraint

$$\vec{\Delta}\cdot\vec{m}_i = \sum_\mu \Delta_\mu m_{i\mu} = \sum_\mu (m_{i+\mu,\mu} - m_{i\mu}) = 0 \Rightarrow \sum_\mu m_{i\mu} = 0 \tag{29}$$

which means the lattice divergence of $\vec{m}$ field of every site is zero.

Next we deal with this constraint. We introduce a dual lattice, where integer variables n defined as:

$$m_{i,x} = n_{i+\frac{x+y}{2}} - n_{i+\frac{x-y}{2}} \tag{30}$$

$$m_{i,y} = n_{i+\frac{y-x}{2}} - n_{i+\frac{x+y}{2}} \tag{31}$$

$$m_{i,-x} = n_{i-\frac{x+y}{2}} - n_{i+\frac{y-x}{2}} \tag{32}$$

$$m_{i,-y} = n_{i+\frac{x-y}{2}} - n_{i-\frac{x+y}{2}} \tag{33}$$

$$\tag{34}$$

so that one can check the above constraint $\sum_\mu m_{i\mu} = 0$ is satisfied automatically.

So we get the partition function defined on the dual lattice

$$Z = \sum_{n_i} e^{-\frac{T}{2J}\sum_{i\mu}(n_{i+\mu}-n_i)^2} \tag{35}$$

$$= \int \prod_i d\phi_i \sum_{n_i} e^{-\frac{T}{2J}\sum_{i\mu}(\phi_{i+\mu}-\phi_i)^2 - 2\pi i \sum_i \phi_i n_i} \tag{36}$$

In the last line, we used the Possion formula:

$$\sum_{n=-\infty}^{\infty} g(n) = \sum_{n=-\infty}^{\infty} \int d\phi g(\phi) e^{-2\pi i n\phi} \tag{37}$$

At this step, if we integral out ϕ field, the partition function is like $\sum_{n_i,n_j} \exp[n_i n_j \ln|\mathbf{r}_i - \mathbf{r}_j|]$ (see the above section), which is like the interaction term of 2D Coulomb gas. This term will be divergent, when $x_i = x_j$. To remove this divergence, we introduce the "core" energy of each vortex E_c, which cancels the divergence when $x_i = x_j$. Adding this term back to the action, we obtain

$$Z = \int \prod_i d\phi_i \sum_{n_i} e^{-\frac{T}{2J}\sum_{i\mu}(\phi_{i+\mu}-\phi_i)^2 - 2\pi i \sum_i \phi_i n_i} e^{-\frac{E_c}{T}\sum_i n_i^2} \tag{38}$$

where $y = e^{-\frac{E_c}{T}}$ is also called fugacity of vortices.

Copyright by Wei Zhu

Since

$$\sum_{n_i} e^{-2\pi i n_i \phi_i} y^{n_i^2} \approx 1 + 2y\cos(2\pi\phi_i) + 2y^4\cos(4\pi\phi_i) + ... \approx e^{2y\cos(2\pi\phi_i)+O(y^2)} \tag{39}$$

we can re-write the partition function as

$$\int \prod_i d\phi_i e^{-\frac{T}{2J}\sum_{i\mu}(\phi_{i+\mu}-\phi_i)^2+2y\sum_i\cos(2\pi\phi_i)} \tag{40}$$

where ϕ_i is dual or disorder variable. ϕ_i are ordered at high T and disordered at low T (opposite to θ_i). In the continuum limit, it is

$$Z = \int D\phi e^{-\int d^2x[\frac{T}{2J}(\nabla\phi)^2+2y\cos(2\pi\phi)]} \tag{41}$$

This is the sin-Gordon model, which is dual to the XY model.

RG flow equations

We separate the fast and slow modes $\phi = \phi_< + \phi_>$, and $\phi_<$ contains only the Fourier components with $k < \Lambda/b$. The partition function becomes

$$Z = \int D\phi_< D\phi_> e^{-\int d^2x[\frac{T}{2J}(\nabla\phi_<)^2+(\nabla\phi_>)^2} e^{2y\int d^2x\cos(2\pi(\phi_<+\phi_>))]} \tag{42}$$

$$\approx \int D\phi_< D\phi_> e^{-\int d^2x[\frac{T}{2J}(\nabla\phi_<)^2+(\nabla\phi_>)^2}\times$$
$$[1+2y\int d^2x\cos(2\pi(\phi_<+\phi_>))+2y^2\int d^2x\int d^2x'\cos(2\pi(\phi_<(x)+\phi_>(x)))\cos(2\pi(\phi_<(x')+\phi_>(x')))]]$$
$$= Z_< \int D\phi_> e^{-\int d^2x\frac{T}{2J}(\nabla\phi_>)^2}[1+2y\int d^2x\cos(2\pi\phi_<)\langle\cos(2\pi\phi_>)\rangle_> +$$
$$2y^2\int d^2x\int d^2x'\cos(2\pi\phi_<(x))\cos(2\pi\phi_<(x')))\langle\cos(2\pi\phi_>(x)\cos(2\pi\phi_>(x'))\rangle_> +$$
$$2y^2\int d^2x\int d^2x'\cos(2\pi\phi_<(x))\cos(2\pi\phi_<(x')))\langle\sin(2\pi\phi_>(x)\sin(2\pi\phi_>(x'))\rangle_>] \tag{43}$$

Defining th correlation function

$$g_>(\mathbf{r}) = (2\pi)^2\langle\phi_>(\mathbf{r})\phi_>(0)\rangle_> \tag{44}$$

and

$$\langle\cos(2\pi\phi_>(\mathbf{r}))\rangle = e^{-\frac{1}{2}g_>(0)} \tag{45}$$

$$\langle\cos(2\pi\phi_>(\mathbf{r}))\cos(2\pi\phi_>(\mathbf{r}'))\rangle = e^{-g_>(0)}\cosh(g_<(\mathbf{x}-\mathbf{x}')) \tag{46}$$

$$\langle\sin(2\pi\phi_>(\mathbf{r}))\sin(2\pi\phi_>(\mathbf{r}'))\rangle = e^{-g_>(0)}\sinh(g_<(\mathbf{x}-\mathbf{x}')) \tag{47}$$

Copyright by Wei Zhu

The action for the slow modes is

$$S_< = \frac{T}{2J}\int d^2x(\nabla\phi_<(\mathbf{r}))^2 - 2ye^{-\frac{1}{2}g_>(0)}\int d^2x\cos(2\pi\phi(x)) - y^2e^{-g_>(0)}\int dxdy[\cos(2\pi(\phi_<(x)+\phi_<(y)))(e^{-g_>} \tag{48}$$

To the first order in fugacity, the result of the momentum shell integration gives the change of fugacity:

$$y \to y(b) = b^2ye^{-\frac{1}{2}g_>(0)} \tag{49}$$

$$g_>(0) = \frac{2\pi}{T}\int_{\Lambda/b}^{\Lambda}\frac{dk}{k} = \frac{2\pi}{T}\ln b \tag{50}$$

The renormalization of temperature derives from the second-order terms in $S_<$. Expanding $\phi_<(y)$ around x, to the leading order in gradients one can write

$$\cos(2\pi(\phi_<(x)-\phi_<(x'))) \approx 1 - \frac{1}{2}(2\pi(x'-x)\cdot\nabla\phi_<(x))^2 \tag{51}$$

$$\cos(2\pi(\phi_<(x)+\phi_<(x'))) \approx \cos(4\pi\phi_<(x)) - 2\pi\sin(4\pi\phi_<(x))((x'-x)\cdot\nabla\phi_<(x)) \tag{52}$$

Then we got

$$T \to T(b) = T + 2\pi^2y^2e^{-g_>(0)}\int d^2x(e^{g_>(x)}-1)x^2 \tag{53}$$

$$g_>(x) = \frac{1}{T}\int_{\Lambda/b}^{\Lambda}\frac{dk}{k}\int_0^{2\pi}d\alpha e^{ikx\cos(\alpha)} = \frac{2\pi}{T}\ln bJ_0(\Lambda x) \tag{54}$$

Here we need treat this integral carefully.

$$g_>(x) = \int_0^{\Lambda}\frac{d^2qe^{i\mathbf{q}\cdot\mathbf{x}}}{Tq^2} - \int_0^{\Lambda/b}\frac{d^2qe^{i\mathbf{q}\cdot\mathbf{x}}}{Tq^2} \tag{55}$$

$$\approx \frac{2\pi}{T}\left(\int_0^{\infty}dq\frac{qJ_0(qx)}{q^2+(\Lambda/b)^2} - \int_0^{\infty}dq\frac{qJ_0(qx)}{q^2+(\Lambda)^2}\right) \tag{56}$$

$$= \frac{2\pi}{T}(K_0(x\Lambda/b) - K_0(x\Lambda)) \qquad = -\frac{2\pi x\Lambda\ln b}{T}\frac{dK_0(z)}{dz}\bigg|_{z=x\Lambda} \tag{57}$$

$$T \to T(b) = T - 2\pi^2y^2\ln b\int d^2xx^2\frac{2\pi x\Lambda}{T}\frac{dK_0(z)}{dz}\bigg|_{z=x\Lambda} \tag{58}$$

$$= T + \frac{1}{2T}\left(\frac{y(4\pi)^2}{\Lambda^2}\right)^2\ln b \tag{59}$$

Copyright by Wei Zhu

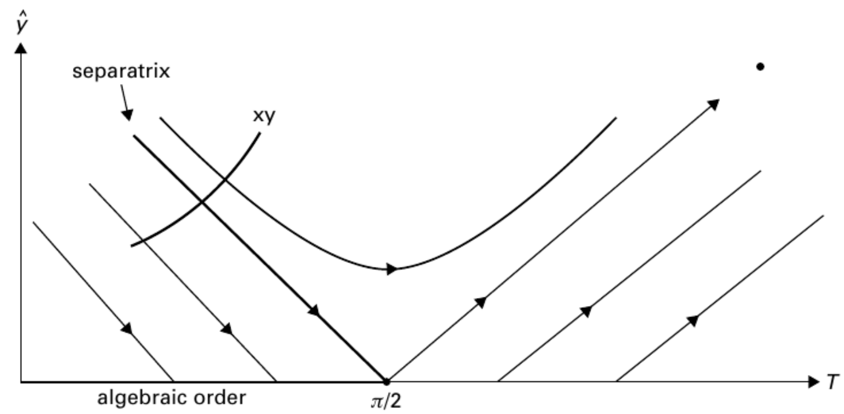

FIG. 1: Renormalization group flow of the temperature and the fugacity in the sine-Gordon model. The thick line separates the flows towards the line of fixed points at $T < T_{KT}$ and $y = 0$ that represent the algebraically ordered superfluid phase from the flow towards a high-temperature high-fugacity sink, representing the exponentially disordered phase. The XY line represents the set of initial values at different temperatures in the XY model.

Define $y = \frac{y(4\pi)^2}{\Lambda^2}$, the flow of couplings in the sine-Gordon theory becomes

$$\begin{aligned} \frac{dT}{d\ln b} &= y^2/2T + O(y^4) \ , \\ \frac{dy}{dl} &= (2 - \pi/T)y + O(y^3) \ , \end{aligned} \tag{60}$$

The critical point is $T_{KT} = \pi/2$. As shown in Figure, in low temperature regime $T < T_{KT}$, the fixed point line relates to $y^* = 0$. $y \to 0$ means vainishing probability to find vortices, or no free vortices in the system. All vortices form vortex-anti-vortices pairs. When $T > T_{KT}$, free vortices appear.

Copyright by Wei Zhu