Advanced Statistical Mechanics

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Week 14: XY model at $d = 2$. Kosterlitz-Thouless transition
1 XY model at $d = 2$ at low temperature

All that was said about the low temperature behavior of the $d > 2$ XY model translates to $d = 2$. The only correction is, we need to recalculate the inverse of the Laplacian in 2D. This gives

$$
\hat{O}^{-1}(r) = \frac{1}{K} \int \frac{d^2p}{(2\pi)^2} e^{ipr}.
$$

(1.1)

This integral formally is divergent at $p \to 0$. Again, we need to recall that this integral is an approximation of really happens. In practice, we are on a lattice of lattice spacing $a$, and the system has a finite size $L$. This means, the momentum magnitude $p$ cannot be smaller than $1/L$ (and larger than $\pi/a$). Then the integral, being taken over finite limits of integration, is convergent. But of course, it’s not easy to compute.

We compute it in the following clever way. Apply a Laplacian to the coordinate $r$ in (1.1). This gives

$$
\Delta \hat{O}^{-1}(r) = -\frac{1}{K} \int \frac{d^2p}{(2\pi)^2} e^{ipr} = -\frac{\delta(r)}{K}.
$$

(1.2)

In other words, the quantity we would like to calculate satisfies the equation for the potential of a charge of size $-1/K$ in a 2D space. This should always be solved using Gauss theorem, or first we find the “electric field”, whose 2D “flux” gives us $-1/K$:

$$
E \cdot (2\pi r) = -\frac{1}{K}.
$$

(1.3)

The potential is the integral of the field, or

$$
\hat{O}^{-1} = -\frac{\ln r}{2\pi K} + \text{const}.
$$

(1.4)

This cannot be the full answer though, because $\ln r$ makes no sense (in other words, there is some “const” we need to determine). We note that if $r \to a$, the integral we are computing reduces to

$$
\frac{1}{K} \int_{p=1/a}^{p=1/L} \frac{dp}{2\pi p} = \frac{1}{2\pi K} \ln \left[ \frac{L}{a} \right].
$$

(1.5)

Matching this gives

$$
\hat{O}^{-1} = \frac{1}{2\pi K} \ln \left( \frac{L}{r} \right).
$$

(1.6)

This gives for the correlation function

$$
\langle \cos(\phi(r_1) - \phi(r_2)) \rangle = e^{\frac{1}{2\pi K} \left( -\ln \frac{L}{a} + \ln \left\| \frac{L}{r_1 - r_2} \right\| \right)} = \frac{a^{\frac{1}{2\pi K}}}{\left\| r_1 - r_2 \right\|^{\frac{1}{2\pi K}}}. \tag{1.7}
$$

The correlation function decays to zero at large distances. Thus there is no long range order, as one should expect.
2 XY model at $d = 2$: vortices

There is no long range order, but the correlation function does look strange. It does not decay exponentially as one might expect, but as a power low. This received the name of “algebraic order” in the literature. There is no order, but no genuine disorder either. As temperature is raised ($K$ is decreased), the correlation function starts decaying faster, but it never decays exponentially.

Kosterlitz and Thouless proved that as temperature is raised, the XY model undergoes a novel type of a transition. At temperatures above the Kosterlitz-Thouless temperature, the correlation function decays exponentially, not algebraically.

To catch this transition, they observed that even when the temperature is not that high so that $\phi$ on the nearby sites are almost the same, sometimes $\phi$ on the nearby sites can be different by $2\pi$. This costs no energy, but then we cannot expand the cosine. In fact, there are configurations, vortices, such that as one goes around the vortex $\phi$ changes by $2\pi$. This does not cost any energy except at the “core” of the vortex, close to its center, where $\phi$ changes very rapidly from 0 to $2\pi$ as one goes around the center of the vortex. But this energy could be thought as finite.

We can split the function $\phi(r)$ into a “smooth” part, and a part which changes by $2\pi$ as we go around certain points, the centers of vortices.

$$\phi(r) = \varphi(r) + v(r),$$

where $v(r)$ is the “vortex part” and $\varphi(r)$ is a “smooth” part. This splitting can be done in many different ways even if the positions of vortices are fixed. We can uniquely do the splitting if we demand that

$$\Delta v = 0.$$ (2.3)

Indeed, $\int (\nabla \phi)^2$ then decomposes into this sum, up to a cross-term $\int \nabla \varphi \nabla v$. This term can be taken by parts, to give $\int \varphi \Delta v$, which is zero by construction.

Suppose $v$ is such “harmonic” function (satisfying the Laplace equation), which changes by $2\pi$ if we go around points $r_k$, $k = 1, 2, \ldots, n$, where $n$ is the number of vortices. Then
it is very easy to find. Namely, introduce complex coordinates $z_k$. These are complex representations of the two-dimensional vector $r_k$. Real part of $z$ is the horizontal component of $r$, and imaginary part of $z$ is the vertical component of $r$. Then

$$v = -i \text{Im} \sum_k \sigma_k \ln (z - z_k). \quad (2.4)$$

Indeed, the logarithm is an analytic function, that is, it satisfies the Laplace equation. In other words, $v(r)$ is the sum of the 2D angles, formed by a point $r$ with the points $r_k$, the centers of vortices. Here $\sigma_k$ takes values either +1 or −1, to give either a clockwise, or counterclockwise vortex.

Suppose we have one such vortex. Let us calculate its energy, or

$$\frac{K}{2} \int d^2 r \left( \nabla v \right). \quad (2.5)$$

For this we need to know the result of applying a gradient to a function such as $-i \text{Im} \ln$. This is easy: it is a vector which is pointing along circles surrounding a vortex, whose magnitude is

$$\frac{1}{|r - r_0|},$$

where $r_0$ is the position of the vortex. Knowing this allows us to conclude that

$$\frac{K}{2} \int d^4 r \left( \nabla v \right)^2 = \frac{K}{2} \int d^4 r \frac{1}{(r - r_0)^2}. \quad (2.7)$$

This integral can be reduced to

$$\frac{K}{2} \int \frac{2\pi r dr}{r^2} = \pi K \ln \frac{L}{a}. \quad (2.8)$$

$L$ is the size of the system, and $a$ is the lattice spacing. This expression allows us to stay whether vortices are generally present or not: the energy cost of having a vortex is given above, but the entropy, or the logarithm of the number of ways to put a vortex on the lattice is $\ln[(L/a)^2] = 2 \ln[L/a]$. The free energy is then (recall that $K = J/T$, and what we calculated above is the ratio of energy to temperature)

$$F = E - TS = \pi J \ln \frac{L}{a} - 2T \ln \frac{L}{a}. \quad (2.9)$$

If $T > \frac{\pi J}{2}$, or if $K < \frac{2}{\pi}$, then vortices proliferate (free energy of inserting a vortex is negative). So we expect that the analysis of the previous section, where we found the algebraic order, is only valid at $K > \frac{2}{\pi}$. This is the famous Kosterlitz-Thouless argument. Amazingly (despite being so crude), it predicts the transition temperature correctly.
3 The phase with vortices

We still need to determine what happens once we have many vortices. We write \( v \) according to (2.4) and substitute into the expression for the energy (now not just one vortex but many). This however is a very difficult calculation. To make it easier, we introduce the so-called “dual” field \( \theta(\mathbf{r}) \). The dual field is such that its gradient is perpendicular to the gradient of \( v \). It can be written as

\[
\theta = -\sum_k \sigma_k \ln \frac{L}{|\mathbf{r} - \mathbf{r}_k|}.
\]  

(3.1)

It is straightforward to see that

\[
\nabla \theta = \nabla v.
\]  

(3.2)

So we see that

\[
\frac{K}{2} \int d^2r \ (\nabla v)^2 = \frac{K}{2} \int d^2r \ (\nabla \theta)^2.
\]  

(3.3)

We can then take the integral by parts and find

\[
-\frac{K}{2} \int d^2r \ \theta \Delta \theta.
\]  

(3.4)

Now \( \Delta \theta \) is easy. We already know that the logarithm is the potential of a charge in 2D. So the Laplacian of a potential is a delta function. More precisely, as follows from (1.4),

\[
\Delta \ln r = 2\pi \delta(\mathbf{r}).
\]  

(3.5)

So

\[
\Delta \theta = 2\pi \sum_k \delta(\mathbf{r} - \mathbf{r}_k).
\]  

(3.6)

Then

\[
\frac{K}{2} \int d^2r \ v(\nabla v)^2 = -\frac{K}{2} \int d^2r \ \theta \Delta \theta = \pi K \sum_{kl} \sigma_k \sigma_l \ln \frac{L}{|\mathbf{r}_k - \mathbf{r}_l|}.
\]  

(3.7)

Armed with this expression we can write down the partition function in the following way. It is given by the integral over all “smooth” functions \( \varphi \) and integral over all positions over vortices plus the sum over all possible number of vortices. This gives

\[
Z = \int \mathcal{D}\varphi \ e^{-\frac{K}{2} \int d^2r(\nabla \varphi)^2} \sum_{n=0}^{\infty} \frac{1}{n!} \left[ \prod_{m=1}^{n} \frac{d^2r_m}{a^2} \right] \sum_{\sigma_{1} \pm 1} e^{-\pi K \sum_{kl} \sigma_k \sigma_l \ln \frac{L}{|\mathbf{r}_k - \mathbf{r}_l|}}.
\]  

(3.8)

1/\( n! \) appears because we do not want to overcount vortices: integrating over their positions counts vortex configurations \( n! \) times too many.
To make further progress in calculating the partition function, we now use the following representation we learned about previously:

\[
e^{-\pi K \sum_{k,l} \sigma_k \sigma_l \ln \frac{1}{|r_k - r_l|}} = \frac{\int \mathcal{D}\theta \, e^{-\frac{1}{8\pi K} \int d^2r (\nabla^2 \theta)^2 + i \sum_{k=1}^n \sigma_k \theta(r_k)}}{\int \mathcal{D}\theta \, e^{-\frac{1}{8\pi K} \int d^2r (\nabla^2 \theta)^2}}. \tag{3.9}
\]

This came from our prior calculations. Indeed, the integral in the numerator on the right is the Gaussian integral. Computed according to the rules of Gaussian integration, which we already invoked last week, reproduces the expression on the left.

We can plug this into the previous expression, to find

\[
Z = \frac{\int \mathcal{D}\varphi \, e^{-\frac{K}{2} \int d^2r (\nabla \varphi)^2} \sum_{n=0}^\infty \frac{1}{n!} \prod_{m=1}^n \frac{d^2r_m}{a^2}}{\int \mathcal{D}\theta \, e^{-\frac{1}{8\pi K} \int d^2r (\nabla^2 \theta)^2 + i \sum_{k=1}^n \sigma_k \theta(r_k)}}. \tag{3.10}
\]

We can now sum over \(\sigma\) and then actually sum over \(n\), with the result

\[
Z = \frac{\int \mathcal{D}\varphi \, e^{-\frac{K}{2} \int d^2r (\nabla \varphi)^2} \sum_{n=0}^\infty \frac{1}{n!} \prod_{m=1}^n \frac{d^2r_m}{a^2}}{\int \mathcal{D}\theta \, e^{-\frac{1}{8\pi K} \int d^2r (\nabla^2 \theta)^2 + i \sum_{k=1}^n \sigma_k \theta(r_k)}} \int \mathcal{D}\theta \, e^{-\frac{1}{8\pi K} \int d^2r (\nabla^2 \theta)^2 + \frac{2}{a^2} \int d^2r \cos(\theta)}. \tag{3.11}
\]

Now we introduce a variable \(\lambda = 2/a^2\). Right now it is just equal to \(2/a^2\), but in the future, its value may change so we call it \(\lambda\). With its help we find

\[
Z = \int \mathcal{D}\theta \, e^{-\frac{1}{8\pi K} \int d^2r (\nabla^2 \theta)^2 + \lambda \int d^2r \cos(\theta)}. \tag{3.12}
\]

(The Gaussian integrals on the left can be omitted because they are not interesting - more precisely they actually cancel each other, although it takes extra work to see that).

What we obtained is an interesting expression. If \(\lambda = 0\), it is at its critical point. \(\lambda \neq 0\) is a perturbation of a theory about its fixed point. If this is an irrelevant perturbation, then the theory is at a fixed point, the correlation functions are power laws, and the theory is not affected by the presence of vortices (that is, it still has long range algebraic order). But if \(\lambda\) is relevant, the theory acquires a correlation length and becomes truly disordered.

We need to deduce if \(\lambda\) is relevant or not. For that, we calculate the correlation function

\[
\langle e^{i\theta(r_1) - i\theta(r_2)} \rangle = \left(\frac{a}{|r_1 - r_2|}\right)^{2\pi K}. \tag{3.13}
\]

The RG dimension of \(\cos(\theta)\) is half of the power which appears in the correlation function. It is equal to \(x = \pi K\). Now we now that the RG dimension of the coupling \(\lambda\) is \(y = d - x = 2 - \pi K\). If \(y > 0\), then the perturbation is relevant and we are in the truly disordered
phase with exponentially decaying correlators. This corresponds to $K < 2/\pi$, just as we expected. $K_c = \frac{2}{\pi}$ corresponds to the Kosterlitz-Thouless transition.

If $K > 2/\pi$, then we are in the fixed point phase with algebraically decaying correlators.

Finally, we can write down the RG equations which follow from these arguments. One is

$$\frac{\partial \lambda}{\partial \ell} = \left(2 - \pi K\right)\lambda = 2\lambda - \pi K\lambda. \quad (3.14)$$

However, $K$ also flows under the renormalization group. To understand how, it is easiest to recognize that $C_{\lambda K \lambda} = \pi/2$. This means that

$$\frac{\partial K}{\partial \ell} = -\frac{\pi}{2}\lambda^2. \quad (3.15)$$

These two sets of equations provide us with all the information we need to know about the Kosterlitz-Thouless transition. They are carefully studied in J. Cardy’s book, chapter 6.4.