Lecture 12: Berezinskii-Kosterlitz-Thouless transition

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In two dimensions, continuous spin models cannot have magnetically ordered state. (Mermin-Wagner theorem)

The XY model, however, has a strange type of phase transition that does not break the symmetry. (BKT transition)

We can understand this transition by mapping the model into the Coulomb gas model. In this mapping, the spin vortices in the XY model corresponds to charges.

By a RGT, we obtain Kosteritz’s RG flow equation, that predicts special characters of the BKT transition.
Mermin-Wagner theorem

**Theorem 1 (Mermin-Wagner(1966))**

*In two dimensions, if the system has a continuous symmetry (represented by a compact connected Lie group), it cannot be spontaneously broken at any finite temperature.* [Pfister, Commun. Math. Phys. 79 181 (1981).]

- Consider the $XY$ model in two dimensions:
  \[ H = -K \sum_{(ij)} \mathbf{S}_i \cdot \mathbf{S}_j = -K \sum_{(ij)} \cos(\theta_i - \theta_j) \]
  where $\mathbf{S}_i \equiv (\cos \theta_i, \sin \theta_i)^T$.

- The $XY$ model has the $U(1)$ symmetry with respect to the transformation $\theta_i \to \theta_i + \alpha$.

- Does the theorem prohibit the phase transition in the $XY$ model?
Berezinskii-Kosterlitz-Thouless transition

- A theoretical proposal of a new type of phase transition without spontaneous symmetry breaking. (Berezinskii (1971), Kosterlitz-Thouless (1973))

- Later the predicted transition was discovered in a thin film experiment of superfluid He4. (Bishop-Reppy (1978))
Vortices

- A typical configuration of 2-component spins near or below the transition temperature consists of a smooth texture with vortices.
- The smooth texture allows the approximation,

\[ \cos(\theta_i - \theta_j) \approx 1 - \frac{1}{2} |\mathbf{r}_{ij} \cdot \nabla \theta|^2 \]

- Therefore, we expect that the Hamiltonian is

\[ \mathcal{H} = -K a^d \sum_{(ij)} \cos(\theta_i - \theta_j) \]

\[ \approx \frac{K}{2} \int d\mathbf{x} |\nabla \theta|^2 + \mu N_v \]

where \( N_v \) is the total number of vortices.
Here we introduce a new field variable $\phi$ that is the deviation of $\theta$ from its stationary solution $\Theta$ for a given vortex configurations:

$$\theta = \Theta + \phi.$$ 

The configuration $\Theta$ is determined by the stationary condition, and it is a harmonic function.

$$0 = \delta E = \frac{K}{2} \int d\mathbf{x} \left\{ |\nabla (\Theta + \delta \Theta)|^2 - |\nabla \Theta|^2 \right\}$$

$$= K \int d\mathbf{x} \nabla \Theta \cdot \nabla \delta \Theta = -K \int d\mathbf{x} \Delta \Theta \delta \Theta$$

$$\Rightarrow \Delta \Theta = 0 \quad (\text{Except at vortices})$$

Note that $\Theta$ can be uniquely determined by the vortex configuration.
Vortex/fluctuation separation

Using $\Theta$, we can separate the vortices from the Gaussian fluctuation:

$$\mathcal{H} = \frac{K}{2} \int d\mathbf{x} \left| \nabla (\Theta + \phi) \right|^2 + \mu N_v = \mathcal{H}_v + \mathcal{H}_G.$$

where

$$\mathcal{H}_v \equiv \frac{K}{2} \int d\mathbf{x} \left| \nabla \Theta \right|^2 + \mu N_v$$

$$\mathcal{H}_G \equiv \frac{K}{2} \int d\mathbf{x} \left| \nabla \phi \right|^2$$

(Note that the term $\nabla \phi \cdot \nabla \Theta$ does not contribute because of the stationary condition for $\Theta$.)
Vortex field $\Omega$

- Since $\Theta$ is a harmonic function, another harmonic function $\Omega$ must exist such that $\frac{\partial \Omega}{\partial x} = -\frac{\partial \Theta}{\partial y}$, and $\frac{\partial \Omega}{\partial y} = \frac{\partial \Theta}{\partial x}$.

- Suppose a region $\Gamma$ that includes a vortex.

\[
I \equiv \oint_{\partial \Gamma} d\mathbf{l} \cdot \nabla \Theta = 2\pi q \quad (q = \pm 1, \pm 2, \cdots)
\]

- Since $d\mathbf{l} \cdot \nabla \Theta = -d\mathbf{n} \cdot \nabla \Omega$,

\[
\int_{\Gamma} d\mathbf{x} \Delta \Omega = \int_{\partial \Gamma} d\mathbf{n}(\mathbf{x}) \cdot \nabla \Omega = -I = -2\pi q \quad (\because \text{Gauss’ theorem})
\]

- Remembering that $\Delta \Omega = 0$ almost everywhere,

\[
\Delta \Omega = -\sum_{i} 2\pi q_i \delta(\mathbf{x} - \mathbf{x}_i) = -2\pi \rho_v(\mathbf{x})
\]
Coulomb gas (1)

- Using Green’s function, \( G(x) \), that satisfies \( \nabla^2 G(x) = -\delta(x) \), we can express \( \Omega \) as

\[
\Omega(x) = 2\pi \int d\mathbf{y} G(x - \mathbf{y}) \rho_v(\mathbf{y}).
\]

- The vortex part in \( \mathcal{H}_v \) can be reformed as

\[
\frac{K}{2} \int d\mathbf{x} |\nabla \Theta|^2 = \frac{K}{2} \int d\mathbf{x} |\nabla \Omega|^2
\]
\[
= -\frac{K}{2} \int d\mathbf{x} \Omega \nabla \Omega = \pi K \int d\mathbf{x} \Omega \rho_v
\]
\[
= 2\pi^2 K \int d\mathbf{x} d\mathbf{y} G(\mathbf{x} - \mathbf{y}) \rho_v(\mathbf{x}) \rho_v(\mathbf{y})
\]
\[
= 4\pi^2 K \sum_{(ij)} \chi_{(i)}(\mathbf{x}_i - \mathbf{y}_i) q_i q_j
\]
Coulomb gas (2)

- Here we introduce the ultra-violet cut-off in the form of the constraint (on the region of the integral with respect to the vortex positions) that no two vortices can be within the mutual distance of \( a \).

- Using

\[
G(r) \approx -\frac{1}{2\pi} \log r
\]

and the charge neutrality condition (\( \sum_i q_i = 0 \)),

\[
\mathcal{H}_v = -2\pi K \sum_{(ij)} \log \frac{|x_i - x_j|}{\Lambda} q_i q_j + \mu N_v \quad (\Lambda \text{ is arbitrary})
\]

Vortices form a Coulomb-gas.

- In what follows, we assume that $q_i = \pm 1$ since vortices $|q_i| > 1$ are energetically unfavorable and would not yield dominant contribution.
- $X_N \equiv (x_1, x_2, \cdots, x_N)$ and $Y_N \equiv (y_1, y_2, \cdots, y_N)$ are the positions of positive and negative vortices, respectively.
- Then, the grand partition function is

$$
\Xi(\zeta, g) = \sum_N \frac{\zeta^{2N}}{(N!)^2} Z_N^a(g) \quad (\zeta \equiv e^\mu)
$$

$$
Z_N^a(g) \equiv \int_{\Omega(a)} dX_N dY_N e^{-g V_N(X_N, Y_N)} \quad (g \equiv 2\pi K)
$$

$$
\Omega(a) \equiv \{ (X_N, Y_N) | \text{Any two elements are apart by more than } a \}
$$

$$
V_N(X_N, Y_N) \equiv -\sum_{(ij)} (\nu(x_i, x_j) + \nu(y_i, y_j)) + \sum_{ij} \nu(x_i, y_j)
$$

$$
\nu(x, y) \equiv \log(|x - y|/\Lambda)
$$
Partial trace — Increasing the cut-off $a$

- Following the general program of the RGT, we first want to take the partial trace with respect to the short-scale degrees of freedom.
- We take the partial integral over the region $\Delta \Omega(a) \equiv \Omega(a) - \Omega(\dot{a})$ where $\dot{a} \equiv (1 + \lambda)a$.
- The region consists of 3 components:

$$\Delta \Omega(a) \approx \sum_{ij} \Omega_{ij}^{+-}(\dot{a}) + \sum_{(ij)} (\Omega_{ij}^{++}(\dot{a}) + \Omega_{ij}^{--}(\dot{a}))$$

$$\Omega_{ij}^{+-}(\dot{a}) \equiv \{ (X_N, Y_N) \in \Omega(a) \mid$$

All pairs are separated by more than $\dot{a}$, except $a < |x_i - y_j| < \dot{a}$. $\}$

$$\Omega_{ij}^{++}(\dot{a}) \equiv \cdots$$
Partial trace — Dipole-mediated interaction

The contribution from $\Omega^{+-}$ should be dominant.

\[ Z_N^a - Z_N^\alpha \approx \sum_{ij} \int_{\Omega_{ij}^{+-}(\alpha)} dX_N dY_N e^{-gV_N} = N^2 \int_{\Omega_{NN}^{+-}(\alpha)} dX_N dY_N e^{-gV_N} \]

\[ = N^2 \int_{\Omega(\alpha)} dX_{N-1} dY_{N-1} e^{-gV_{N-1}} \int_{a<|x_N-y_N|<\hat{a}} dX_N dY_N e^{-g \sum_i [\Delta v(x_i) - \Delta v(y_i)]} \]

\[ (\Delta v(x_i) \equiv v(x_i, x_N) - v(x_i, y_N)) \]

\[ \approx N^2 \int_{\Omega(\alpha)} dX_{N-1} dY_{N-1} e^{-gV_{N-1}} \]

\[ \times \int_{a<|x_N-y_N|<\hat{a}} dX_N dY_N \left\{ 1 + \frac{g^2}{2} \left( \sum_{i=1}^{N-1} (\Delta v(x_i) - \Delta v(y_i)) \right)^2 \right\} \]

\[ \approx \left( \frac{\pi a^2}{\lambda} \right) + \frac{4\pi^2 a^4 \lambda g^2 V_{N-1}}{2} \]

(contribution to the regular part is omitted)
Partial trace — Screening effect

\[ \Xi(\zeta, g) = \sum_N \frac{\zeta^{2N}}{(N!)^2} Z_N^a(g) \]

\[ \simeq \sum_N \frac{\zeta^{2N}}{(N!)^2} \left( Z_N^a(g) + N^2 \int_{\Omega(\phi)} dX_{N-1} dY_{N-1} e^{-gV_{N-1}} \gamma g^2 \lambda V_{N-1} \right) \]

\[ (\gamma \equiv 4\pi^2 a^4; (N - 1) \rightarrow N) \]

\[ = \sum_N \frac{\zeta^{2N}}{(N!)^2} \int_{\Omega(\phi)} dX_N dY_N e^{-gV_N} (1 + \gamma g^2 \lambda \zeta^2 V_N) \]

\[ \simeq \sum_N \frac{\zeta^{2N}}{(N!)^2} \int_{\Omega(\phi)} dX_N dY_N e^{-(g - \gamma g^2 \lambda \zeta^2) V_N} \]

The 2nd order perturbation screens the Coulomb interaction
Rescaling of the interaction

We rescale the length so that $\dot{a}$ comes back to $a$.

$$\dot{x}_i = \frac{a}{\dot{a}} x_i = e^{-\lambda} x_i$$

By this replacement, the interaction becomes

$$V_N(X_N, Y_N)$$

$$= - \sum_{(ij)} \left( \log \frac{x_i - x_j}{\Lambda} + \log \frac{y_i - y_j}{\Lambda} \right) + \sum_{ij} \log \frac{x_i - y_j}{\Lambda}$$

$$= - \sum_{(ij)} \left( \log \frac{\dot{x}_i - \dot{x}_j}{\Lambda} + \log \frac{\dot{y}_i - \dot{y}_j}{\Lambda} + 2\lambda \right) + \sum_{ij} \left( \log \frac{\dot{x}_i - \dot{y}_j}{\Lambda} + \lambda \right)$$

$$= V_N(\dot{X}_N, \dot{Y}_N) + (-N(N - 1) + N^2)\lambda$$

$$= V_N(\dot{X}_N, \dot{Y}_N) + N\lambda$$
Rescaling

Now, we can summarize the RGT as

$$\Xi(\zeta, g)$$

$$= \sum_N \frac{\zeta^{2N}}{(N!)^2} e^{2dN\lambda} \int_{\Omega(a)} d\dot{X}_N d\dot{Y}_N e^{-(g-\gamma g^2 \zeta^2 \lambda)} V_N(\dot{X}_N, \dot{Y}_N) e^{-gN\lambda}$$

$$= \sum_N \frac{1}{(N!)^2} \left( \zeta e^{(d-\frac{g}{2})\lambda} \right)^{2N} \int_{\Omega(a)} dX_N dY_N e^{-(g-\gamma g^2 \zeta^2 \lambda)} V_N(X_N, Y_N)$$

$$= \Xi(\zeta', g') \times e^{(\text{regular term})}$$

where

$$\zeta' = \zeta e^{(d-\frac{g}{2})\lambda} \quad \text{and} \quad g' = g - \gamma g^2 \zeta^2 \lambda$$

In the form of differential equations,

$$\frac{d\zeta}{d\lambda} = \left( 2 - \frac{g}{2} \right) \zeta \quad \text{and} \quad \frac{dg}{d\lambda} = -\gamma g^2 \zeta^2$$
RG flow equation

It is convenient to use \( x \equiv 2 - g/2 \) instead of \( g \), and focus on the vicinity of \( x = \zeta = 0 \).

\[
\frac{d\zeta}{d\lambda} = x\zeta \quad \text{and} \quad \frac{dx}{d\lambda} = -\frac{1}{2} \frac{dg}{d\lambda} \approx 8\gamma\zeta^2
\]

We can remove the factor \( 8\gamma \) by defining \( y \equiv \sqrt{8\gamma}\zeta \):

\[
\begin{align*}
\frac{dx}{d\lambda} &= y^2 \\
\frac{dy}{d\lambda} &= xy
\end{align*}
\]

\( \left( \begin{array}{l} x = 2 - \pi K \\ y = (\text{const}) \times e^\mu \end{array} \right) \)  \quad \text{(Kosterlitz’s RG eq.)}
The constant of motion of the RG equation
\[ \frac{dx}{d\lambda} = y^2, \quad \frac{dy}{d\lambda} = xy \]
can be given by \( t \equiv y^2 - x^2 \).

The value of \( t \) depends only on the initial values of the parameter, \( \mu \) and \( K = 1/T \). Schematically, the initial points are located on the \( t \) axis.

There are two cases: \( t < 0 \) \( y \) goes to zero (no vortices) and \( t > 0 \) \( y \) goes to infinity (vortex proliferation). The separatorix, \( t = 0 \), corresponds to the BKT transition.
In the case where \( t \equiv y^2 - x^2 > 0 \), \( \frac{dx}{d\lambda} = y^2 = t + x^2 \). This equation has the solution \( x(\lambda) = \sqrt{t} \tan \left( \sqrt{t} (\lambda - \lambda_0) \right) \).

Note that \( x_0 \equiv x(0) \sim -O(1) \), and \( x(\log \xi) \sim O(1) \). (\because In the initial state, there is no reason to assume that any one of the parameter is extremely large or small. The same is true for a system with the correlation length of \( O(1) \).)

The first condition means \( \tan(\sqrt{t}\lambda_0) \sim \frac{1}{\sqrt{t}} \gg 1 \), which is satisfied only when \( \sqrt{t}\lambda_0 \sim \frac{\pi}{2} \), or, \( \lambda_0 \sim \frac{\pi}{2\sqrt{t}} \).

The second condition means \( \log \xi - \lambda_0 \sim \frac{\pi}{2\sqrt{t}} \).

From these we have
\[
\xi \sim e^{\frac{\pi}{\sqrt{t}}} \sim \exp \left( \frac{\text{const}}{\sqrt{T - T_c}} \right). \quad \text{(More divergent than any power-law)}
\]
Correlation function below the transition temperature

- When $T < T_c$, the system flows to the vortex free states, i.e., it is asymptotically described by the Gaussian fixed-point Hamiltonian.

- Therefore, the 2-point correlation function is

$$\langle S^x(x)S^x(y) + S^y(x)S^y(y) \rangle = \langle e^{i(\phi(x) - \phi(y))} \rangle$$

$$= Z_G^{-1} \int d\phi \ e^{-K \frac{1}{2} \int dx|\nabla \phi|^2 - i\omega \cdot \phi}$$

where $\omega(x) \equiv 1$, $\omega(y) \equiv -1$, and $\omega(r) \equiv 0$ everywhere else.

- The lattice Laplacian is the inverse of the lattice Green function, $G(x, y) = G(r) \sim -\frac{1}{2\pi} \log r + (\text{const}) \ (r \equiv |x - y|)$. Therefore,

$$= Z_G^{-1} \int d\phi \ e^{-K \frac{1}{2} \phi^\top G^{-1} \phi - i\omega \cdot \phi}$$

$$= e^{-\frac{1}{2K} \omega^\top G \omega} = e^{-\frac{1}{K} (G(0) - G(r))} \propto r^{-\frac{1}{2\pi K}}.$$

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Statistical Mechanics I

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Universal jump

- Thus, we have obtained the correlation function $\sim r^{-\eta}$ with
  
  $$\eta = \frac{1}{2\pi K} = \frac{k_B T}{2\pi J}.$$ 

  This type of correlation is called “quasi-long-range order”.

- In particular, at the transition point, $K_c \equiv \frac{2}{\pi}$, the exponent takes a universal value, $\eta(K = K_c) = 1/4$.

- In the context of 2D superfluidity, the superfluid density $\rho_s$ is, when it is finite, related to $K$ as
  
  $$K = \frac{\hbar^2 \rho_s}{mk_B T}$$

  where $m$ is the mass of a constituent particle. Therefore, $\rho_s$ has a jump with a universal magnitude at the BKT transition.
Supplement: Screening by dimers

\[
I \equiv \int_{a<|x_N-y_N|<\hat{a}} dxdy \sum_{ij} \left( \Delta v(x_i) - \Delta v(y_i) \right) \left( \Delta v(x_j) - \Delta v(y_j) \right)
\]

- We use approximation

\[
\Delta v(r) \equiv \log(r - x_N) - \log(r - y_N), \approx -\frac{x_i - x_N}{|x_i - x_N|^2} \cdot d. \quad (d \equiv y_N - x_N.)
\]

- Consider a single term

\[
l_{ij} \equiv \int_{a<|x_N-y_N|<\hat{a}} dxdy \sum_{ij} \Delta v(x_i) \Delta v(y_i)
\]

\[
\approx \int d x_N \int_{a<|d|<\hat{a}} dd \left( \frac{x_i - x_N}{|x_i - x_N|^2} \cdot d \right) \left( \frac{y_i - x_N}{|y_i - x_N|^2} \cdot d \right)
\]

\[
= 2\pi a^4 \lambda \int d x_N \frac{x_i - x_N}{|x_i - x_N|^2} \cdot \frac{y_i - x_N}{|y_i - x_N|^2}
\]
Supplement: Screening by dimers (2)

\[ l_{ij}(x_i, y_j) \approx 2\pi a^4 \lambda \int d\mathbf{x}_N \frac{x_i - x_N}{|x_i - x_N|^2} \cdot \frac{y_i - x_N}{|y_i - x_N|^2} \]

\[ \approx 2\pi \log \frac{L}{|x_i - y_j|} \]

\[ l = \sum_{ij} (l_{ij}(x_i, x_j) + l_{ij}(y_i, y_j) - l_{ij}(x_i, y_j) - l_{ij}(y_i, x_j)) \]

\[ = 2\pi a^4 \lambda \left[ 4\pi \left\{ \sum_{(ij)} (v(x_i, x_j) + v(y_i, y_j)) - \sum_{ij} v(x_i, y_j) \right\} \right] \]

\[ = 8\pi^2 a^4 \lambda \times V_{N-1}(X_{N-1}, Y_{N-1}) \]
Supplement: An integral formula

\[ I \equiv \int dx \frac{\cos \theta}{R_1 R_2} \]

\[ = \int dx \frac{R^2 - r^2/4}{((\frac{r}{2})^2 + R^2)^2 - r^2 R^2 \cos^2 \phi} \]

\[ I = \int_0^L dR \frac{R^2 - r^2/4}{4} \]

\[ \times \int_0^{2\pi} \frac{d\phi}{(r^2/4 + R^2)^2 - r^2 R^2 \cos^2 \phi} \]

\[ = \int_0^L dR \frac{2\pi R}{R^2 + r^2/4} = \pi \log \frac{L^2 + r^2/4}{r^2/4} \approx 2\pi \log \frac{L}{r} \]

We’ve used \[ \int_0^{2\pi} \frac{d\phi}{a + b \cos^2 \phi} = \frac{2\pi}{\sqrt{a(a + b)}}. \]
Summary

- The $XY$ model is mapped to a composite system of vortices and fluctuations.
- The vortices behave as a 2D Coulomb gas.
- The fluctuations are governed by the massless Gaussian model.
- The RGT to the 2D Coulomb gas yields a set of RG flow equation.
- Above the transition temperature, the correlation length diverges as $\xi \sim \exp(c/\sqrt{T - T_c})$.
- Below the transition temperature, the system flows into the vortex-less Gaussian FP, where the spin-spin correlation obeys power-law with the exponent $\eta$ varying with temperature.
- Its value is 1/4 at the transition point. This means the universal jump in the superfluid density.