

Lecture 12: Berezinskii-Kosterlitz-Thouless transition

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[12-1] XY model in two dimensions

- 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:

$$\mathcal{H} = -K \sum_{(ij)} \mathbf{s}_i \cdot \mathbf{s}_j = -K \sum_{(ij)} \cos(\theta_i - \theta_j)$$

where $\mathbf{s}_i \equiv (\cos \theta_i, \sin \theta_i)^\top$.

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

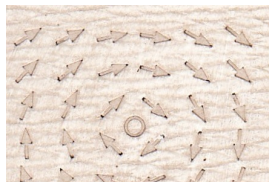
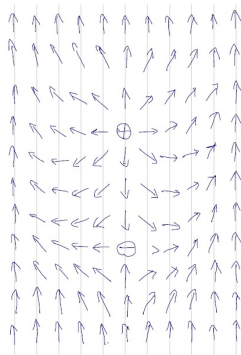
- A typical configuration of 2-component spins near or below the transition temperature consists of a smooth texture with vortices.
- The smooth texture allows the approximation,

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

- Therefore, we expect that the Hamiltonian is

$$\begin{aligned} \mathcal{H} &= -Ka^d \sum_{(ij)} \cos(\theta_i - \theta_j) \\ &\approx \frac{K}{2} \int d\mathbf{x} |\nabla\theta|^2 + \mu N_v \end{aligned}$$

where N_v is the total number of vortices.



Stationary configuration and fluctuation around it

- Here we introduce a new field variable ϕ that is the deviation of θ from its stationary solution Θ for a given vortex configurations:

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

- The configuration Θ is determined by the stationary condition, and it is a harmonic function.

$$\begin{aligned} 0 = \delta E &= \frac{K}{2} \int d\mathbf{x} \left\{ |\nabla(\Theta + \delta\Theta)|^2 - |\nabla\Theta|^2 \right\} \\ &= K \int d\mathbf{x} \nabla\Theta \cdot \nabla\delta\Theta = -K \int d\mathbf{x} \Delta\Theta\delta\Theta \\ &\Rightarrow \Delta\Theta = 0 \quad (\text{Except at vortices}) \end{aligned}$$

- Note that Θ can be uniquely determined by the vortex configuration.

Vortex/fluctuation separation

- Using Θ , we can separate the vortices from the Gaussian fluctuation:

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

where

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

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

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

Vortex field Ω

- Since Θ is a harmonic function, another harmonic function Ω 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 Γ that includes a vortex.

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

- 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, $G(\mathbf{x})$, that satisfies $\Delta G(\mathbf{x}) = -\delta(\mathbf{x})$, we can express Ω as

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

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

$$\begin{aligned} \frac{K}{2} \int d\mathbf{x} |\nabla\Theta|^2 &= \frac{K}{2} \int d\mathbf{x} |\nabla\Omega|^2 \\ &= -\frac{K}{2} \int d\mathbf{x} \Omega \Delta\Omega = \pi K \int d\mathbf{x} \Omega \rho_v \\ &= 2\pi^2 K \int d\mathbf{x} d\mathbf{y} G(\mathbf{x} - \mathbf{y}) \rho_v(\mathbf{x}) \rho_v(\mathbf{y}) \\ &= 4\pi^2 K \sum_{(ij)} G(\mathbf{x}_i - \mathbf{y}_j) q_i q_j \end{aligned}$$

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 ($\sum_i q_i = 0$),

$$\mathcal{H}_v = -2\pi K \sum_{(ij)} \log \frac{|\mathbf{x}_i - \mathbf{x}_j|}{\Lambda} q_i q_j + \mu N_v \quad (\Lambda \text{ is arbitrary})$$

Vortices form a Coulomb-gas.

Grand partition function (J. M. Kosterlitz: J. Phys. C 7 1046 (1974))

- In what follows, we assume that $q_i = \pm 1$ since vortices $|q_i| > 1$ are energetically unfavorable and would not yield dominant contribution.
- $X_N \equiv (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N)$ and $Y_N \equiv (\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_N)$ are the positions of positive and negative vortices, respectively.
- Then, the grand partition function is

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

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

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

$$V_N(X_N, Y_N) \equiv - \sum_{(ij)} (v(\mathbf{x}_i, \mathbf{x}_j) + v(\mathbf{y}_i, \mathbf{y}_j)) + \sum_{ij} v(\mathbf{x}_i, \mathbf{y}_j)$$

$$v(\mathbf{x}, \mathbf{y}) \equiv \log(|\mathbf{x} - \mathbf{y}|/\Lambda)$$

Partial trace — Increasing the cut-off a

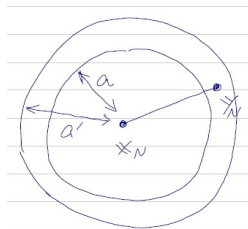
- Following the general program of the RGT, we first want to take the partial trace with respect to the short-scale degrees of freedom.
- We take the partial integral over the region $\Delta\Omega(a) \equiv \Omega(a) - \Omega(\acute{a})$ where $\acute{a} \equiv (1 + \lambda)a$.
- The region consists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

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

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

All pairs are separated by more than \acute{a} ,
except $a < |\mathbf{x}_i - \mathbf{y}_j| < \acute{a}$. }

$$\Omega_{ij}^{++}(\acute{a}) \equiv \dots$$



Partial trace — Dipole-mediated interaction

The contribution from Ω^{+-} should be dominant.

$$\begin{aligned}
 Z_N^a - Z_N^{\dot{a}} &\approx \sum_{ij} \int_{\Omega_{ij}^{+-}(\dot{a})} dX_N dY_N e^{-gV_N} = N^2 \int_{\Omega_{NN}^{+-}(\dot{a})} dX_N dY_N e^{-gV_N} \\
 &= N^2 \int_{\Omega(\dot{a})} dX_{N-1} dY_{N-1} e^{-gV_{N-1}} \int_{a < |\mathbf{x}_N - \mathbf{y}_N| < \dot{a}} d\mathbf{x}_N d\mathbf{y}_N e^{-g \sum_i [\Delta v(\mathbf{x}_i) - \Delta v(\mathbf{y}_i)]} \\
 &\quad (\Delta v(\mathbf{x}_i) \equiv v(\mathbf{x}_i, \mathbf{x}_N) - v(\mathbf{x}_i, \mathbf{y}_N)) \\
 &\approx N^2 \int_{\Omega(\dot{a})} dX_{N-1} dY_{N-1} e^{-gV_{N-1}} \\
 &\quad \times \int_{a < |\mathbf{x}_N - \mathbf{y}_N| < \dot{a}} d\mathbf{x}_N d\mathbf{y}_N \left\{ 1 + \frac{g^2}{2} \left(\sum_{i=1}^{N-1} (\Delta v(\mathbf{x}_i) - \Delta v(\mathbf{y}_i)) \right)^2 \right\} \\
 &\stackrel{(*)}{\approx} N^2 \int_{\Omega(\dot{a})} dX_{N-1} dY_{N-1} e^{-gV_{N-1}} \times \left(\frac{2\pi\hbar^2 \lambda N^2}{M^2} + 4\pi^2 a^4 \lambda g^2 V_{N-1} \right) \\
 &\quad \text{(contribution to the regular part is omitted)}
 \end{aligned}$$

Partial trace — Screening effect

$$\begin{aligned}\Xi(\zeta, g) &= \sum_N \frac{\zeta^{2N}}{(N!)^2} Z_N^a(g) \\ &\approx \sum_N \frac{\zeta^{2N}}{(N!)^2} \left(Z_N^a(g) + N^2 \int_{\Omega(\dot{a})} dX_{N-1} dY_{N-1} e^{-gV_{N-1}} \gamma g^2 \lambda V_{N-1} \right) \\ &\quad (\gamma \equiv 4\pi^2 a^4; (N-1) \rightarrow N) \\ &= \sum_N \frac{\zeta^{2N}}{(N!)^2} \int_{\Omega(\dot{a})} dX_N dY_N e^{-gV_N} (1 + \gamma g^2 \lambda \zeta^2 V_N) \\ &\approx \sum_N \frac{\zeta^{2N}}{(N!)^2} \int_{\Omega(\dot{a})} dX_N dY_N e^{-(g - \gamma g^2 \lambda \zeta^2) V_N}\end{aligned}$$

The 2nd order perturbation screens the Coulomb interaction

Rescaling of the interaction

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

$$\acute{\mathbf{x}}_i = \frac{a}{\acute{a}} \mathbf{x}_i = e^{-\lambda} \mathbf{x}_i$$

By this replacement, the interaction becomes

$$\begin{aligned} V_N(X_N, Y_N) &= - \sum_{(ij)} \left(\log \frac{\mathbf{x}_i - \mathbf{x}_j}{\Lambda} + \log \frac{\mathbf{y}_i - \mathbf{y}_j}{\Lambda} \right) + \sum_{ij} \log \frac{\mathbf{x}_i - \mathbf{y}_j}{\Lambda} \\ &= - \sum_{(ij)} \left(\log \frac{(\acute{\mathbf{x}}_i - \acute{\mathbf{x}}_j)}{\Lambda} + \log \frac{(\acute{\mathbf{y}}_i - \acute{\mathbf{y}}_j)}{\Lambda} + 2\lambda \right) + \sum_{ij} \left(\log \frac{(\acute{\mathbf{x}}_i - \acute{\mathbf{y}}_j)}{\Lambda} + \lambda \right) \\ &= V_N(\acute{X}_N, \acute{Y}_N) + (-N(N-1) + N^2)\lambda \\ &= V_N(\acute{X}_N, \acute{Y}_N) + N\lambda \end{aligned}$$

Rescaling

Now, we can summarize the RGT as

$$\begin{aligned}\Xi(\zeta, g) &= \sum_N \frac{\zeta^{2N}}{(N!)^2} e^{2dN\lambda} \int_{\Omega(a)} dX_N dY_N e^{-(g-\gamma g^2 \zeta^2 \lambda) V_N(X_N, Y_N)} e^{-gN\lambda} \\ &= \sum_N \frac{1}{(N!)^2} \left(\zeta e^{(d-\frac{g}{2})\lambda} \right)^{2N} \int_{\Omega(a)} dX_N dY_N e^{-(g-\gamma g^2 \zeta^2 \lambda) V_N(X_N, Y_N)} \\ &= \Xi(\zeta', g') \times e^{\text{(regular term)}}\end{aligned}$$

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 8γ by defining $y \equiv \sqrt{8\gamma}\zeta$:

$$\left\{ \begin{array}{l} \frac{dx}{d\lambda} = y^2 \\ \frac{dy}{d\lambda} = xy \end{array} \right. \quad \left(\begin{array}{l} x = 2 - \pi K \\ y = (\text{const}) \times e^{\mu} \end{array} \right) \quad (\text{Kosterlitz's RG eq.})$$

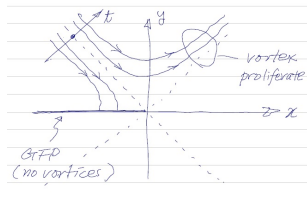
RG flow diagram

- 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, μ 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 separator, $t = 0$, corresponds to the BKT transition.



Solution and correlation length

- 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

$$\begin{aligned}\langle S^x(\mathbf{x})S^x(\mathbf{y}) + S^y(\mathbf{x})S^y(\mathbf{y}) \rangle &= \langle e^{i(\phi(\mathbf{x})-\phi(\mathbf{y}))} \rangle \\ &= Z_G^{-1} \int d\phi e^{-\frac{K}{2} \int d\mathbf{x} |\nabla\phi|^2 - i\omega \cdot \phi}\end{aligned}$$

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

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

$$\begin{aligned}&= Z_G^{-1} \int d\phi e^{-\frac{K}{2} \phi^T G^{-1} \phi - i\omega \cdot \phi} \\ &= e^{-\frac{1}{2K} \omega^T G \omega} = e^{-\frac{1}{K} (G(0) - G(r))} \propto r^{-\frac{1}{2\pi K}}.\end{aligned}$$

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 ρ_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, ρ_s has a jump with a universal magnitude at the BKT transition.

Supplement: Screening by dimers

$$I \equiv \int_{a < |\mathbf{x}_N - \mathbf{y}_N| < \acute{a}} d\mathbf{x} d\mathbf{y} \sum_{ij} (\Delta v(\mathbf{x}_i) - \Delta v(\mathbf{y}_i)) (\Delta v(\mathbf{x}_j) - \Delta v(\mathbf{y}_j))$$

- We use approximation

$$\Delta v(\mathbf{r}) \equiv \log(\mathbf{r} - \mathbf{x}_N) - \log(\mathbf{r} - \mathbf{y}_N), \approx -\frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \mathbf{d}. \quad (\mathbf{d} \equiv \mathbf{y}_N - \mathbf{x}_N.)$$

- Consider a single term

$$\begin{aligned} I_{ij} &\equiv \int_{a < |\mathbf{x}_N - \mathbf{y}_N| < \acute{a}} d\mathbf{x} d\mathbf{y} \sum_{ij} \Delta v(\mathbf{x}_i) \Delta v(\mathbf{y}_i) \\ &\approx \int d\mathbf{x}_N \int_{a < |\mathbf{d}| < \acute{a}} d\mathbf{d} \left(\frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \mathbf{d} \right) \left(\frac{\mathbf{y}_i - \mathbf{x}_N}{|\mathbf{y}_i - \mathbf{x}_N|^2} \cdot \mathbf{d} \right) \\ &= 2\pi a^4 \lambda \int d\mathbf{x}_N \frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \frac{\mathbf{y}_i - \mathbf{x}_N}{|\mathbf{y}_i - \mathbf{x}_N|^2} \end{aligned}$$

Supplement: Screening by dimers (2)

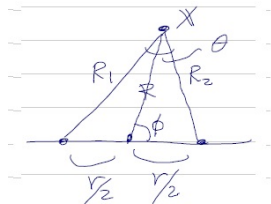
$$l_{ij}(\mathbf{x}_i, \mathbf{y}_j) \approx 2\pi a^4 \lambda \int d\mathbf{x}_N \frac{\mathbf{x}_i - \mathbf{x}_N}{|\mathbf{x}_i - \mathbf{x}_N|^2} \cdot \frac{\mathbf{y}_j - \mathbf{x}_N}{|\mathbf{y}_j - \mathbf{x}_N|^2}$$
$$\underset{(*)}{\approx} 2\pi \log \frac{L}{|\mathbf{x}_i - \mathbf{y}_j|}$$

$$I = \sum_{ij} (l_{ij}(\mathbf{x}_i, \mathbf{x}_j) + l_{ij}(\mathbf{y}_i, \mathbf{y}_j) - l_{ij}(\mathbf{x}_i, \mathbf{y}_j) - l_{ij}(\mathbf{y}_i, \mathbf{x}_j))$$
$$= 2\pi a^4 \lambda \left[4\pi \left\{ \sum_{(ij)} (v(\mathbf{x}_i, \mathbf{x}_j) + v(\mathbf{y}_i, \mathbf{y}_j)) - \sum_{ij} v(\mathbf{x}_i, \mathbf{y}_j) \right\} \right]$$
$$= 8\pi^2 a^4 \lambda \times V_{N-1}(X_{N-1}, Y_{N-1})$$

Supplement: An integral formula

$$\begin{aligned} I &\equiv \int dx \frac{\cos \theta}{R_1 R_2} \\ &= \int dx \frac{R^2 - r^2/4}{\left(\left(\frac{r}{2}\right)^2 + R^2\right)^2 - r^2 R^2 \cos^2 \phi} \\ I &= \int_0^L dR R \frac{R^2 - r^2/4}{4} \\ &\quad \times \int_0^{2\pi} \frac{d\phi}{(r^2/4 + R^2)^2 - r^2 R^2 \cos^2 \phi} \\ &= \int_0^L dR \frac{2\pi R}{R^2 + r^2/4} = \pi \log \frac{L^2 + r^2/4}{r^2/4} \approx 2\pi \log \frac{L}{r} \end{aligned}$$

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-low with the exponent η varying with temperature.
- Its value is $1/4$ at the transition point. This means the universal jump in the superfluid density.