Phase transitions in models with continuous symmetry

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In the previous chapters, we mainly focus on the Ising model with discrete Z_2 symmetry. We have been familiar with the properties of phase transition in the Ising model. Moreover, We have mentioned the the properties of phase transition are different in continuous symmetric models and in the discrete symmetric model. To illustrate this difference, we will discuss the statistical models with continuous symmetry in this chapter.

We will first discuss the Mermin-Wegner theorem, i.e. "In one or two dimension, no stable ordered phase at finite temperature can exist if the system is invariant under a continuous symmetry". We will provide some discussion on the Mermin-Wegner theorem, based on the spherical model, XY model, and O(N) model.

Accordingly to the Mermin-Wegner theorem, 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 finite critical temperature T_c, below which there is long-range order. The feat of Berezinskii, Kosterlitz and Thouless in the late 1970s was to show that XY model instead shows a 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. More interestingly, KT transition is a topological transition, which is beyond the description of Landau phase transition theory.

MERMIN-WAGNER THEOREM

Mermin-Wegner theorem: *In one and two dimensions, continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions.* (Please be aware the "continuous" condition here.)

The theorem says that if we try to break the symmetry by imposing a field and then letting the field go to zero, the symmetry remains unbroken in the sense that the average manetization is zero.

Formally, this theorem can be understood by the spherical model and the XY model below.

Next, we will approach the Mermin-Wagner theorem via the non-linear sigma model.

Non-linear sigma model

For continuous spins, the lowest energy excitations are long-wavelength Goldstone modes (as shown in the Laudau theory). We consider unit n-component spins on the sites of a lattice, i.e.

$$\mathbf{s}_i = (s_1, s_2, ..., s_n)_i, |\mathbf{s}_i|^2 = s_1^2 + s_2^2 + ... + s_n^2 = 1 \tag{1}$$

The nearest-neighbor Hamiltonian can be written as

$$-\beta H = K \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j = K \sum_{\langle i,j \rangle} (1 - \frac{(\mathbf{s}_i - \mathbf{s}_j)^2}{2}) \approx -\beta E_0 - \frac{K}{2} \int d^d x (\nabla s(\mathbf{x}))^2. \tag{2}$$

Therefore the partition function is

$$Z = \int D[\mathbf{s}(x)] \delta(|\mathbf{s}(x)|^2 - 1) e^{-\frac{K}{2} \int d^d x (\nabla \mathbf{s}(\mathbf{x}))^2}. \tag{3}$$

For a possible magnetic order, say $\mathbf{s}(\mathbf{x}) = (1, 0, 0, ...)$, there are $n-1$ Goldstone modes describing the transverse fluctuations. To examine these fluctuations close to zero temperature, we set

$$\mathbf{s}(\mathbf{x}) = (\sigma(x), \pi_1(x), \pi_2(x), ...) \equiv (\sigma(x), \vec{\pi}(x)) \tag{4}$$

where $\vec{\pi}$ is an $n-1$ component vector describing transverse fluctuations. For each degree of freedom, $(\delta(ax) = \frac{1}{|a|}\delta(x))$

$$\begin{aligned} \int D[\mathbf{s}] \delta(|s|^2 - 1) &= \int d\vec{\pi} d\sigma \delta(\pi^2 + \sigma^2 - 1) \\ &= \int d\vec{\pi} d\sigma \delta((\sigma - \sqrt{1-\pi^2})(\sigma + \sqrt{1-\pi^2})) = \int d\vec{\pi} \frac{1}{2\sqrt{1-\pi^2}} \end{aligned} \tag{5}$$

Using this result, the partition function can be written as

$$\begin{aligned} Z &= \int D[\mathbf{s}(x)] \delta(|\mathbf{s}(x)|^2 - 1) e^{-\frac{K}{2} \int d^d x (\nabla \mathbf{s}(\mathbf{x}))^2} \\ &= \int d\vec{\pi} \frac{1}{2\sqrt{1-\pi^2}} e^{-\frac{K}{2} \int d^d x (\nabla \pi(\mathbf{x}))^2 + (\nabla \sqrt{1-\pi^2(\mathbf{x})})^2} \\ &= \int d\vec{\pi} \exp[-\int d^d x [\frac{K}{2} (\nabla \pi(\mathbf{x}))^2 + \frac{K}{2} (\nabla \sqrt{1-\pi^2(\mathbf{x})})^2 + \frac{\rho}{2} \ln(1-\pi^2)]] \end{aligned} \tag{6}$$

where $\rho = N/V$ is density of lattice sites. Here we see, while the original Hamiltonian is quite simple, the effective Hamiltonian describing Goldstone modes $\vec{\pi}(x)$ is rather complicated.

We can expand the nonlinear terms in powers of $\vec{\pi}(x)$, resulting in a series

$$\beta H[\vec{\pi}(x)] \approx \beta H_0 + U_1 + U_2 + ... \tag{7}$$

$$H_0 = \frac{K}{2}\int d^dx(\nabla\pi(\mathbf{x}))^2 \tag{8}$$

$$U_1 = \int d^dx[\frac{K}{2}(\pi(\mathbf{x})\cdot\nabla\pi(\mathbf{x}))^2 - \frac{\rho}{2}\pi^2(\mathbf{x})] \tag{9}$$

Here H_0 is independent Goldstone modes, and U_1 is the first order perturbation when the terms in the series due to $\ln(1-x) \approx -x, \nabla\sqrt{1-x^2} = \frac{x\nabla x}{\sqrt{1-x^2}} \approx x\nabla x$.

In the language of Fourier modes,

$$\beta H_0 = \frac{K}{2}\int \frac{d^dq}{(2\pi)^d} q^2|\vec{\pi}(\mathbf{q})|^2 \tag{10}$$

$$U_1 = -\frac{K}{2}\int \frac{d^dq_1}{(2\pi)^d}\frac{d^dq_2}{(2\pi)^d}\frac{d^dq_3}{(2\pi)^d}\frac{d^dq_4}{(2\pi)^d}\pi_\alpha(\mathbf{q}_1)\pi_\alpha(\mathbf{q}_2)\pi_\beta(\mathbf{q}_3)\pi_\beta(\mathbf{q}_4)(\mathbf{q}_1\cdot\mathbf{q}_3)\delta(\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4)$$
$$-\frac{\rho}{2}\int \frac{d^dq}{(2\pi)^d}|\vec{\pi}(\mathbf{q})|^2 \tag{11}$$

For non-interacting part, the correlation function of the Goldstone modes are

$$\langle \pi_\alpha(q)\pi_\beta(q')\rangle_0 = \frac{\delta_{\alpha\beta}(2\pi)^d\delta(\mathbf{q}+\mathbf{q}')}{Kq^2} \tag{12}$$

which leads to the fluctuation taking the order of

$$\rightarrow \langle \vec{\pi}(x=0)^2\rangle = \int \frac{d^dq}{(2\pi)^d}\langle|\pi_\alpha(q)|^2\rangle_0$$
$$\frac{n-1}{K}\int_{1/L}^{\Lambda=1/a}\int \frac{d^dq}{(2\pi)^d}\frac{1}{q^2} = \frac{n-1}{K}\frac{S^d(a^{2-d}-L^{2-d})}{d-2} \tag{13}$$

For this estimation, we can deduce: For $d > 2$, the fluctuations are proportional to T, but for $d < 2$, the fluctuations diverge since $L \to \infty$. This manifests the Mermin-Wagner theorem, i.e. the absence of long-range order in $d \leq 2$.

Moreover, an RG expansion in powers of T provides a systematic way to explore critical behavior close to two dimensions. By skipping the RG details, one can obtain the RG equation for the temperature as

$$\frac{dK}{d\ell} = (d-2)K - (n-2)S^d\Lambda^{d-2} \leftrightarrow \frac{dT}{d\ell} = -\frac{dK}{K^2d\ell} = -(d-2)T + (n-2)S^d\Lambda^{d-2}T^2. \tag{14}$$

Here we see, the RG equation changes behavior drastically at $d = 2$. For $d < 2$, the flow is away from zero, indicating that the ordered phase is unstable and there is no broken symmetry. For $d > 2$, small T flows back to zero, implying that the ordered phase is stable. At $d = 2$, the first term in the RG equation vanishes so that the flow is controlled by the second term, which changes sign at $n = 2$. For $n > 2$ the flow is towards high temperatures, so that Heisenberg and higher spin models are disordered. The situation of $d = 2, n = 2$ is special, and it is marginal in the RG calculations. This special case will be discussed in more detail in the XY model.

SPHERICAL MODEL

The spherical model was introduced by Berlin and Kac by relaxing the rigid Ising constraint $\sigma_i^2 = 1$ (or $\sigma_i = \pm$), and replacing it by the overall spherical constraint

$$\sum_{i=1}^{N} (s_i)^2 = N \tag{15}$$

where s_i are taken as continuous variables. One can further reduce this condition, and replace it by mean constraint:

$$\langle \sum_{i=1}^{N} (s_i)^2 \rangle = N \tag{16}$$

Furthermore, this condition can be formulated by the Hamiltonian

$$H = -\sum_{(i,j)} J_{ij} s_i s_j - h \sum_i s_i + \lambda \sum_{i=1}^{N} (s_i)^2 \tag{17}$$

where $-\infty < s_i = s(\mathbf{r}_i) < +\infty$ describing the spin on lattice site i. This model is called the spherical model, where the free energy per spin is given by

$$f(\beta, h, \lambda) = -\frac{1}{\beta N} \ln Z_N(\beta, h, \lambda) \tag{18}$$

$$Z_N(\beta, h, \lambda) = \int_{-\infty}^{+\infty} ds_1 ... \int_{-\infty}^{+\infty} ds_N \exp[-\beta H] \tag{19}$$

In particular, the mean value condition Eq. 16 can be derived by $-\frac{1}{\beta}\frac{\partial \ln Z_N}{\partial \lambda} = N$.

The Hamiltonian is a symmetric quadratic form and hence be diagonalized by an orthogonal matrix $[U_{qi}]$:

$$UJU^{-1} = D \Rightarrow J_{ij} = (U^{-1})_{iq} D_q U_{qj} \tag{20}$$

The proof next makes use of the fact that H can be diagonalized by orthogonal transformation, $J = U^T D U$, where the matrix U is orthogonal, and all elements of the diagonal matrix $D = diag(\mu_q), q = 0, 1, ..., N-1$ are positive. In terms of μ_q, the free energy may be evaluated as

$$Z_N(\beta, h, \lambda) = (2\pi)^{N/2}\sqrt{\Pi_q \frac{1}{\lambda - \mu_q}} e^{\frac{1}{2}h^2 \sum_q \frac{|\epsilon_q|^2}{\lambda - \mu_q}} \tag{21}$$

$$\rightarrow f = \frac{1}{2\beta N}\sum_{q=0}^{N-1} \ln[\beta(\lambda - \mu_q)] - \frac{h^2}{4N}\sum_{q=0}^{N-1}\frac{|\epsilon_q|^2}{\lambda - \mu_q} \tag{22}$$

where we made a transformation $h\epsilon_q = \sum_i U_{qi} h_i$, and we used the Gaussian integeral

$$\int d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T A \mathbf{v} + \mathbf{j}^T \mathbf{v}} = (2\pi)^{N/2}[detA]^{-1/2} e^{\frac{1}{2}\mathbf{j}^T A^{-1}\mathbf{j}} \tag{23}$$

where $\mathbf{v}, \mathbf{j}$ are N-component vector

In this context, the mean spherical constraint Eq. 16 ($-\frac{1}{\beta}\frac{\partial \ln Z_N}{\partial \lambda} = N$) becomes

$$\frac{1}{2\beta N}\sum_{q=0}^{N-1}\frac{1}{\lambda - \mu_q} + \frac{h^2}{4N}\sum_{q=0}^{N-1}\frac{|\epsilon_q|^2}{(\lambda - \mu_q)^2} = 1 \tag{24}$$

through which we can get the expression of $\lambda = \lambda(\beta, h)$.

The thermal quantities can be calculated as follows. The magnetization per spin now follows

$$m(\beta, h) = \frac{\partial f}{\partial h} = \frac{h}{2N}\sum_{q=0}^{N-1}\frac{|\epsilon_q|^2}{\lambda - \mu_q} \tag{25}$$

and susceptibility

$$\chi(T) = \lim_{h \to 0}\frac{\partial m}{\partial h} = \lim_{h \to 0}\frac{m}{h} \tag{26}$$

Especially, for a uniform magnetic field, we have $\epsilon_q = \sum_i U_{qi} h_i = \delta_{q,0}\epsilon_0$, so that $\chi \sim \frac{1}{\lambda - \mu_0}$.

The entropy per spin is given by

$$S(\beta, h) = -\frac{\partial f}{\partial T} = \frac{k_B}{2} - \frac{k_B}{2N}\sum_q \ln[\beta(\lambda - \mu_q)] \tag{27}$$

From this it follows, the zero field specific hear per spin is

$$c = T\frac{\partial S}{\partial T} = \frac{1}{2}k_B \sum_q [1 - \frac{T(\partial \lambda / \partial T)}{\lambda - \mu_q}] \tag{28}$$

Next we consider $h = 0$ and we set the largest eigenvalue of $\{\mu_q\}$ is μ_0, the reduced eigenvalues is

$$\Omega_q = (\mu_0 - \mu_q)J \geq 0. \tag{29}$$

On a hypercubical lattice with periodic boundary conditions we easily find

$$\Omega_q = 2\sum_{j=1}^{d}[1 - \cos(2\pi k_j a)] \tag{30}$$

In the thermodynamic limit ($N \to \infty$), the spherical constraint in zero field becomes

$$\frac{1}{2\beta N}\sum_{q=0}^{N-1}\frac{1}{\lambda - \mu_q} = 1 \to 2\beta J = W_d(\phi) \tag{31}$$

$$W_d(z) = \frac{1}{(2\pi)^2}\int_0^{2\pi}...\int_0^{2\pi} d\theta_1...d\theta_d \frac{1}{z + 2\sum_{j=1}^{d}(1-\cos\theta_j)} = \int_0^{\infty} e^{-zx}[e^{-x}I_0(x)]^d dx \tag{32}$$

where we introduce a reduced spherical field $\phi = (\lambda - \mu_0)/J$. $W_d(\phi)$ is called Watson function, which has the behavior when $\phi \ll 1$:

$$W_d(\phi) = \begin{cases} (2\pi)^{-d/2}\Gamma((2-d)/2)\phi^{-(2-d)/2} + const., d < 2 \\ (2\pi)^{-1}\ln(1/\phi) + const, d = 2 \\ W_d(0) - (2\pi)^{-d/2}|\Gamma((2-d)/2)|\phi^{(d-2)/2}, 2 < d < 4 \\ W_d(0) - |W_d'(0)|\phi, d > 4 \end{cases} \tag{33}$$

where $W_d(0)$ exists (it is finite) when $d > 2$ and $W_d'(0)$ is well defined in $d > 4$.

Then we can discuss the critical behaviors.

- $d < 2$. $\phi \approx [\frac{\Gamma((2-d)/2)}{2(2\pi)^{d/2}\beta J}]^{2/(2-d)} \sim (\frac{kT}{J})^{2/(2-d)}$
  $\chi \approx \frac{N}{2J\phi} = (\frac{kT}{J})^{-2/(2-d)}$ which is divergent only when $T = T_c = 0$. So the ciritical temperture is $T_c = 0$.

- $d = 2$. $\phi \approx \exp(-4\pi J\beta)$.
  $\chi \sim \exp(4\pi J/kT)$, which is divergent at $T = T_c = 0$. The critical temperature is $T_c = 0$.

- $2 < d < 4$. $W_d(0) - (2\pi)^{-d/2}|\Gamma((2-d)/2)|\phi^{(d-2)/2} = 2\beta J$.
  So we get the critical temperature is around $kT_c \approx W_d(0)/2J$. Near the critical point,

we have

$$\phi \sim \begin{cases} (\beta_c - \beta)^{2/(d-2)}, T > T_c \\ 0, T < T_c \end{cases} \tag{34}$$

and

$$\chi \sim (\beta_c - \beta)^{-2/(d-2)} = (T - T_c)^{-2/(d-2)} \tag{35}$$

From this we obtain the critical exponent $\gamma = \frac{2}{d-2}$.

- $d > 4$. T_c is finite, and $\phi = \beta_c - \beta$, so we have $\chi \sim (T - T_c)^{-1}$, giving $\gamma = 1$. In this case, the result recover the mean field calculation that we see for Landau theory.

Finally, we move to discuss the physics behind these results.

- Models with continuous symmetry is different that of discrete symmetry (e.g. Ising model).
- There is no finite temperature transition, i.e. $T_c = 0$, in dimension $d \leq 2$, in the model with continuous symmetry. In sharp contrast, in the model with discrete symmetry (e.g. Ising model), there is a finite temperature transition $T_c \neq 0$ at $d = 2$.
- In the model with conintuous symmetry, the critical exponent depends on dimension d, when $2 < d < 4$, but not when $d > 4$. Especially, for $d > 4$, critical exponent is constant with the mean field calculation. The physical reason is, fluctuation is less important in higher dimension, so mean-field works very well.

Although we obtain these from a specific model, i.e. spherical model, the above conclusion is general, which is widely confirmed by $O(n)(n \geq 2)$ model with continuous symmetry.

Why the continuous model is different from the discrete model? Why Ising model is so special? The answer is Goldstone mode! This gapless mode only appears in the continuous symmetry spontaneously broken, but not exists in the case of discrete symmetry.

XY MODEL

Let us consider the XY (or rotator) model with periodic boundary conditions. (Actually, this is a preparation for future study. We will come back to this model again in future.) We include an external field in the x direction:

$$H = -\sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j - \sum_j \vec{h} \cdot \vec{S}_j = -\sum_{\langle i,j\rangle} \cos(\theta_i - \theta_j) - h \sum_j \cos\theta_j \tag{36}$$

where $\vec{S}_i = (\cos\theta_i, \sin\theta_i)$ lays down in the xy plane. Let N denote the number of sites in the rectangle and define

$$m = \frac{1}{N} \sum_j \langle \cos\theta_j \rangle \tag{37}$$

Then, Mermin-Wegner theorem states

$$\lim_{h\to 0} m = 0 \tag{38}$$

There are two ways to calculate it. One is to prove it using a phenomenogical method, and the other one is a direct calculation.

Operator method based on Cauchy-Schwarz inequality

In the first method, we define two quantity:

$$A = \sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j} \sin\theta_j \tag{39}$$

$$B = -\sum_j e^{-i\mathbf{k}\cdot\mathbf{r}_j} \frac{\partial H}{\partial \theta_j} \tag{40}$$

Here $\mathbf{k}$ is summed of the appropriate set of momenta. For simplicity, we take a square lattice, $\mathbf{k} = (k_1, k_2)$ with $k_i = 2\pi l_i / L$ where $l_i = 0, 1, 2, ..., L-1$.

The proof will rely on the Cauchy Schwarz inequality

$$\langle \overline{A} B \rangle^2 \leq \langle \overline{A} A \rangle \langle \overline{B} B \rangle \tag{41}$$

Next we calculate the different terms one by one. We need one trick as

$$e^{-\beta H} \frac{\partial H}{\partial \theta_l} = -\frac{1}{\beta} \frac{\partial}{\partial \theta_l} e^{-\beta H} \tag{42}$$

$$
\begin{aligned}
\langle \overline{A} B\rangle &= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\langle \sin\theta_j \frac{\partial H}{\partial \theta_l}\rangle \\
&= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z}\int d\theta e^{-\beta H}\sin\theta_j \frac{\partial H}{\partial\theta_l} \\
&= \sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z\beta}\int d\theta \sin\theta_j \frac{\partial e^{-\beta H}}{\partial\theta_l} \\
&= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z\beta}\int d\theta e^{-\beta H} \frac{\partial}{\partial\theta_l}\sin\theta_j \\
&= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{\beta}\delta_{j,l}\langle\cos\theta_j\rangle = -\frac{Nm}{\beta}
\end{aligned} \tag{43}
$$

For another term,

$$
\begin{aligned}
\langle \overline{B} B\rangle &= \sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\langle \frac{\partial H}{\partial\theta_j}\frac{\partial H}{\partial\theta_l}\rangle \\
&= \sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z}\int d\theta e^{-\beta H}\frac{\partial H}{\partial\theta_j}\frac{\partial H}{\partial\theta_l} \\
&= -\sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z}\int d\theta \frac{\partial H}{\partial\theta_j}\frac{\partial e^{-\beta H}}{\partial\theta_l} \\
&= \sum_{j,l} e^{i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_l)}\frac{1}{Z}\int d\theta \frac{\partial}{\partial\theta_j}\frac{\partial}{\partial\theta_l}e^{-\beta H}
\end{aligned} \tag{44}
$$

Since

$$
\frac{\partial H}{\partial\theta_j} = \sum_{|m-j|=1}\sin(\theta_j-\theta_m) + h\sin\theta_l \tag{45}
$$

$$
\frac{\partial^2 H}{\partial\theta_j\partial\theta_l} = \delta_{j,l}\sum_{|m-l|=1}\cos(\theta_l-\theta_m) - \delta_{|j-l|=1}\cos(\theta_l-\theta_j) + \delta_{j,l}h\cos\theta_l \tag{46}
$$

we have

$$
\begin{aligned}
\langle \overline{B} B\rangle &= \frac{1}{\beta}[\sum_l\sum_{|m-l|=1}\langle\cos(\theta_l-\theta_m)\rangle - \sum_{j,l,|j-l|=1} e^{ik(j-l)}\langle\cos(\theta_j-\theta_l)\rangle + h\sum_l\langle\cos\theta_l\rangle] \\
&= \frac{1}{\beta}\sum_{j,l,|j-l|=1}(1-e^{ik(j-l)})\langle\cos(\theta_j-\theta_l)\rangle + hNm/\beta
\end{aligned} \tag{47}
$$

The last one

$$
\begin{aligned}
&\langle \overline{A} A\rangle = \sum_{j,l} e^{ik(j-l)}\langle\sin\theta_j\sin\theta_l\rangle \\
&\Rightarrow \sum_k\langle \overline{A} A\rangle = N\sum_l\langle\sin^2\theta_j\rangle \le N^2
\end{aligned} \tag{48}
$$

Then we can write the Cauthy inequality as

$$\begin{aligned}
&\langle \overline{A}A\rangle \geq \frac{\langle \overline{A}B\rangle^2}{\langle \overline{B}B\rangle}\\
&N^2 \geq \sum_k \frac{\langle \overline{A}B\rangle^2}{\langle \overline{B}B\rangle}\\
&= \frac{1}{\beta}\sum_k \frac{N^2m^2}{\sum_{j,l,|j-l|=1}(1-e^{ik(j-l)})\langle\cos(\theta_j-\theta_l)\rangle + hNm}\\
&(\langle\cos(\theta_j-\theta_l)\rangle \leq 1) \Rightarrow 1 \geq \frac{1}{\beta}\sum_k \frac{m^2}{\sum_{j,l,|j-l|=1}(1-e^{ik(j-l)}) + hNm}
\end{aligned} \tag{49}$$

Then we use the condition $1-\cos x \leq x^2/2$, we have

$$\begin{aligned}
&\sum_{j,l,|j-l|=1}(1-e^{ik(j-l)}) \leq Nk^2\\
&\Rightarrow 1 \geq \frac{1}{\beta}\int d^2k \frac{m^2}{ck^2+hm}
\end{aligned} \tag{50}$$

At last we take the zero field limit,

$$1 \geq \frac{1}{\beta}\int d^2k \frac{m^2}{ck^2} \tag{51}$$

Since $\int d^2k \frac{1}{k^2} = \infty$, this implies that

- $T = 0, m \neq 0$: The magnetic order is possible only at zero temperature;
- $T \neq 0, m = 0$: At finite temperature, the magnetic order should be zero.

Another point is interesting, the integral $\int d^dk \frac{1}{k^2}$ is divergent when $d \leq 2$, but it is regular $d > 2$. So, in three dimension, the order at finite temperature is possible.

Low-temperature expansion

The second method to calculate the magnetization is shown below.

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.

$$H = -J \sum_{<i,j>} \cos(\theta_i - \theta_j)$$
$$= -JN + \frac{J}{2} \sum_{<i,j>} (\theta_i - \theta_j)^2$$
$$= E_0 + \frac{J}{4} \sum_{\mathbf{r},\mathbf{a}} (\theta(\mathbf{r}+\mathbf{a}) - \theta(\mathbf{r}))^2$$
$$\simeq E_0 + \frac{J}{2} \int d^2r (\nabla\theta(\mathbf{r}))^2 \ . \tag{52}$$

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:

$$\langle S_x \rangle = < \cos\theta(\mathbf{r}) > = < \cos\theta(0) > \tag{53}$$
$$= \frac{Tr_{\{\theta_i\}} \cos\theta(0) e^{-\beta H}}{Tr_{\{\theta_i\}} e^{-\beta H}} \tag{54}$$
$$= Re\left(\frac{1}{\mathcal{Z}} \int \mathcal{D}[\theta_i] e^{-\beta H + i\theta(0)} \right) \tag{55}$$

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

$$\theta(\mathbf{r}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \theta_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \ , \tag{56}$$
$$\theta(\mathbf{r}=0) = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} \theta_{\mathbf{k}} \tag{57}$$

This leads to, after Gaussian integral:

$$< S_x > = \exp\left(-\frac{T}{2J} I_d(L) \right) \ , \tag{58}$$

with $I_d(L)$ a geometric factor written as (by setting a momentum UV cut-off $\Lambda \sim \pi/a$)

$$I_d(L) = S_d \int_{\pi/L}^{\pi/a} dk k^{d-3} = \begin{cases} L^{2-d}, d < 2 \\ \ln\left(\frac{L}{a}\right), d = 2 \\ \frac{1}{d-2}\left(\frac{\pi}{a}\right)^{d-2}, d > 2 \end{cases} \tag{59}$$

Therefore,

$$\lim_{L\to\infty} \langle S_x \rangle = \begin{cases} 0, d \leq 2 \\ \exp(-\frac{S_d}{2Ja^{2-d}} AT), d > 2 \end{cases} \tag{60}$$

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 in $d = 2$:

$$\begin{aligned} g(r) &=< \exp\{i(\theta(\mathbf{r}) - \theta(0))\} >=< \frac{Tr_{\{\theta_i\}} e^{i(\theta(\mathbf{r})-\theta(0))} e^{-\beta H}}{Tr_{\{\theta_i\}} e^{-\beta H}} > \\ &= e^{-\frac{1}{2}<[\theta(\mathbf{r})-\theta(0)]^2>} = e^{-<\theta^2(0)-\theta(\mathbf{r})\theta(0)>}. \end{aligned} \tag{61}$$

This is a conclusion for a Gaussian Hamiltonian: $< \exp\{i(\theta(\mathbf{r}) - \theta(0))\} >= e^{-\frac{1}{2}<[\theta(\mathbf{r})-\theta(0)]^2>}$. Then we have

$$\begin{aligned} < \theta^2(0) - \theta(\mathbf{r})\theta(0) > &= \int \frac{d^2k_1}{(2\pi)^2} \int \frac{d^2k_2}{(2\pi)^2} < \theta(k_1)\theta(k_2) > (1 - e^{i\mathbf{k_1}\cdot\mathbf{r}}) \\ &= T \int_0^\Lambda \frac{1 - e^{i\mathbf{k_1}\cdot\mathbf{r}}}{k^2} \\ &= T \frac{1}{4\pi^2} \int_0^{2\pi} d\phi \int_0^\Lambda dk \frac{1}{k}(1 - e^{ikr\cos\phi}) = T \frac{1}{2\pi} \int_0^\Lambda dk \frac{1 - J_0(kr)}{k} \\ &\approx \frac{T}{2\pi} \ln\frac{r}{a} \end{aligned} \tag{62}$$

So

$$g(r) = e^{-\frac{T}{2\pi}\ln\frac{r}{a}} = \left(\frac{r}{a}\right)^{-\eta(T)}, \eta = \frac{T}{2\pi} \tag{63}$$

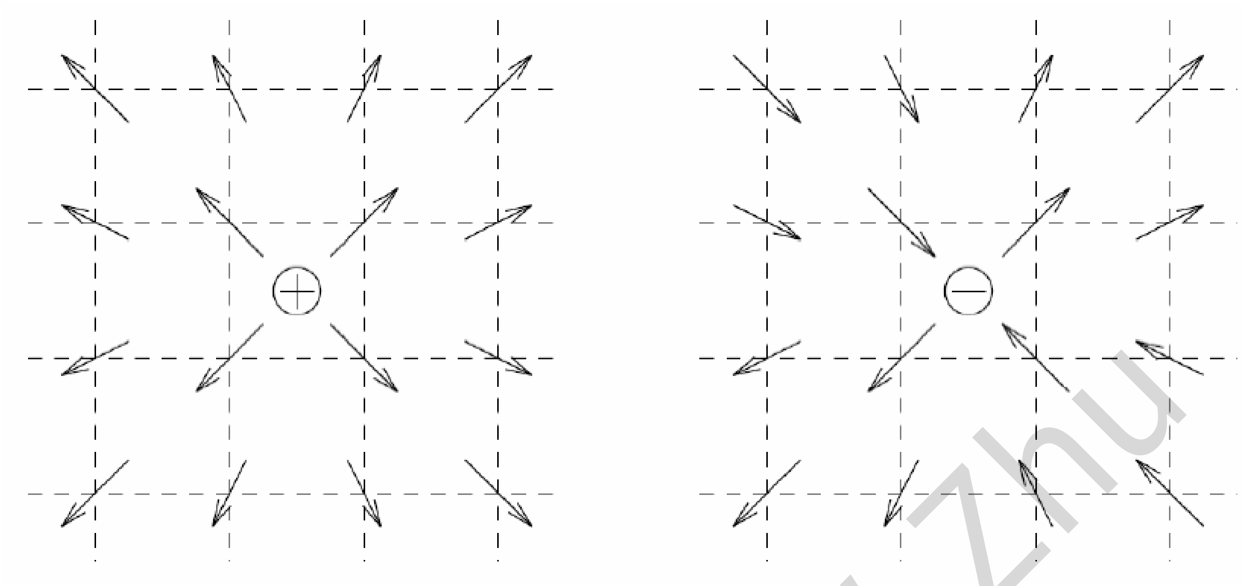

FIG. 1: (a) Following the vectors around the plaquette in a counterclockwise way, the vectors turn 2π while we circle 2π. This is a vortex. Its core radius is r, therefore the energy of such a vortex is $E \sim \ln(R/r)$. In (b), the vectors wind by -2π while we circle counterclockwise - this is an antivortex.

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.

◇ Think about is: *How can there be a finite temperature transition in two-dimension?*

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:

$$\oint_{\mathbf{r}_0} \nabla\theta(\mathbf{r}) \cdot d\mathbf{l} = 2\pi n, \tag{64}$$

with $n < 0$ corresponding to clockwise winding vortices, and $n > 0$ to anticlockwise. Such configurations are illustrated in Fig. 1.

Can the proliferation of these objects be a reason for the 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 into a system without vortex. In order to estimate the energy generated by the presence of an isolated vortex, we must first estimate $\nabla\theta$. We use our equation 64, 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

$$\Delta E = \frac{J}{2}\int d^2r(\nabla\theta(\mathbf{r}))^2 = \pi J n^2 \int_a^L \frac{dr}{r} = \pi J n^2 \ln\frac{L}{a} \ , \tag{65}$$

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:

$$\Delta S = k_B \ln{(L/a)^2} = 2k_B \ln L/a \ . \tag{66}$$

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

$$\Delta F = \Delta E - T\Delta S = (\pi J n^2 - 2k_B T)\ln\frac{L}{a} \ . \tag{67}$$

We can clearly see the following two regimes:

- For $k_BT < \pi J/2$, $\Delta F > 0$, 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;
- 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.

KOSTERLITZ-THOULESS TRANSITION

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

$$Z = \int \prod_i \frac{d\theta_i}{2\pi} e^{\frac{J}{T}\sum_{i,\mu}\cos(\theta_i - \theta_{i+\mu})} = \int \prod_i \frac{d\theta_i}{2\pi} e^{\frac{J}{T}\sum_{i,\mu}\cos(\Delta_\mu \theta_i)} \tag{68}$$

Next we would like to introduce a Fourier transformation:

$$F(m_{i\mu}) = \frac{1}{2\pi}\int_0^{2\pi} d(\Delta_\mu \theta_i) e^{-i m_{i\mu}\Delta_\mu \theta_i} e^{\frac{J}{T}\cos(\Delta_\mu \theta_i)} = I_{m_{i\mu}}(\frac{J}{T}) \tag{69}$$

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,

$$e^{\frac{J}{T}\cos(\Delta_\mu \theta_i)} \approx \sqrt{\frac{T}{2\pi J}} e^{\frac{J}{T}} \sum_{m_{i\mu}=-\infty}^{+\infty} e^{i m_{i\mu}\Delta_\mu \theta_i - \frac{T m_{i\mu}^2}{2J}} \tag{70}$$

$$\begin{aligned} Z &= \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \sum_{m_{i\mu}} e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2 + i\sum_{i\mu} m_{i\mu}\Delta_\mu \theta_i} \\ &= \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \sum_{m_{i\mu}} e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2 + i\sum_{i\mu} m_{i\mu}(\theta_{i+\mu} - \theta_i)} \\ &= \int_0^{2\pi} \prod_i \frac{d\theta_i}{2\pi} \sum_{m_{i\mu}} e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2 + i\sum_{i\mu}(m_{i\mu} - m_{i-\mu,\mu})\theta_i} \\ &= \sum_{m_{i\mu}} \delta(\vec{\Delta}\cdot \vec{m}_i) e^{-\frac{T}{2J}\sum_{i\mu} m_{i\mu}^2} \end{aligned} \tag{71}$$

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

$$\vec{\Delta}\cdot\vec{m}_i = \sum_\mu \Delta_\mu m_{i\mu} = \sum_\mu (m_{i+\mu,\mu} - m_{i\mu}) = 0 \Rightarrow \sum_\mu m_{i\mu} = 0 \tag{72}$$

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:

$$m_{i,x} = n_{i+\frac{x+y}{2}} - n_{i+\frac{x-y}{2}} \tag{73}$$

$$m_{i,y} = n_{i+\frac{y-x}{2}} - n_{i+\frac{x+y}{2}} \tag{74}$$

$$m_{i,-x} = n_{i-\frac{x+y}{2}} - n_{i+\frac{y-x}{2}} \tag{75}$$

$$m_{i,-y} = n_{i+\frac{x-y}{2}} - n_{i-\frac{x+y}{2}} \tag{76}$$

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

$$Z = \sum_{n_i} e^{-\frac{T}{2J}\sum_{i\mu}(n_{i+\mu}-n_i)^2} \tag{77}$$

$$= \int \prod_i d\phi_i \sum_{n_i} e^{-\frac{T}{2J}\sum_{i\mu}(\phi_{i+\mu}-\phi_i)^2 - 2\pi i \sum_i \phi_i n_i} \tag{78}$$

In the last line, we used the Possion formula:

$$\sum_{n=-\infty}^{\infty} g(n) = \sum_{n=-\infty}^{\infty} \int d\phi g(\phi) e^{-2\pi i n\phi} \tag{79}$$

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

$$Z = \int \prod_i d\phi_i \sum_{n_i} e^{-\frac{T}{2J}\sum_{i\mu}(\phi_{i+\mu}-\phi_i)^2 - 2\pi i \sum_i \phi_i n_i} e^{-\frac{E_c}{T}\sum_i n_i^2} \tag{80}$$

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

Next we have to use an approximation as

$$\sum_{n_i} e^{-2\pi i n_i \phi_i} y^{n_i^2} \approx 1 + 2y\cos(2\pi\phi_i) + 2y^4\cos(4\pi\phi_i) + ... \approx e^{2y\cos(2\pi\phi_i) + O(y^2)} \tag{81}$$

and we re-write the partition function as

$$\int \prod_i d\phi_i e^{-\frac{T}{2J}\sum_{i\mu}(\phi_{i+\mu}-\phi_i)^2 + 2y\sum_i \cos(2\pi\phi_i)} \tag{82}$$

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

$$Z = \int D\phi e^{-\int d^2x [\frac{T}{2J}(\nabla\phi)^2 + 2y\cos(2\pi\phi)]} \tag{83}$$

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

Renormalization-group analysis

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

$$Z = \int D\phi_< D\phi_> e^{-\int d^2x[\frac{T}{2J}(\nabla\phi_<)^2 + (\nabla\phi_>)^2} e^{2y\int d^2x \cos(2\pi(\phi_< + \phi_>))]} \tag{84}$$

$$\approx \int D\phi_< D\phi_> e^{-\int d^2x[\frac{T}{2J}(\nabla\phi_<)^2 + (\nabla\phi_>)^2} \times$$
$$[1 + 2y\int d^2x \cos(2\pi(\phi_< + \phi_>)) + 2y^2\int d^2x \int d^2x' \cos(2\pi(\phi_<(x) + \phi_>(x))) \cos(2\pi(\phi_<(x') + \phi_>(x')))]$$
$$= Z_< \int D\phi_> e^{-\int d^2x \frac{T}{2J}(\nabla\phi_>)^2}[1 + 2y\int d^2x \cos(2\pi\phi_<)\langle\cos(2\pi\phi_>)\rangle_> +$$
$$2y^2 \int d^2x \int d^2x' \cos(2\pi\phi_<(x))\cos(2\pi\phi_<(x'))\langle\cos(2\pi\phi_>(x)\cos(2\pi\phi_>(x'))\rangle_> +$$
$$2y^2 \int d^2x \int d^2x' \cos(2\pi\phi_<(x))\cos(2\pi\phi_<(x'))\langle\sin(2\pi\phi_>(x)\sin(2\pi\phi_>(x'))\rangle_>] \tag{85}$$

Defining th correlation function

$$g_>(\mathbf{r}) = (2\pi)^2\langle\phi_>(\mathbf{r})\phi_>(0)\rangle_> \tag{86}$$

and

$$\langle\cos(2\pi\phi_>(\mathbf{r}))\rangle = e^{-\frac{1}{2}g_>(0)} \tag{87}$$
$$\langle\cos(2\pi\phi_>(\mathbf{r}))\cos(2\pi\phi_>(\mathbf{r}'))\rangle = e^{-g_>(0)}\cosh(g_<(\mathbf{x} - \mathbf{x}')) \tag{88}$$
$$\langle\sin(2\pi\phi_>(\mathbf{r}))\sin(2\pi\phi_>(\mathbf{r}'))\rangle = e^{-g_>(0)}\sinh(g_<(\mathbf{x} - \mathbf{x}')) \tag{89}$$

The action for the slow modes is

$$S_< = \frac{T}{2J}\int d^2x(\nabla\phi_<(\mathbf{r}))^2 - 2ye^{-\frac{1}{2}g_>(0)}\int d^2x \cos(2\pi\phi(x)) - y^2e^{-g_>(0)}\int dxdy[\cos(2\pi(\phi_<(x) + \phi_<(y)))(\tag{90}$$

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

$$y \to y(b) = b^2ye^{-\frac{1}{2}g_>(0)} \tag{91}$$
$$g_>(0) = \frac{2\pi}{T}\int_{\Lambda/b}^{\Lambda}\frac{dk}{k} = \frac{2\pi}{T}\ln b \tag{92}$$

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

$$\cos(2\pi(\phi_<(x)-\phi_<(x'))) \approx 1-\frac{1}{2}(2\pi(x'-x)\cdot\nabla\phi_<(x))^2 \tag{93}$$

$$\cos(2\pi(\phi_<(x)+\phi_<(x'))) \approx \cos(4\pi\phi_<(x)) - 2\pi\sin(4\pi\phi_<(x))((x'-x)\cdot\nabla\phi_<(x)) \tag{94}$$

Then we got

$$T \to T(b) = T + 2\pi^2 y^2 e^{-g_>(0)} \int d^2x (e^{g_>(x)}-1)x^2 \tag{95}$$

$$g_>(x) = \frac{1}{T}\int_{\Lambda/b}^{\Lambda}\frac{dk}{k}\int_0^{2\pi} d\alpha e^{ikx\cos(\alpha)} = \frac{2\pi}{T}\ln b J_0(\Lambda x) \tag{96}$$

Here we need treat this integral carefully.

$$\begin{aligned} g_>(x) &= \int_0^{\Lambda}\frac{d^2q e^{i\mathbf{q}\cdot\mathbf{x}}}{Tq^2} - \int_0^{\Lambda/b}\frac{d^2q e^{i\mathbf{q}\cdot\mathbf{x}}}{Tq^2} \\ &\approx \frac{2\pi}{T}(\int_0^{\infty} dq\frac{qJ_0(qx)}{q^2+(\Lambda/b)^2} - \int_0^{\infty} dq\frac{qJ_0(qx)}{q^2+(\Lambda)^2}) \\ &= \frac{2\pi}{T}(K_0(x\Lambda/b)-K_0(x\Lambda)) \qquad = -\frac{2\pi x\Lambda\ln b}{T}\frac{dK_0(z)}{dz}_{z=x\Lambda} \end{aligned} \tag{97}$$

$$\begin{aligned} T \to T(b) &= T - 2\pi^2 y^2 \ln b \int d^2x x^2 \frac{2\pi x\Lambda}{T}\frac{dK_0(z)}{dz}_{z=x\Lambda} \\ &= T + \frac{1}{2T}(\frac{y(4\pi)^2}{\Lambda^2})^2 \ln b \end{aligned} \tag{98}$$

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

$$\begin{aligned} \frac{dT}{d\ell} &= y^2/2T + O(y^4)\ , \\ \frac{dy}{d\ell} &= (2-\pi/T)y + O(y^3)\ , \end{aligned} \tag{99}$$

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.

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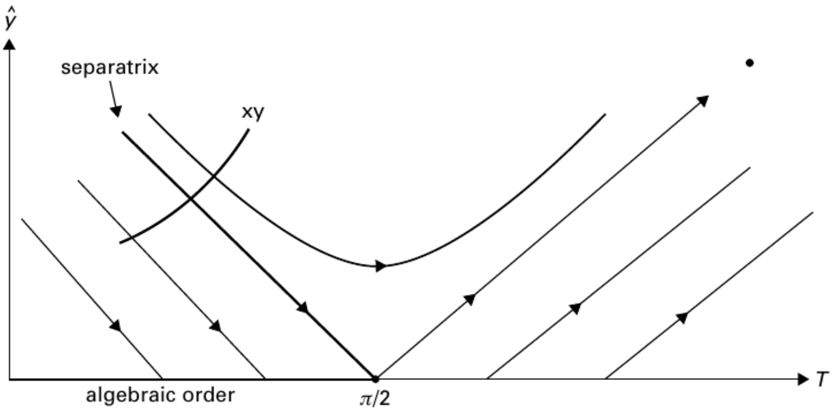

FIG. 2: Renormalization group flow of the temperature and the fugacity in the sine-Gordon model. The thick line separates the flows towards the line of fixed points at $T < T_{KT}$ and $y = 0$ that represent the algebraically ordered superfluid phase from the flow towards a high-temperature high-fugacity sink, representing the exponentially disordered phase. The XY line represents the set of initial values at different temperatures in the XY model.