The Berezinskii–Kosterlitz–Thouless transition

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Contents

1 Introduction

The Berezinskii–Kosterlitz–Thouless (BKT) transition was the first example of a topological phase transition studied in condensed matter systems. In these types of transitions there is no spontaneous symmetry breaking (SSB) differentiating the phases, and the underlying mechanism separating these phases can be well explained by the existence of topologically stabilized excitations called vortex. The origin of these defects are purely topological and can be explained in a more general set with the theory of homotopy groups. In this work we will discuss a particular system known as the XY-model that exhibit these topological phases.

2 Aspects of the XY-model

The goal of this section is to present the general aspects of the XY-model and its phase transition phenomenologically, with some brief explanations on the origins of the topological defects.

2.1 Mermin-Wagner theorem

There is a result proved first by Mermin and Wagner [5], which says that it is not possible to have SSB in short-ranged interacting theories for dimensions $d \leq 2$. This is expected since the two-point function of the Nambu-Goldstone bosons generated by the SSB have an infrared divergence.

The lack of symmetry breaking in two dimensions can be rigorously proved with the Bogoliubov inequality as in [1]. Here we will show a particular case of the theorem: Consider the n-vector model in d dimensions:

$$H = -J \sum_{\langle ij \rangle} S_i \cdot S_j \tag{2.1}$$

where the sum is taken over neighboring points. The hamiltonian naturally has a global $O(n)$ symmetry that we expect will break in a transition to an ordered state. Suppose, by contradiction, that there is an ordered phase in the x direction meaning that the spin fields can be written as $S = \left(\sqrt{1 - \sum_\alpha \sigma_\alpha^2}, \sigma_\alpha \right)$, $\alpha \in \{1, ..., n-1\}$, where $|\sigma_\alpha| << 1$. Expanding the hamiltonan (2.1) in the σ fields and taking the continuum limit approximation we arrive at the following field theory

$$H = \frac{J}{2} \int \mathrm{d}^d \mathbf{r} \sum_\alpha (\nabla \sigma_\alpha)^2$$

Where σ_α are the corresponding Nambu-Goldstone bosons. Our hypothesis must be at least self-consistent, meaning that to first order in perturbation the magnetization $\langle S \cdot \hat{x} \rangle \approx 1 - \frac{1}{2} \sum_\alpha \langle \sigma_\alpha^2 \rangle$ should be finite (and non-zero). On the other hand

$$\left\langle \sigma_\alpha^2(0) \right\rangle = \frac{1}{\beta J} \int_{1/L}^{1/a} \frac{\mathrm{d}^d \mathbf{k}}{(2\pi)^d} \frac{1}{k^2}$$

is divergent for dimensions $d \leq 2$ in the thermodynamic limit. Note that although there is no SSB we may still look for some sort of phase transition. In seminal works of Kosterlitz and Thouless [2], they proposed "a new definition of order" that does not involve any symmetry breaking. The $O(2)$ version of (2.1) in $d = 2$, know as the XY-model, exhibit these sort of phases.

2.2 Spin-spin correlation function

To see why the XY-model have a unique status among other types in (2.1) we analyse the behaviour at high and low temperatures of the spin-spin correlation function $\langle S_0 \cdot S_x \rangle = \langle \cos(\theta_x - \theta_0) \rangle$. The corresponding hamiltonian can be written in terms of the angles $H = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$. At high temperatures we can expand the exponential in the partition function of the system[1]:

$$\mathcal{Z} = \int \mathcal{D}S e^{-S_E} = \int_0^{2\pi} \Pi_k \frac{d\theta_k}{2\pi} \Pi_{\langle ij \rangle} \left(1 + J \cos(\theta_i - \theta_j) + O(J^2) \right)$$

where β was absorbed in the definition of $J \to \beta J$. It's clear that only "loop" terms connecting neighboring sites in the lattice will contribute to $\mathcal{Z}$ [2]. To leading order in J we observe an exponential decay

$$\langle S_0 \cdot S_x \rangle \approx \left(\frac{J}{2} \right)^{|x|} = e^{-\frac{|x|}{\xi}} \tag{2.2}$$

where the correlation length is defined as $\xi^{-1} = \ln(2/J)$. Now in the low temperature limit fluctuations between neighboring sites are strongly penalized so we can recover the continuum limit $H = \frac{J}{2} \int \mathrm{d}^2 r \, (\nabla \theta)^2$ and arrive at

[1] In the following discussion we use the Euclidean space formulation of QFT.

[2] This is easy to see with the identity $\int_0^{2\pi} \frac{d\theta_k}{2\pi} \cos(\theta_i - \theta_k) \cos(\theta_k - \theta_j) = \frac{1}{2} \cos(\theta_i - \theta_j)$

$$\langle S_0 \cdot S_x \rangle \sim e^{-\frac{1}{2J}\int_{1/|x|}^{1/a}\frac{d^2k}{(2\pi)^2}\frac{1}{k^2}} = \left(\frac{a}{|x|}\right)^{\frac{T}{4\pi J}} \tag{2.3}$$

which is exactly the behaviour of correlation functions near the critical point of some phase transition. Although the correlations goes to zero when $|x| \to \infty$ for any non-zero temperature, the singular behaviour of (2.3) motivates the search for a new kind of long range order where it's possible to have phase transitions independent of the asymptotics of the two-point function.

2.3 Phenomenology of the BKT phase transition

The mechanism behind such transition can be understood by looking at the flow of couplings in parameter space with the renormalization procedure, and this is done in detail on the next section. For now we can make the calculations with an intuitive line of reasoning. The topological structure of the target manifold S^1 related to the angular field $\theta : \mathbb{R}^2 \to S^1$ allows for the possibility of special field configurations.

(a) Vortex of charge $n = 1$. The black circle encloses the topological defect core

(b) Vortex of charge $n = -1$

Figure 1: Vortex and antivortex configurations

In figure (1) we see that it's possible to have field configurations that cannot be deformed continuously to the "ordered state" and also cannot be deformed into each other. These field configurations are topological defects called vortices.[3]. Given a closed curve γ that encircles the topological defect core (see figure 1a), we define its line integral as:

$$\int \nabla\theta \cdot \mathrm{d}\mathbf{l} = 2\pi n \tag{2.4}$$

where $n \in \mathbb{Z}$ is called a topological charge. To see how these vortices can be used to describe the transition we proceed to calculate the free energy associated with the creation of one vortex of charge $n = 1$. Choosing γ as a circle, far away from the center $\nabla\theta$ is approximately constant in the azimuthal direction so that:

$$\nabla\theta = \frac{n}{r}\mathbf{e}_z \times \mathbf{e}_r \tag{2.5}$$

The action takes a simple form

$$S = S^{\text{core}}(a) + \frac{J}{2}\int_a d^2r(\nabla\theta)^2 = S^{core}(a) + \pi J \ln(L/a)$$

We separate terms close to the center $S^{\text{core}}(a)$ where details of the lattice geometry matters, and far from the center where we substitute (2.5). Then the partition function and free energy are given by:

[3]The ordered state here is defined as a vortex with topological charge $n = 0$.

$$\mathcal{Z}_1 \approx \left(\frac{L^2}{a^2}\right) e^{-S^{core}(a) - \pi J \ln(L/a)}$$

$$F \approx (\pi J - 2T) \ln(\frac{L}{a})$$

The first factor in the partition function accounts for the configurational entropy: the number of possible places to accommodate the vortex on the lattice. We see from the free energy that low temperatures regimes are not favorable to create vortices given the required energy to do so. However at high temperatures the configurational entropy is favorable for the creation of vortices. The critical temperature where the free energy changes sign and there is a phase transition happens at $T_c = \frac{\pi J}{2}$.

Therefore we see that the condensation of vortices-antivortices pairs is what characterises the ordered phase, and at high temperatures these pairs have enough energy to unbound and create some form of plasma. The arguments given here covers much of the phenomenology of the BKT phase transition. However one may question if high order terms in the gradient expansion of S can attenuate or even destroy the transition, so we need the machinery of perturbation theory to answer these questions.

2.4 Topological Defects

Before we start the discussion in the language of perturbation theory it's interesting to question the origin of these topological stable solutions. We saw that the general arguments for the existence of a phase transition in the XY-model relies on the assumption that topological defects of different charges cannot be deformed into each other and equation (2.4) holds. Note that since θ is not defined in the vortex core we can cut it off of the domain $\theta : \mathbb{R}^2 \setminus \{0\} \to S^1$. To better understand the connection with topology we have to define some keys concepts:

Definition 2.1. *Two maps $\phi_1, \phi_2 : X \to T$ are homotopy equivalent $\phi_1 \sim \phi_2$ if there exists a continuous map H such that:*

$$H : X \times [0,1] \to T$$
$$H(.,0) = \phi_1(.),\ \ H(.,1) = \phi_2(.)$$

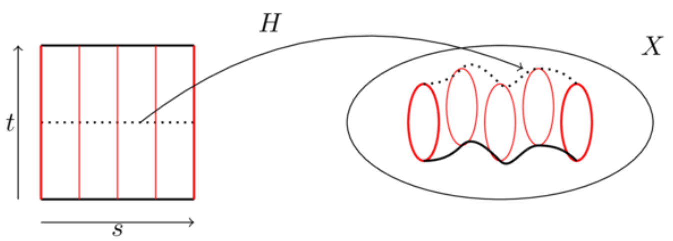

Figure 2: Visualizing the homotopy map

Definition 2.2. *Let $\phi_i : S^1 \to T$ then the set of all equivalent classes generated by the equivalent relation above $\sim$ is called the first homotopy group $\pi_1(T)$. This set acquires a group structure with the composition law*

$$\phi_1 * \phi_2 = \begin{cases} \phi_1(s), & s \in [0, 1/2] \\ \phi_2(2s-1), & s \in [1/2, 1] \end{cases} \tag{2.6}$$

The first definition allows us to make sense of deforming field configurations into each other as can be seen in figure 2. Since the punctured plane $\mathbb{R}^2 \setminus \{0\}$ is homotopy equivalent to S^1 [4] they have the same (up to an isomorphism) homotopy group which in this particular case is given by $\pi_1(S^1) = \mathbb{Z}$ [4]. Therefore each field can be assigned to a unique topological sector $n \in \pi_1(S^1)$ and different classes are all **homotopically distinct**. This is exactly the characterization we did before with the winding number in (2.4).

3 Perturbation theory of the XY-model

To treat the problem perturbatively we need to rearrange and separate the different channels in $\mathcal{Z}$ corresponding to harmonic fluctuations (spin waves) and the topological defects. Furthermore we will see how the screening effect in the stiffness J is generated by the unbound of charged pairs $n = \pm 1$.

3.1 Harmonic and topological channels

We can separate the fields $\nabla\theta = \nabla\phi - \nabla \times (\hat{\mathbf{e}}_{\mathbf{z}}\psi)$ in irrotational spin wave fluctuations ϕ and a rotational part where ψ is defined through

$$\int \nabla^2\psi \, \hat{\mathbf{e}}_{\mathbf{z}} \cdot d\mathbf{S} = \oint \nabla\theta \cdot \mathrm{d}l = 2\pi n$$
$$\implies \nabla^2\psi = 2\pi \sum_i n_i \delta^2(r - r_i)$$

that possess a simple solution $\psi = \sum_i n_i \ln(|r - r_i|)$ given by the sum of 2D Couloumb potentials. We can then calculate the total action assuming that $\sum_i n_i = 0$:

$$\begin{aligned} S =& \frac{J}{2} \int \mathrm{d}^2 r \, (\nabla\phi - \nabla \times (\hat{\mathbf{e}}_{\mathbf{z}}\psi))^2 \\ =& \frac{J}{2} \int \mathrm{d}^2 r \, (\nabla\phi)^2 - 2\nabla\phi \cdot \nabla \times (\hat{\mathbf{e}}_{\mathbf{z}}\psi) + (\nabla \times (\hat{\mathbf{e}}_{\mathbf{z}}\psi))^2 \\ =& \frac{J}{2} \int \mathrm{d}^2 r \, (\nabla\phi)^2 + \sum_i S^{core}_{n_i} - 2\pi^2 J \sum_{i<j} n_i n_j C(r_i - r_j) \\ \doteq& S_{\text{s.w}} + S_t \end{aligned}$$

where we integrate by parts in the third equality and define $C(r_i - r_j) = \frac{\ln|r_i - r_j|}{2\pi}$ as the Coulomb potential. The S_i^{core} terms comes from the regularization at points located in the vortex core where $C(x)$ has a singular behaviour. The partition function is then factorized in these two channels $\mathcal{Z} = \mathcal{Z}_{\text{s.w}}\mathcal{Z}_t$ [5] where:

$$\mathcal{Z}_{\text{s.w}} = \frac{J}{2} \int \mathrm{d}^2 r (\nabla\phi)^2, \quad \mathcal{Z}_t = \sum_{N=0}^{\infty} \frac{1}{(N!)^2} \int \Pi_{i=1}^{2N} d^2 r_i e^{-S_t}$$

and r_i are the scaled positions of the vortex centers. To simplify our analysis we consider only charges $n_i = \pm 1$ and define $y_0 = e^{-S^{\text{core}}_{\pm 1}}$ as the fugacity. Then

[4] The definition of homotopy equivalence in sets are similar to that of functions: Two topological spaces X, Y are homotopy equivalent if there exists continuous maps $f : X \to Y$, $g : Y \to X$ such that $f \circ g \sim id_Y$ and $g \circ f \sim id_X$.

[5] Recall that the spin wave fluctuations corresponds to a different homotopy class so we can separate the degrees of freedom

$$\mathcal{Z}_t = \sum_{N=0}^{\infty} \frac{y_0^{2N}}{(N!)^2} \int \Pi_{i=1}^{2N} d^2 r_i e^{4\pi^2 J \sum_{i<j} n_i n_j C(r_i - r_j)} \tag{3.1}$$

is the relevant partition function that will have the non-analytical properties required for a phase transition. An important feature of the partition function (3.1) is that it describes exactly the same physics of a neutral Coulomb plasma, i.e, a grand canonical ensemble of charges $n = \pm 1$ with a 2D Coulomb interaction.

3.2 Insulating to metallic transition

There is a simple way to compute the difference between the phases. Suppose that we put two test charges separated by a distance x. At low temperatures we expect that they feel the bare potential $C(x)$. As the temperature increases the formation of internal pairs is energetically favorable and consequently there will be a screening effect changing the interaction between the test charges $C'(x) = C(x)/\epsilon$. The phenomena is analogous to that of a transition from an insulating phase to a metallic one where $\epsilon \to \infty$.

If the test charges are located at r and r' we can measure the effective interaction between them by the following equation

$$e^{-S_{eff}(r-r')} \doteq \left\langle e^{-4\pi^2 J C(r-r')} \right\rangle_t$$

Since at low temperatures $y_0 \to 0$ the problem can be treated perturbatively to lowest order in the fugacity. Moreover one can measure the screening effect using only one pair of internal charges s,s':

$$\begin{aligned} & e^{-S_{eff}(r-r')+4\pi^2 J C(r-r')} \\ &= \frac{1 + y_0^2 \int d^2 s d^2 s' e^{4\pi^2 J(-C(s-s')+C(r-s)-C(r-s')-C(r'-s)+C(r'-s'))} + O(y_0^4)}{1 + y_0^2 \int d^2 s d^2 s' e^{-4\pi^2 J C(s-s')} + O(y_0^4)} \\ &= 1 + y_0^2 \int d^2 s d^2 s' e^{-4\pi^2 J C(s-s')} \left(e^{4\pi^2 J D} - 1 \right) + O(y_0^4) \end{aligned}$$

where $D = C(r-s) - C(r-s') - C(r'-s) + C(r'-s') \approx -\mathbf{x} \cdot \nabla_{\mathbf{X}} (C(\mathbf{r} - \mathbf{X}) - C(\mathbf{r}' - \mathbf{X}))$ in the limit of small separations $\mathbf{x} = \mathbf{s}' - \mathbf{s}$ when we change to the center of mass coordinates $\mathbf{X} = \frac{\mathbf{s}+\mathbf{s}'}{2}$. Expanding $\exp[4\pi^2 J D]$ to second order, all the terms linear in $\mathbf{x}$ vanishes after the integration, and the second order contribution simplifies to $\frac{x^2 (\nabla_X C)^2}{2}$ when integrated in the angular variables. After these manipulations we arrive at the effective action for the interacting charges:

$$e^{-S_{eff}(r-r')} = e^{-4\pi^2 J C(r-r')} \left[1 + 16\pi^5 J^2 y_0^2 C(r-r') \int_1^{\infty} dx\, x^3 e^{-2\pi J \ln x} + O(y_0^4) \right]$$

Assuming that the effective action can be written as $S_{\text{eff}} = 4\pi^2 J_{\text{eff}} C(r-r')$ and exponentiating the right hand side we get:

$$J_{\text{eff}} = J - 4\pi^3 J^2 y_0^2 \int_1^{\infty} dx x^3 e^{-2\pi J \ln x} \tag{3.2}$$

While the integral above converges for large values of x, it diverges for $J \leq \frac{2}{\pi}$ similar to what happens in perturbation calculations of the ϕ^4-theory for $d < 4$. Note that this is the same value where the free energy changes its sign and the plasma phase is expected to dominate. To overcome the divergences we have to use a renormalization procedure.

4 Renormalization of the XY-model

To calculate the β function of the couplings J^{-1} and y_0 [6] we can slip the integral (3.2) into two parts and rescale the variable of integration:

$$\int_1^\infty = \int_1^b + \int_b^\infty$$
$$x \to x/b$$

With this procedure we can absorb the finite part of the integral in the definition of $\tilde{J} = J - 4\pi^3 J^2 y_0^2 \int_1^b dx x^3 e^{-2\pi J \ln x}$ and rescale $\tilde{y_0} = b^{2-\pi J} y_0$. Then

$$J_{\text{eff}}^{-1} = \tilde{J}^{-1} + 4\pi^3 \tilde{y}_0^2 \int_1^\infty dx x^{3-2\pi J} + O(y_0^4) \tag{4.1}$$

Consider that the renormalization scale is $b = e^l \approx 1 + l$ so we can calculate the running of couplings:

$$\frac{dJ^{-1}}{d\ln b} = 4\pi^3 y_0^2 + O(y_0^4)$$
$$\frac{dy_0}{d\ln b} = (2 - \pi J) y_0 + O(y_0^3)$$

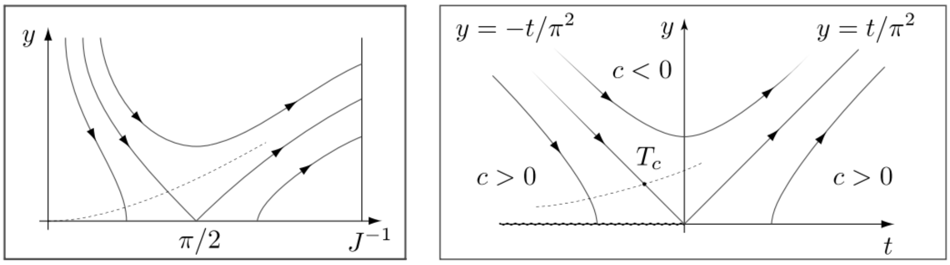

Figure 3: Renormalization group flow

Figure 3 show the renormalization group flow in parameter space. There is a fixed line $y_0 = 0$ where, at low temperatures, the flow terminates and $J_{eff} \geq 2/\pi$. This is the insulating regime. However at some temperature T_c the coupling y_0 becomes relevant and the flow asymptote to large values of J^{-1} indicating a phase transition. We can study the critical behavior changing variables $t = J^{-1} - 2/\pi$ and linearizing the system:

$$\frac{dt}{d\ln b} = 4\pi^3 y^2 + O(ty^2) \tag{4.2}$$
$$\frac{dy}{d\ln b} = \frac{4}{\pi} t y + O(t^2 y) \tag{4.3}$$

we see that the dynamical system is inherently non-linear, in contrast with the other types of phase transitions we studied before. The conserved quantity $c \doteq t^2 - \pi^4 y^2$ separate the flows at the critical trajectory $c = 0$, hence in low temperatures close to T_c we set $c \sim -b^2(T_c - T)$. Therefore we can estimate the effective stiffness

[6] Since J^{-1} scales with the temperature it is more convenient to consider the inverse rather than J.

$$J_{\text{eff}} = \frac{2}{\pi} + \frac{4b}{\pi^2}\sqrt{T_c - T}$$

so J_{eff} will have a square root singularity. At high temperatures we can set $c = b^2(T - T_c)$ and integrate the second differential equation (4.3):

$$\frac{4l}{\pi} \approx \frac{1}{b\sqrt{T - T_c}} \arctan\left(\frac{t}{b\sqrt{T - T_c}}\right)$$

The maximum scale up to where perturbation theory breaks is $l^* \approx \frac{\pi^2}{8b\sqrt{T-T_c}}$ so the resulting correlation lenght is given by:

$$\xi \approx ae^{l^*} \approx ae^{\frac{\pi^2}{8b\sqrt{T-T_c}}}$$

showing that the divergence in ξ is not a power law in consequence of the non-linearity in (4.2),(4.3).

5 Conclusion

As we saw before the consequences of topologically stabilized solutions in the long range behaviour of these systems are highly non-trivial. The non-linearity of the RG flow indicates that when considering these types of topological phases a plethora of novel phenomena may appear.

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