Berezinskii-Kosterlitz-Thouless transition in superconductors*

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(Dated: May 17, 2019)

Despite it has been almost a half century since Berezinskii, Kosterlitz and Thouless (BKT) published their seminal work on phase transitions in 2D systems, BKT transition is still an active area of research. BKT transition happens in vortex unbinding in 2D XY-model; dipole unbinding in 2D Coulomb gas and metal-insulator transition (MIT) in 1D chain. These three physically distinct phenomena belong to the same universality class, hence can be interchangeably mapped one into another. In this work, we show mapping procedure from 2D XY-model into 1D chain with sine-Gordon potential. We will focus on one advantage of performing this mapping; ability to assign correct core energies to topological defects in these systems. This is motivated by recent experimental works, which report significantly different defect core energies than predicted by XY-model.

I. INTRODUCTION

One of the lessons we learnt in class is dimensionality plays a key role in identifying the nature of order in various systems. In 3D systems there is a true long-range order at low temperatures and thermal fluctuations destroy the order, making two-point correlation functions decay exponentially at high temperatures. For systems of $d \leqslant 2$ with continuous symmetry, as Mermin and Wagner showed [5], there cannot be a true long-range order due to high level of thermal fluctuations in these dimensions. In 2D XY model, correlations exhibit power law decay at low temperatures, while above certain temperature, correlations decay exponentially. Berezinskii [2], Kosterlitz and Thouless [3], introduced topological defects to explain the nature of this phase transition; from quasi-long-range order to disorder. This transition is called Berezinskii-Kosterlitz-Thouless (BKT) transition and still remains to be a topic of active research.

One of the most exciting areas to study BKT transition is 2D or layered 2D (quasi-two-dimensional) superconducting systems. 2D XY-model was extensively studied to capture the nature of BKT transition in these systems. Although the model was successful in correctly identifying the critical behavior, recently there emerged some discrepancies between theory and experimental findings [6], which we will discuss below.

In this report, we will map BKT transition in 2D XY-model into (1+1)D quantum phase transition in sine-Gordon model. One of the several reasons of doing this, sine-Gordon model gives a flexibility in assigning a core energy to a vortex, whereas in XY-model it is defined solely by a coupling constant between spins. We will also discuss briefly a recent experimental work [6], which demonstrates a BKT transition in copper oxide ultrathin films, a high-T_c superconductor.

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II. MAPPING ON SINE-GORDON MODEL

A sine-Gordon model can be used to describe quantum phase transition in 1D systems. One can find a vast number of works [1] that show analogy between 1D quantum system and 2D classical cases as vortex-unbinding in superfluids. In this section, we will go through steps of this mapping.

We will start with low temperature phase of XY-model.

$$-\beta H_{XY} = J \sum_{<i,j>} \vec{\sigma_i} \cdot \vec{\sigma_j} = J \sum_{<i,j>} \cos(\theta_i - \theta_j) \tag{1}$$

where θ_i is angle of a given spin with respect to some direction, and $< i, j >$ means nearest neighbours.

At low temperatures, we assume θ_i varies very slowly within order of lattice constant a and we can rewrite Hamiltonian in the following form [4] by expanding cosine:

$$-\beta H_{XY} = \frac{J}{2} \int d^2x (\nabla\theta(\vec{x}))^2 \tag{2}$$

If there exist vortices in the lattice, then following equality is satisfied for a closed loop integral around the defect:

$$\oint (\nabla\theta) \cdot ds = 2\pi \sum_i q_i \tag{3}$$

with q_i being the charge, a winding number of a given vortex.

In one of the Problem sets, we have explicitly shown that a interaction between a pair of vortices is Coulombic and system of large number of well separated defects we can treat as a 2D Coulomb gas. We have derived an expression for total energy of system of vortices:

$$-\beta H = \pi J \sum_{i \neq j} q_i q_j \ln(\frac{\vec{r_i} - \vec{r_j}}{a}) + \frac{\pi^2 J}{2} \sum_i |q_i| \tag{4}$$

The first term in above expression describes interaction, second term stands for sum of core energies of defects. Hence in 2D XY-model core energy is solely fixed by coupling constant J and reads as:

$$E_{core} = \frac{\pi^2 J}{2} \tag{5}$$

In the following, we will make two assumptions: i) defects are of only $q_i = \pm 1$; ii) number of positive and negative charges are equal, a neutrality condition. Thus partition function reads as:

$$Z = \sum_{N=1}^{\infty} \frac{1}{(N!)^2} \cdots$$
$$\int D\vec{r} \exp\left[-\beta N E_{core} + \beta\pi J \sum_{i\neq j} q_i q_j \ln(\frac{\vec{r_i} - \vec{r_j}}{a})\right] \tag{6}$$

where N is total number of defects. To compensate for double counting, we need to divide by $(N!)^2$. We define defect fugacity as:

$$y_0 = e^{-\beta E_{core}} \tag{7}$$

and partition function reads:

$$Z = \sum_{N=1}^{\infty} \frac{1}{(N!)^2} y_0^N \int D\vec{r} \exp\left[\beta\pi J \sum_{i\neq j} q_i q_j \ln(\frac{\vec{r_i} - \vec{r_j}}{a})\right] \tag{8}$$

Next we will write a partition function for 1D chain, and analogy between XY and sine-Gordon models will become apparent.

Hamiltonian for 1D chain of length L [1]:

$$-\beta H_{sG} = \frac{v_s}{2\pi} \int_0^L dx \left[K(\partial_x \theta)^2 + \frac{1}{K}(\partial_x \phi)^2 - \frac{2g_u}{a^2}\cos(2\phi)\right] \tag{9}$$

where K is the Luttinger liquid parameter, v_s is the velocity of 1D fermion, last term of the integrand is a sine-Gordon potential with g_u defining strength of the potential.

Next we will show that a partition function of ϕ will have exactly the same form as in Eq.(8). For this we integrate over θ, and partition function for ϕ, will be:

$$Z =$$
$$\int D\phi e^{-W} \sum_{l=0}^{\infty} \frac{1}{l!} d\vec{r_1} \cdots \vec{r_l} (\frac{g_u}{2\pi})^l \cos(2\phi(\vec{r_1})) \cdots \cos(2\phi(r_l)) \tag{10}$$

with:

$$W = \frac{K}{2\pi} \int dx (\partial_x \theta)^2 \tag{11}$$

By decomposing cosines into exponential functions and inspecting that the expression for partition function Eq. [10] is basically an average of exponential functions with Gaussian weights:

$$\left\langle \exp(2i \sum_i \epsilon_i \phi(\vec{r_i})) \right\rangle = \exp\left[2K \sum_{i<j} \epsilon_i \epsilon_j \ln(\frac{r_{ij}}{a})\right] \tag{12}$$

Here we have denoted a variable by ϵ_i, which actually comes from decomposition of cosine:

$$\cos(2\phi(\vec{r_i})) = \sum_{\epsilon_i = \pm 1} \frac{e^{2i\epsilon_i \phi(\vec{r_i})}}{2} \tag{13}$$

Finally, partition function, with some modifications of dummy variables will be:

$$Z = \sum_{N=1}^{\infty} \frac{1}{(N!)^2} (\frac{g}{2\pi})^N \int D\vec{r} \exp\left[2K \sum_{i<j} \ln(\frac{\vec{r_i} - \vec{r_j}}{a})\right] \tag{14}$$

By comparing equations [8] and [14], we can see that 2D XY-model can be mapped into 1D chain with sine-Gordon potential, given:

$$K = \pi\beta k_B J \tag{15}$$

$$g = 2\pi y_0 = 2\pi e^{-\beta E_{core}} \tag{16}$$

The important message that should be taken from this mapping is that in XY-model, core energy of a vortex is fixed by interaction coupling constant, while after mapping the core energy is defined by sine-Gordon potential strength g_u, which can be used to as a fitting parameter for core energy. This flexibility of assigning an energy to the defect is actually hinted by many experiments, i.e. experimental results mostly deviate from XY-model predictions.

III. SUPERFLUID DENSITY JUMP

One of the direct demonstrations of BKT transition is a sudden jump of superfluid density at $T = T_{BKT}$. The analysis of spin system that we have started our discussion with, we can actually directly apply to superfluid in two dimensions. So in this case, J will play a role of superfluid stiffness and we will show that J disappears suddenly at $T = T_{BKT}$, which is also indication of superfluid density n_s jump.

To study the phase transition, we look at coupling constants K and g under renormalization group flow, whose recursion relations reads as [1]:

$$\frac{dK}{dl} = -K^2 g^2 \tag{17}$$

$$\frac{dg}{dl} = (2 - K) g \tag{18}$$

The stiffness (from Eq. [15]) of superfluid is given as:

$$J = \frac{TK(l)}{\pi} \tag{19}$$

As clearly seen from above equations, behavior of RG flow changes at $K = 2$. For $K > 2$ the vortex fugacity goes to zero ($g \to 0$), consequently K will have some finite value and stiffness J^* as well. Instead in the case of $K < 2$, g flows to infinity, K flows to zero, consequently stiffness drops to zero as well. Hence at point $(2, 0)$ in the (K, g) plane, there occurs a phase transition, where superfluid stiffness J jumps from some finite value J^* to zero.

$$K(T_{BKT}) = \frac{\pi J(T_{BKT})}{T_{BKT}} = 2 \tag{20}$$

The relation between stiffness and temperature at the transtion $J(T_{BKT}) = \frac{2T_{BKT}}{\pi}$ is a so called universal relation. One of the things that we have achieved by mapping into sine-Gordon model is that now stiffness at the transition is not fixed, as opposed to original result of Kosterlitz and Thouless [3]. One assumption we made implicitly is superfluid density drop is originating only from vortex anti-vortex unbinding, while in real materials there are other contributions, such as quasiparticle excitations. For the sake of simplicity we neglected those effects.

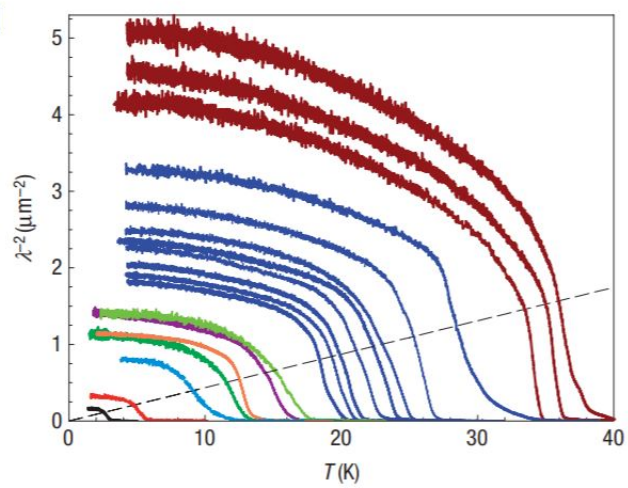

FIG. 1. Figure 1. Superfluid density as a function of temperature [6]

IV. EXPERIMENTAL WORK

Hetel et al.[6] demonstrates BKT transition in ultrathin high-quality copper-oxide superconductor, $YBa_2Cu_3O_{7-\delta}$. They use two-coil mutual-conductance method to measure the penetration depth λ, of the sample. The superfluid density is obtained from penetration depth measurements with relation $n_s \propto 1/\lambda^2$. A direct signature of BKT transition, as was predicted by Nelson and Kosterlitz [7], there must be a sudden sharp drop in superfluid density at the critical point. In this experimental work authors show this phenomenon. We note that, cuprate superconductors have many other competing phases and it is hard single out only one contribution. As a result of these effects, the superfluid density drop is broadened (see FIG. 1). The things we want to emphasize are i) superfluid density drop is mostly dominated by BKT transition; ii) estimate of vortex core energy by XY-model is larger by a factor of 5 [6] than experiment. This indicates the need for more rigorous theories beyond XY-model, and our approach, though not new, can serve as one possibility. Obviously, in strongly correlated materials, as cuprate superconductors, things get more complex. To treat these systems, one needs to take into account: quantum phase fluctuations [6]; Josephson coupling between copper oxide layers; quasiparticle excitations and etc.

V. CONCLUSION

In this report we show one limitation of XY-model for the description of cuprate superconductors; the core energy of a vortex if fixed and deviates significantly from experimental results. To address this issue, we provide a framework, where mapping from 2D XY-model into 1D sine-Gordon model can give one a flexibility of assigning a correct core energy.

Acknowledgement: this work was mostly motivated by "*Quantum physics in one dimension*" by T. Giamarchi [1].

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