

Topological phase transitions (BKT)

Statistical physics seminar by Prof. Wolschin

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Abstract:

The Berezinski Kosterlitz Thouless (BKT) transition is a phase transition in 2D, without the breaking of symmetry and without true long range order. In 2016 Kosterlitz, Thouless and (Haldane) received the nobel prize for the BKT transition and related work. In this work, which is an extended summary of a seminar presentation, the basic theoretical concepts to understand the BKT transition are introduced in the XY model and experimental evidence is discussed.

Essential to the understanding of the BKT transition are vortices, which are topological defects that interact with an interaction energy $\sim \ln(r)$. Because of this logarithmic energy dependence, vortex-antivortex pairs unbind at T_c , causing a transition between a quasi long range order and a more disordered state. Experimental evidence supports that the occurrence of free topological defects causes this transition in the order of the system.

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1 Introduction

1.1 General introduction

The Berezinski Kosterlitz Thouless (BKT) transition is a new type of phase transition which occurs in many physical systems (2D vector spin systems, superfluid films, 2D crystals, superconductors etc.). Kosterlitz, Thouless (and Haldane) received the nobel prize in 2016 for the BKT transition and related work.

The BKT transition is new in the sense that it is a 2D phase transition without the breaking of a symmetry, which does not possess a true long range order below T_c . The system only has a quasi long range order.

For a two dimensional spin vector model on a 2D lattice this means that at the transition the average magnetization still vanishes (no true long range order), but the spin-spin correlation function only decreases algebraically (quasi long range order). The $O(2)$ symmetry of the spin system (i.e. turning all spins at their position) remains unbroken at the transition.

Thus, the BKT transition shows that there can be a phase transition in 2D. It is not forbidden by the Mermin-Wagner theorem since no continuous symmetry is broken.

The transition will turns out to be due to topological defects, more exactly due to the unbinding of vortex pairs.

1.2 Structure

The work is an extended summary of a seminar presentation, it is therefore structured similarly.

First, the XY model is discussed with a strong focus on the important details for the BKT transition. Therefore, the algebraic decay of the correlations at low T and the exponential decay at high T are derived. Next, the notion of a vortex is introduced and the energy of single vortex and of a vortex-antivortex pair is derived. Finally, the BKT transition can be discussed and experimental evidence is presented.

2 XY model

2.1 The XY model

The XY model is a model of 2 dimensional normalised vectors (spins) placed at each side of a square lattice (spacing a). Only the next neighbour spins (i.e. four surrounding spins) interact with each other (short range interaction). The interaction tends to align neighbouring spins ($J > 0$) along the same direction. The hamiltonian βH is given by

$$\beta H = -J \sum_{\langle ij \rangle} \vec{S}_i \vec{S}_j = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) . \quad (1)$$

A typical spin configuration for high T and for $T = 0$ is given by the picture below.

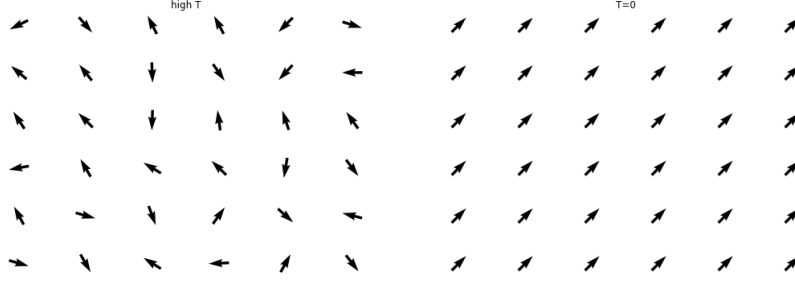


Figure 1: Typical configuration high T (left) and $T = 0$ (right)

2.2 Correlations at high T

The goal is to show that the correlation function decreases exponentially with separation (argument similar to [1]). For high T (i.e. $J \ll 1$) the Boltzmann weight can be approximated to

$$e^{-\beta H} = \prod_{\langle ij \rangle} (1 + J \cos(\theta_i - \theta_j) + \mathcal{O}(J^2)). \quad (2)$$

Furthermore,

$$\int_0^{2\pi} \frac{d\theta_2}{2\pi} \cos(\theta_1 - \theta_2) = 0 \quad (3)$$

and

$$\int_0^{2\pi} \frac{d\theta_2}{2\pi} \cos(\theta_1 - \theta_2) \cos(\theta_2 - \theta_3) = \cos(\theta_1 - \theta_3)/2 \quad (4)$$

can be used to calculate $\langle \vec{S}(0) \vec{S}(x_i) \rangle = \langle \cos(\theta_0 - \theta_i) \rangle$. To obtain the average one integrates over the angle of each spin at each lattice site the factor $e^{-\beta H} \cos(\theta_0 - \theta_i)$ and uses the approximation of equation 2. Therefore one has to integrate many $J \cos$ factors at each order in J and tries to find the non vanishing contribution at leading order.

The idea is now to think of an angle integral as node of the lattice and a factor $\cos(\theta_i - \theta_j)$ as connection between the nodes i and j . Then, equation 3 says that if there is a node which has only one connection, then the contribution of this term vanishes. If a node has two connections, the node goes away and the two connections become one long connection (equation 4).

The $\langle S(0) S(x_i) \rangle = \langle \cos(\theta_0 - \theta_i) \rangle$ factor connects node 0 to node i , the lowest (non vanishing) contribution is therefore shortest path of connections which closes the "loop". The lowest order term is thus of order $\approx J^{\frac{x_i}{a}}$, i.e. the correlation decreases exponentially (x_i is in the exponent) with distance.

2.3 Correlations at low T

At low temperature the angles are assumed to be slowly varying and the configuration is close to figure 1 (right picture). A continuum approximation of the angles and hamiltonian can be made.

$$\begin{aligned} \beta H &= -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \approx \text{const.} + J \sum_{\langle ij \rangle} (\theta_i - \theta_j)^2 / 2 \\ &\approx \frac{J}{2} \int (\nabla \theta)^2 dx^2, \end{aligned} \quad (5)$$

where $\theta(x)$ is now a continuum field which gives the values of the angle at position x . Using this low T approximation, the behavior of the correlation function can be calculated.

$$\begin{aligned}
\langle \vec{S}(0) \vec{S}(x) \rangle &= \langle \cos(\theta(0) - \theta(x)) \rangle = \text{Re}(\langle e^{i(\theta(0) - \theta(x))} \rangle) \\
&= \text{Re}\left(\frac{1}{Z} \int_{\text{angle fields}} \exp(-I(x))\right)
\end{aligned} \tag{6}$$

with

$$I(x) = \int \frac{J}{2} (\nabla \theta)^2 dx^2 + i(\theta(x) - \theta(0)). \tag{7}$$

By going to Fourier space and completing the square, $I(x)$ can be further simplified.

$$\begin{aligned}
I(x) &= \int \left(-\frac{J}{2} k^2 \theta(k) \theta(-k) + i(e^{ikx} - 1) \theta(k) \right) \frac{dk^2}{(2\pi)^2} \\
&= \int -\frac{J}{2} k^2 (\theta(-k) - i(e^{ikx} - 1) \frac{1}{Jk^2}) (\theta(k) - i(e^{-ikx} - 1) \frac{1}{Jk^2}) \frac{dk^2}{(2\pi)^2} \\
&\quad - \int \frac{1}{2Jk^2} (e^{ikx} - 1)(e^{-ikx} - 1) \frac{dk^2}{(2\pi)^2}
\end{aligned} \tag{8}$$

The important thing to notice is that the last line of the expression for $I(x)$ is independent of θ , while the first line only has a constant function added to $\theta(k)$. The latter can be seen as a change of variable in $\int_{\text{angle fields}}$, while the former can be pulled in front of $\int_{\text{angle fields}}$. Using these observations and normalisation equation 6 becomes

$$\begin{aligned}
\langle \vec{S}(0) \vec{S}(x) \rangle &= \text{Re}(\exp \int \frac{1}{2Jk^2} (e^{ikx} - 1)(e^{-ikx} - 1) \frac{dk^2}{(2\pi)^2}) \\
&= \exp\left(\frac{1}{J} \int \frac{1 - e^{ikx}}{k^2} \frac{dk^2}{(2\pi)^2}\right).
\end{aligned} \tag{9}$$

The integral $I(x)$ in the exponential is finite for small k , but it diverges for large k . If a large k cutoff Λ is introduced, then the large $|x|$ asymptotics of $I(x)$ can be obtained. It involves a small analysis of the Bessel function of order 0, more details are in [2] on p.295/296. It turns out

$$I(x) = \frac{1}{2\pi J} \ln(\Lambda|x|) \text{ for } |x| \rightarrow \infty. \tag{10}$$

This result shows that the correlation function decreases algebraically in 2D (the dimension was essential for the integral $I(x)$).

3 Vortices

3.1 Vortices

Vortices are stable defects that satisfy specific boundary conditions. Stable means that they satisfy

$$\frac{\delta(\beta H)}{\delta \theta} = 0 \iff 0 = \Delta \theta. \tag{11}$$

The boundary conditions that they satisfy are

$$\oint \nabla \theta \, ds = \theta(\gamma(1)) - \theta(\gamma(0)) = n 2\pi, \quad n \in \mathbb{Z}, \tag{12}$$

if the vortex is encircled and $\oint \nabla \theta \, ds = 0$ otherwise. Fields with $n = 1$ are called vortex and fields with $n = -1$ antivortex. A possible gradient field, $\nabla \theta$, can be calculated from equation 12 if one assumes $\nabla \theta(x) = \nabla \theta(\rho) = f(\rho) e_\phi$.

$$\oint \nabla \theta \, ds = 2\pi \rho f(\rho) = n 2\pi \Rightarrow \nabla \theta = \frac{n}{\rho} e_\phi \tag{13}$$

As an illustration a possible configuration of spins forming a vortex $n = 1$ and an antivortex $n = -1$ is shown below.

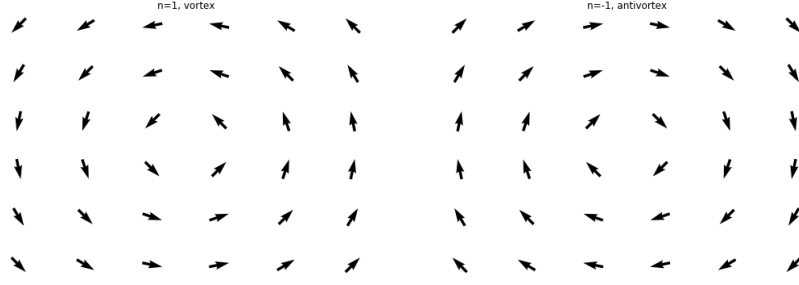


Figure 2: Spin configuration for a vortex (left) and an antivortex (right)

From figure 2 and equation 12 (otherwise it would vanish due to Stokes or alternatively because the angular direction is not well defined in the center) it is clear that one introduces a singularity at the core of the vortex (in the continuum approximation). As the figure shows, the associated divergence of the energy in the continuum approximation is not physical since at the center the approximation simply fails (the system is defined on a lattice, there is no center). Therefore it makes sense to introduce a short distance cutoff a beyond which the details of the core matter.

3.2 Energy vortex and antivortex

There are different ways to calculate the energy. The presented path (which follows [2]) allows for an easy generalisation to more complicated situations.

$$E_v = E_{core} + \frac{J}{2} \int_A (\nabla \theta)^2 dx \quad (14)$$

The area A (see picture below) is chosen such that core of the vortex is left out to avoid the singular behavior and to avoid that θ is not continuous on the full circle. Then all integral theorems can be applied without problem.

$$E_v = E_{core} + \frac{J}{2} \int_{\partial A} \theta \nabla \theta \, d\Sigma - \frac{J}{2} \int_A \theta \Delta \theta \, dx \quad (15)$$

$$= E_c + \frac{J}{2} (\theta^+ - \theta^-) \int_a^R f(\rho) \, d\rho \quad (16)$$

$$= E_c + Jn\pi \int_a^R \frac{n}{\rho} d\rho = E_c + J\pi n^2 \ln\left(\frac{R}{a}\right), \quad (17)$$

with R a finite system size. This result is very important for the BKT transition. The energy of a single vortex diverges logarithmically in a system of infinite size.

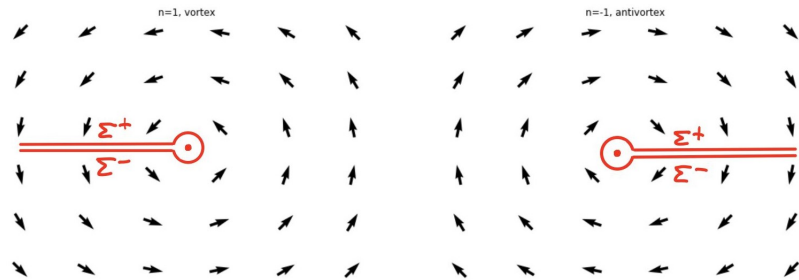


Figure 3: Boundaries of integration Area A for vortex (left) and antivortex (right)

3.3 Energy vortex-antivortex pair

For the statistical discussion of the occurrence of vortices, it is important to study what the energy of multiple vortices is. As an elementary building block the energy of two vortices with charges n_1 and n_2 is calculated.

$$\beta E = 2\beta E_c + \frac{J}{2} \int_A (\nabla\theta^{(1)} + \nabla\theta^{(2)})^2 dx \quad (18)$$

$$= \beta E_1 + \beta E_2 + \frac{J}{2} \int_A (\nabla\theta^{(1)} \nabla\theta^{(2)}) dx, \quad (19)$$

where A is now the union of both picture from figure 3.2. The calculation is identical to the one from the previous subsection, except for the fact that there are two boundaries, the integration starts from r (separation of the two vortices) and $n^2 \leftrightarrow n_1 n_2$.

$$\begin{aligned} \Rightarrow \beta E &= \beta E_1 + \beta E_2 + J n_1 n_2 2\pi \ln\left(\frac{R}{r}\right) \\ &= \beta E_{\text{cores}} + J\pi(n_1 + n_2)^2 \ln\left(\frac{R}{a}\right) + J 2\pi n_1 n_2 \ln\left(\frac{a}{r}\right) \end{aligned} \quad (20)$$

This formula for the energy merits a small discussion.

A neutral vortex pair (i.e. $n_1 = -n_2$) has finite energy (the energy does not depend on $\ln(\frac{R}{a})$) and can therefore appear at every finite temperature T . A vortex-antivortex pair ($n_1 = 1$, $n_2 = -1$) has the lowest energy and therefore appears more often. The spins get aligned fairly quickly far away from the cores for a neutral pair.

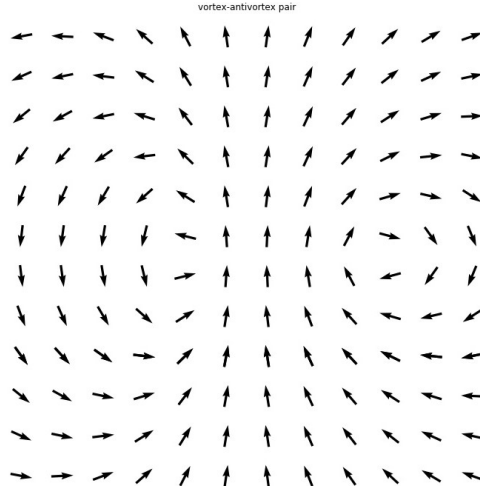


Figure 4: Spin configuration of a vortex-antivortex pair

There is also an attractive/repulsive force between two vortices due to the $n_1 n_2$ term. For a neutral system of multiple vortices, the interaction hamiltonian can be written in the form

$$\beta H_v = J \sum_{ij} \pi n_i n_j \ln\left(\frac{a}{|x_i - x_j|}\right). \quad (21)$$

4 BKT in XY model

4.1 Phenomenology

The description of the BKT transition that will now be presented needs further justification, some additional justification is in the next two subsections.

At very low temperatures (i.e. below T_c) only vortex- antivortex pairs are important because of their finite energy. They do not disorder the system sufficiently to cause a breakdown of the low T approximation. The correlation function decreases algebraically with distance. As the temperature is increased further and further, the average separation of the pairs increase until the pairs unbind at T_c .

After the unbinding, there are free vortices in the system, which disorder the system enough to cause a breakdown of the low temperature approximation. The correlation decreases now exponentially with distance.

At T_c there is a phase transition, the rotational symmetry of the system is not broken spontaneously, $\langle s(x) \rangle$ still vanishes.

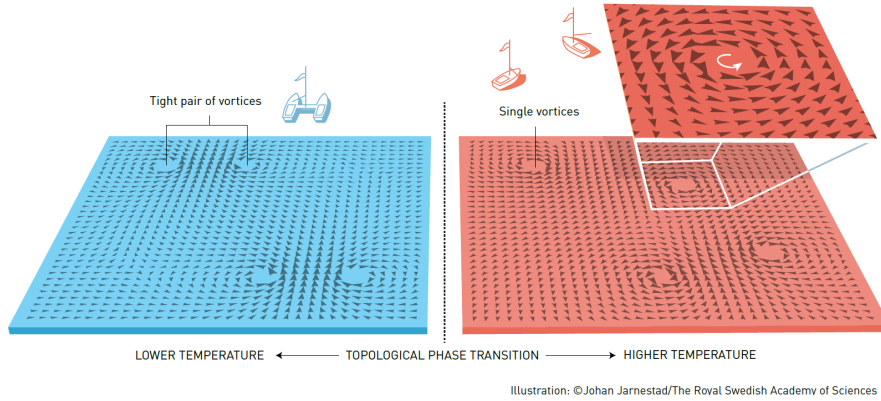


Figure 5: Diagram BKT transition [3]

4.2 Vortex unbinding - simple argument

A system at thermal equilibrium prefers to be in states with low free energy F . The free energy associated to the creation of a free vortex is

$$F_{vortex} = E_v - TS_v = J\pi \ln\left(\frac{R}{a}\right) - TS_v. \quad (22)$$

The entropy associated to the creation of a vortex can be estimated to

$$S_v = \ln\left(\left(\frac{R}{a}\right)^2\right), \quad (23)$$

i.e. the vortex can be centered at every lattice side.

$$\begin{aligned} \Rightarrow F &= J\pi \ln\left(\frac{R}{a}\right) - 2T \ln\left(\frac{R}{a}\right) \\ &= (J\pi - 2T) \ln\left(\frac{R}{a}\right) \end{aligned} \quad (24)$$

$$\Rightarrow T_c = \frac{\pi}{2} J \quad (25)$$

Above T_c it is therefore favorable to create free vortices. This estimate turns out to be actually quite good.

It is important to point out that the only crucial ingredient was the logarithmic dependence of the energy (not the nature (i.e. microscopic details)) of a vortex. Other systems with which also have such an energy dependence may therefore also exhibit such a transition. An example is given in the section about experimental evidence.

4.3 Vortex unbinding - more complex argument

So far, many important features have been pointed out (the transition in the correlation behavior), but not been properly argued for. Only a sketch of a more complex argument providing the necessary arguments is given, the full argument can be found in [2]. It makes sense, however, to read [4] first.

The constant J measures how much energy it costs to turn neighbouring spins against each other at fixed T . If one wants to incorporate the effect of vortices into the low T approximation, then one has to incorporate them into J . It is then called J^R . One would expect J^R to decrease, since if vortices are present the system is already more disordered and turning spins against each other should cost less energy.

One can calculate how J^R changes due to the presence of vortices. Then, the vortex interaction hamiltonian (equation 21) and an expansion in fugacity $y = e^{\beta\mu}$ can be used to calculate J^R . Incorporating the effects due to vortices one after another, differential equations for J^R and y can be obtained.

It turns out that the transition temperature is given by

$$J^R(T_c^-)/T = 2/\pi \quad (26)$$

and J^R jumps to zero above T_c . Giving an explicit formula for $J^R(T_c^-)$ is not easy because it depends on y /the core energy. Moreover, the change in behavior of the correlation can also be predicted and connected to the transition.

5 Experimental evidence

5.1 Experimental evidence

Very good experimental evidence for the underlying mechanism of the BKT transition can be found in [5]. Reasons why the arguments given for the XY model should work are given in the next subsection.

The experiment first cools a 3D quantum gas (^{87}Rb), thereby creating a condensate of many atoms. Then, the gas is separated into two clouds, which are compressed into the 2D regime. Finally, after giving the clouds time to equilibrate, the two clouds are put on top of each other and their interference is observed.

The experimental setup looks the following, where the two red planes in a are the compressed clouds.

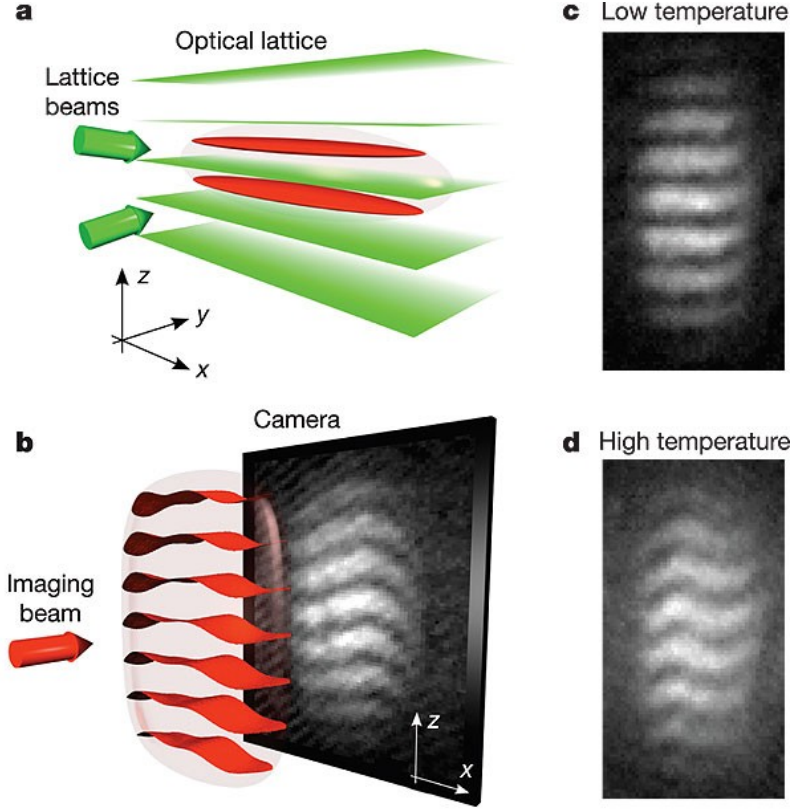


Figure 6: Images from [5] describing the experimental setup (a), the observational method (b) and examples of interference patterns (c,d)

The goal is to extract the correlation behavior of the wavefunction describing the condensate and to measure the interference patterns as a function of temperature. Then, by looking for vortices in the interference pattern, it can be tested, whether, as predicted, the change of decay behavior occurs coincidentally to an onset of free vortices.

As a measure for the temperature the contrast C_0 (higher C_0 means lower temperature, more atoms were condensed which interfere) is used. For the correlation some function obtained from the interference pattern is averaged over different integration lengths L_x , obtained values are plotted as a function of L_x . The functions for different T values are each one fit with $((\frac{1}{L_x})^{2\alpha})$. It can be argued that $\alpha = 0$ corresponds to long range order, $\alpha = 0.5$ to exponential decay and values in between are interpolations thereof. The exponent α obtained from the fit therefore represents some measure for how fast the decay is.

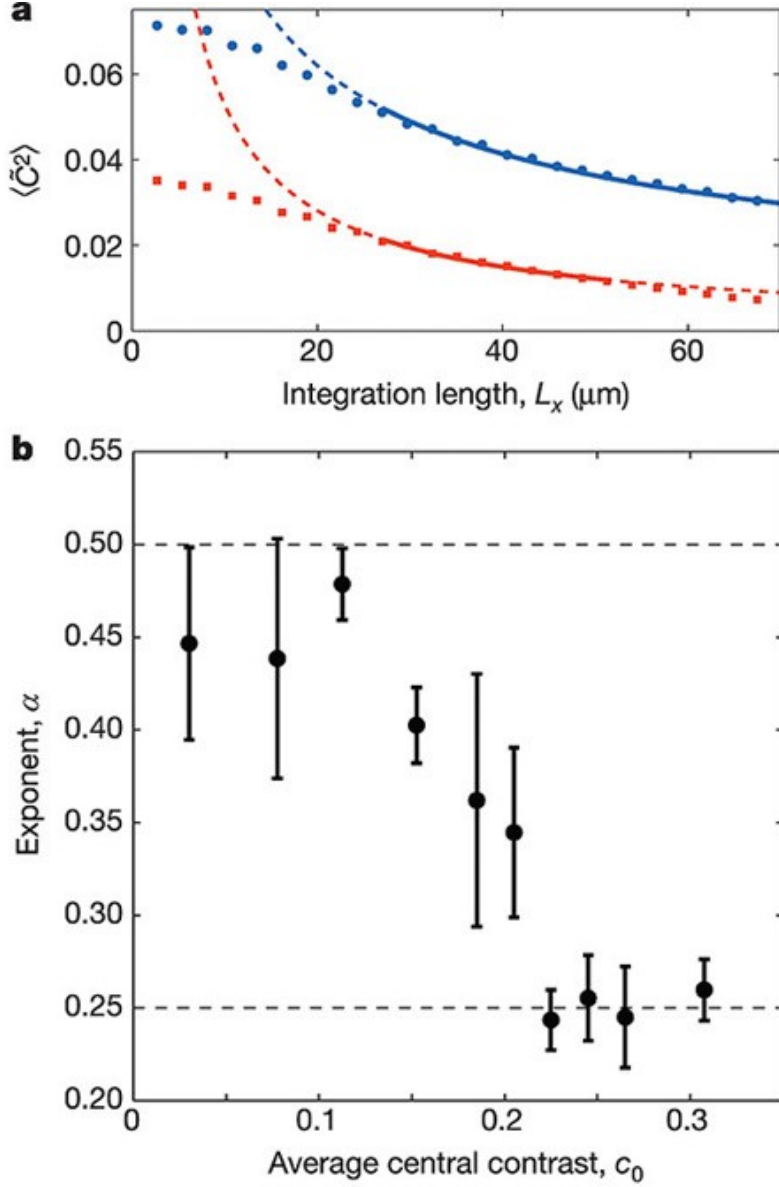


Figure 7: Measurements of the correlations from [5], from a the exponents α are extracted, in b α is plotted as function of T (increase in $c \iff$ decrease in T)

There seems to be a transition in the behavior to the exponential ($\alpha = 0.5$) regime if the temperature is lowered.

Next, the number of free vortices (vortex-antivortex pairs are unobservable, they cause small changes) can be counted as a function of temperature. Vortices cause abrupt change in the interference pattern in contrast to smooth changes due to phonons etc. The results are shown in the following diagram.

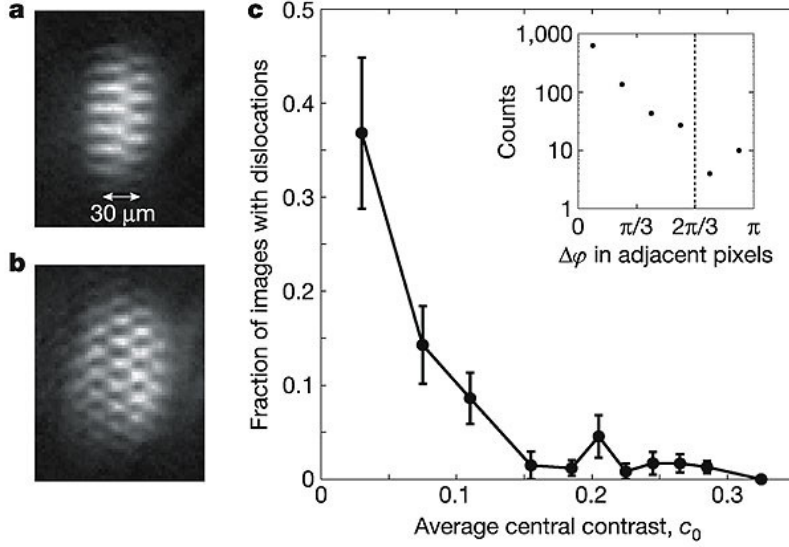


Figure 8: Images and a diagram from [5], a and b show a sharp dislocation and several sharp dislocations, c shows the fraction of images with dislocations as a function of T

There seems to be an onset of free vortices coincidentally to the change in the correlation behavior. This confirms the main prediction of the BKT mechanism, which predicts that the change in decay behavior is due to the unbinding of vortex-antivortex pairs. The obtained transition temperature (for scale $C_0 = 0.15$ corresponds to (290 ± 40) nK) is also within the rather large experimental errors conform with the theory prediction.

The presented discussion of the experiment is not very detailed (merely sketched) and some of the presented arguments need further justification (e.g. there is not a sharp transition temperature, possible reasons: finite system size, residual heating etc.). For a more detailed discussion of the experiment it is recommendable to read [5].

5.2 BKT in superfluid films

The arguments presented for the XY model carry over by replacing J by ρ , the superfluid density, and some prefactors. $\nabla\theta$ becomes the velocity of the superfluid, also written as $\nabla\theta$ and some prefactors, where θ is the phase of the wavefunction describing the superfluid. There is the possibility for the superfluid to form quantized vortices (in the center of the vortex the superfluid is absent, e.g. a rod), these vortices also have a logarithmic dependence of the energy. Therefore, except for some reinterpretations, the arguments really are identical.

6 Summary and outlook

The occurrence of a phase transition in the 2D XY model due to the unbinding of vortex pairs was predicted (BKT transition). From a simple free energy argument an estimate for T_c was obtained $T_c = \frac{\pi}{2}J$. Central to this argument was that the energy of the vortices grows logarithmically, as does the entropy. Nothing else was relevant for the argument, so, other systems (e.g. superfluid films) can also exhibit this transition. A more complex argument, which was only sketched, gave an even better estimate for T_c and also connected the change of the behavior in the correlation function to the transition.

Good experimental evidence ([5]) was presented supporting this phase transition. The experimental evidence confirmed the change in the correlation behavior and also confirmed it's

connection to the occurrence of topological defects. Also, the T_c prediction was confirmed within very loose experimental bounds.

Although the presented experimental evidence supports many central aspects of the BKT mechanism, some details of the theory are simply not tested well enough by the presented experiment. For example the relation for T_c definitely needs more experimental and theoretical investigations as also pointed out in the paper of the experiment. Also, there is a lack of direct evidence for the transition in the XY model, because it is experimentally hard to properly realise such a 2D system.

Since the first prediction of the BKT transition in the early 70's there have been many developments in the field. The BKT transition turned out to be relevant for quite a big set of system, 2D superconductors as another example, because the nature of the charge is not relevant. Therefore, it is very probable that in the future other systems, maybe also important for technical applications (often in 2D), will be discovered that also exhibit a BKT type transition.

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