Seminar on Statistical Physics

University of Heidelberg
Lecturer: Prof. Dr. Georg Wolschin

Topological Phase Transitions

Melda Akyazi

Summer Semester 2020

Abstract

Considering the two-dimensional XY model the Berezinskii-Kosterlitz-Thouless transition is introduced. As the Hohenberg-Mermin-Wagner theorem forbids phase transitions resulting from a transition from a disordered to an ordered state with rising temperature, a new state called quasi-ordered state is defined and the crossover to the disordered high-temperature phase is shown to be due to the unbinding of pairs of vortices and antivortices.

Contents

1. Motivation

Before the 1970s, when topological phase transitions were found, the conventional type of phase transitions was based on the idea of symmetry breaking since the critical point was thought of as the crossover from an ordered to a disordered state. Therefore, if there was no long-range order (LRO) in the low-temperature phase, there should be no phase transition at all. Furthermore, it was expected and rigorously shown in 1966 by Mermin and Wagner in the case of the XY and Heisenberg model that there is no LRO at nonzero temperatures in one and two dimensions [11]. In the same year, Hohenberg showed rigorously that there can be no superfluidity and superconductivity at nonzero temperatures in one and two dimensions [4]. Nevertheless, numerical results and series expansions seemed to be in a contradiction to these results (cf. [9] and references therein), therefore, it was clear that under the assumption that the Hohenberg-Mermin-Wagner theorem was true the investigation of some other kind of phase transition was missing. In the year 1971 Berezinskii first came up with the idea that there has to be another kind of phase transition due to topological defects [1] and two years later Kosterlitz and Thouless had the same idea and expanded the theory [9]. In the following year Kosterlitz used renormalisation group techniques to investigate this problem in some more detail [7]. Since then topological defects became very important and had a wide impact on a large number of systems due to the concept of universality classes which allows to describe systems having the same dimension and nature of order parameter by the same effective theory. This made it possible to use this kind of theory to describe, for instance, two-dimensional superfluids.

In the following we will investigate therefore the simplest model showing a topological phase transition, namely the two-dimensional XY model. The difference in the spin-spin correlations at high and low temperatures will lead us to the definition of a new kind of order and a new kind of phase transition due to topological defects.

2. Two-Dimensional XY Model

We begin our investigations with a regular two-dimensional square lattice Λ with lattice spacing a and assign to each site $\mathbf{x} \in \Lambda$ a two-component unit vector $\mathbf{s}_\mathbf{x}$, interpreted as a classical spin:

$$\mathbf{s}_\mathbf{x} = (\cos(\theta_\mathbf{x}), \sin(\theta_{\mathbf{x}'})), \quad \theta_\mathbf{x} \in [0, 2\pi],$$

where the spin is constrained to rotate in the (XY-) plane of the lattice and $\theta_\mathbf{x}$ is the angle the spin of site $\mathbf{x}$ makes with some arbitrary axis. This classical spin model is therefore called XY model or rotator model and has a continuous symmetry. It is a special case of the n-vector model for $n = 2$.

The Hamiltonian of this system is given by

$$\begin{aligned}\mathcal{H} &= -J \sum_{\langle \mathbf{x},\mathbf{x}' \rangle} \mathbf{s}_{\mathbf{x}} \cdot \mathbf{s}_{\mathbf{x}'} \\ &= -J \sum_{\langle \mathbf{x},\mathbf{x}' \rangle} \cos(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'}),\end{aligned}$$

where $\langle \mathbf{x}, \mathbf{x}' \rangle$ denotes nearest neighbour pairs. In the last line we used a trigonometric identity. In the following we consider only the ferromagnetic case, therefore J is a positive interaction term.

This system has two important invariances (cf. [5]): first, we have a *global invariance* which causes that a rotation of every spin by the very same amount, say α,

$$\theta_{\mathbf{x}} \to \theta_{\mathbf{x}} + \alpha$$

leaves the Hamiltonian unchanged. In addition, there is a *gauge invariance* as the Hamiltonian is invariant under

$$\theta_{\mathbf{x}} \to \theta_{\mathbf{x}} + 2\pi$$

for any site $\mathbf{x}$. The latter invariance is important for us as it is responsible for the occurrence of vortices.

As we are interested in the possibility of a phase transition at finite temperature, we want to know how spin-spin correlations behave at low and high temperatures. We expect no LRO at low temperatures and thus we suspect that the correlation function of the spins fall off for largely separated lattice sites at all temperatures. Nevertheless it is insightful to examine whether there is a change in correlations at all and, as we will see, there is indeed a difference.

2.1. High Temperature Phase

Although it should be clear that at high temperatures there can be no LRO due to thermal fluctuations and therefore spins on lattice sites which are far apart from each other should not be correlated, we will show for the sake of completeness a way to see this in the case of the two-dimensional XY model immediately by looking at the spin-spin correlation function. We follow here [6] and consider the spins at the lattice sites $\mathbf{0}$ and $\mathbf{r}$. Defining $K := \frac{J}{k_B T}$ for k_B being the Boltzmann constant, we see that for a lattice with N lattice sites

$$\begin{aligned}\langle \mathbf{s}_{\mathbf{0}} \cdot \mathbf{s}_{\mathbf{r}} \rangle &= \langle \cos(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}) \rangle \\ &= \frac{1}{Z} \int_0^{2\pi} \cos(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}) \exp\Big(K \sum_{\langle \mathbf{x},\mathbf{x}' \rangle} \cos(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'}) \Big) \prod_{i=1}^{N} \frac{d\theta_i}{2\pi} \\ &= \frac{1}{Z} \prod_{i=1}^{N} \int_0^{2\pi} \cos(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}) \prod_{\langle \mathbf{x},\mathbf{x}' \rangle} \Big[1 + K \cos(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'}) + \mathcal{O}\big(K^2\big) \Big] \frac{d\theta_i}{2\pi} \qquad (1)\end{aligned}$$

for Z being the partition function. In the last line, we used that we are allowed to expand the exponential function around zero at high temperatures. Neglecting higher order terms in the expansion we see that each bond on the lattice, i.e., each pair of nearest neighbours, contributes either a factor one or $K\cos(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'})$. The product over nearest neighbours leads to a large sum with the first term being equal to one and the others depending on K or higher orders of K. We enumerate the lattice sites and see immediately that, for example,

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

By using this we do not only see that terms depending on K and with endpoints within the lattice sites $\mathbf{0}$ and $\mathbf{r}$ should vanish, but also paths of such internal points as, for example,

$$\begin{aligned}
\int_0^{2\pi} \cos(\theta_1 - \theta_2)\cos(\underbrace{\theta_2 - \theta_3}_{:=\phi})\frac{d\theta_2}{2\pi} &= \int_0^{2\pi} \cos(\theta_1 - \theta_3 - \phi)\cos(\phi)\frac{d\phi}{2\pi} \\
&= \cos(\theta_1 - \theta_3)\int_0^{2\pi} \cos^2(\phi)\frac{d\phi}{2\pi} \\
&\quad + \sin(\theta_1 - \theta_3)\underbrace{\int_0^{2\pi} \sin(\phi)\cos\phi\frac{d\phi}{2\pi}}_{=0} \\
&= \frac{1}{2}\cos(\theta_1 - \theta_3).
\end{aligned}$$

We used in the second step that according to trigonometric identities $\cos(\theta_1 - \theta_3 - \phi) = \cos(\theta_1 - \theta_3)\cos(\phi) + \sin(\theta_1 - \theta_3)\sin(\phi)$. But comparing this result with (1) we see, how non-vanishing terms resulting from the product over nearest neighbours have to look like: we need a term which depends on $\cos(\theta_{\mathbf{0}} - \theta_{\mathbf{r}})$ such that it adds up to a quadratic term after being multiplicated with the cosine in (1). Integrating over a quadratic cosine would not vanish, therefore the only integrals which are nonzero are those connecting paths between the sites $\mathbf{0}$ and $\mathbf{r}$ such as

$$\int_0^{2\pi} \cos^2(\theta_{\mathbf{0}} - \theta_{\mathbf{r}})\frac{d\theta_{\mathbf{0}} d\theta_{\mathbf{r}}}{(2\pi)^2} = \frac{1}{2}.$$

Hence each bond along the path contributes $K/2$ and as we are in the high temperature phase, i.e. $K \ll 1$, the leading term will be the shortest path $|\mathbf{r}|$. Therefore to lowest order we have

$$\langle \mathbf{s}_{\mathbf{0}} \cdot \mathbf{s}_{\mathbf{r}} \rangle \approx \left(\frac{K}{2}\right)^{|\mathbf{r}|} = e^{-|\mathbf{r}|/\xi} \quad \text{with} \quad \xi \approx (\ln(2/K))^{-1}.$$

Hence we see that spins at lattice sites of far distance are not correlated and that the correlation falls off very fast as the correlation function tends *exponentially* to zero for $\mathbf{r} \to \infty$, just as expected.

2.2. Low Temperature Phase

At low temperatures we have a quite different situation. It is important to bear in mind that we are only considering the ferromagnetic case of this model, thus the ground state is the fully aligned state $\theta_{\mathbf{x}} = \theta$ for all $\mathbf{x}$, where $\theta \in [0, 2\pi]$ is a fixed value. Assuming low temperatures there will be only slowly varying configurations, i.e. adjacent angles nearly equal. Therefore we expand the cosine up to terms quadratic in the angles

$$\cos(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'}) \approx 1 - \frac{1}{2}(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'})^2.$$

Furthermore, as the range of $\theta_{\mathbf{x}}$ is otherwise inconvenient, we extend the range to go from minus infinity to infinity resulting now in a completely Gaussian problem which can be solved. Therefore this is called Gaussian or spin wave approximation to the XY model and is reliable for all dimensions if the temperature is low enough. We go on by considering the spin-spin correlation function again:

$$\begin{aligned}
\langle \mathbf{s_0} \cdot \mathbf{s_r} \rangle &= \langle \cos(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}) \rangle \\
&= \Re \Big\langle \exp(i(\theta_{\mathbf{0}} - \theta_{\mathbf{r}}) \Big\rangle \\
&= \Re \Big(\exp \Big(-\langle (\theta_{\mathbf{0}} - \theta_{\mathbf{r}})^2 \rangle / 2 \Big) \Big) \\
&\approx \left(\frac{|\mathbf{r}|}{a} \right)^{-\frac{k_B T}{4\pi J}},
\end{aligned}$$

where we used in the penultimate step that we have a set of Gaussian distributed variables with zero mean because of symmetry such that we are able to use the results of section A.1, especially equation (2). In the last step, we used that Gaussian fluctuations grow logarithmically in two dimensions, a proof can be found in the appendix, section A.2, especially equation (5). Now we see that the decay of correlations is *algebraic* rather than exponential implicating the possibility of a phase transition. We say that this low-temperature phase has *quasi-LRO* or *topological-LRO* in contrast to the totally disordered, high-temperature phase.

3. Vortices

The results from the low-temperature phase showed an algebraic behaviour of spin-spin correlations as one would expect according to the theory of conventional phase transitions from the spin-spin correlation at a critical point. Therefore the resulting temperature-dependent exponent is reminiscent of a critical exponent with the important difference that in the spin wave approximation the system seems to be at a critical point for all temperatures, which is clearly unphysical. Hence, as Berezinskii, Kosterlitz, and Thouless argued [1], [9], there has to exist another set of excitations. The disordering at low temperatures is, according to them, caused by topological defects, or more explicit vortices in the case of the XY model, that can not be regarded as simple deformations of the ground state. Those vortex excitations are responsible for the change in the correlations as the critical temperature for the phase transitions is the one at which vortex-antivortex pairs unbind, whereas at higher temperatures there is a plasma of free vortices and antivortices.

Before continuing we consider the Hamiltonian using the spin wave approximation and defining the ground state energy $E_0 = -JN_{nn}$ with N_{nn} being the number of nearest neighbours

$$\begin{aligned}\mathcal{H} - E_0 &\approx \frac{1}{2}J\sum_{\langle \mathbf{x},\mathbf{x}'\rangle}(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'})^2 \\ &\overset{continuum\ limit}{\rightarrow} J\int(\nabla\theta_{\mathbf{r}})^2 d^2\mathbf{r}.\end{aligned}$$

For the continuum limit we assumed that the lattice spacing a is infinitesimal, then one gets according to [13]:

$$\begin{aligned}\mathcal{H} - E_0 &\approx \frac{1}{2}J\sum_{\langle \mathbf{x},\mathbf{x}'\rangle}(\theta_{\mathbf{x}} - \theta_{\mathbf{x}'})^2 \\ &= \frac{1}{2a^2}\sum_{i=1}^{N}\Big[\Big(\frac{\theta_i - \theta_R}{a}\Big)^2 + \Big(\frac{\theta_i - \theta_T}{a}\Big)^2 + \Big(\frac{\theta_i - \theta_L}{a}\Big)^2 + \Big(\frac{\theta_i - \theta_B}{a}\Big)^2\Big] \\ &\approx a^2\sum_{i=1}^{N}|\nabla\theta_i|\end{aligned}$$

where we enumerated each of the n lattice sites and where $\theta_R, \theta_T, \theta_L, \theta_B$ represent some θ_j being the right, top, left, or bottom nearest neighbour of θ_i. The first two and the last two terms in the large bracket represent the one-sided gradient at the site i. Finally we want to replace the sum by an integral and have to divide by a^2(size of an elementary cell in the lattice):

$$a^2\sum_{i=1}^{N}|\nabla\theta_i| \rightarrow J\int(\nabla\theta_{\mathbf{r}})d^2\mathbf{r}.$$

In some literature, such as in [6], the continuum limit is taken in a different way such that there is an additional factor of one half. This leads to slightly different results but does not change the nature of topological phase transitons. The way we took the continuum limit leads to the same results as in the original paper of Kosterlitz and Thouless [9].

3.1. Topological Charge

We follow here [6] and [12] and recall that we already mentioned that the XY model has a gauge invariance and therefore the angle θ describing the orientation of a spin is defined

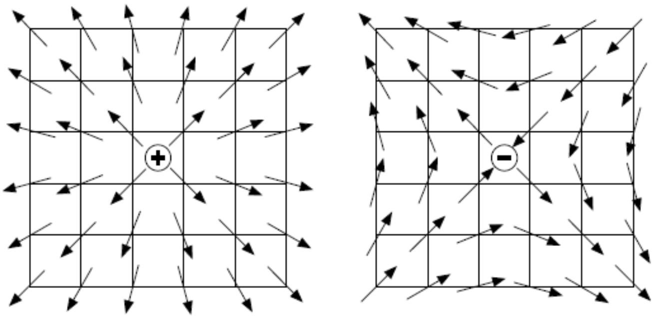

Figure 1: Vortex and antivortex in the two-dimensional XY model [6].

up to an integer multiple of 2π. As a result we are able to construct spin configurations for which going around a closed path the angle rotates by $2\pi q$ if we define $q \in \mathbb{Z}$ to be the topological charge or winding number. For instance, in figure (1) there are elementary defects which can not be destroyed by small fluctuations of the neighbouring spins and going around a closed path around these causes a change in the orientation of spin by 2π respectively -2π, thus we call the left one a vortex and the right one an antivortex. In contrast to that integrating along a closed path if there is no topological defect leads to a topological charge equal to zero. In the continuum limit, we expect

$$\begin{aligned} q &= \frac{1}{2\pi} \oint \nabla\theta \cdot d\ell = \frac{1}{2\pi}\frac{d\theta}{dr}(2\pi r) = \frac{1}{2\pi}|\nabla\theta| 2\pi r \\ \Rightarrow |\nabla\theta| &= \frac{q}{r}, \end{aligned}$$

as θ has a spherical symmetry and for r being a radial coordinate. This approximation clearly fails close to the center of the vortex due to the lattice structure which becomes more important.

Using this result we can now calculate the energy cost of a single vortex. We neglect the contributions from the core region as this will only lead to a constant which will anyway cancel out when we are considering the change in the free energy.

3.2. Energy Cost of Vortices and Vortex-Antivortex Pairs

We now want to check whether it is favourable that the system makes these vortex-excitations. Therefore we calculate the cost to create a single vortex of topological charge q according to [6] and [12]. Although we expect to have contributions not only from the relatively uniform distortions away from the center but also from the core region, we use without loss of generality a circle of radius r_0, a cutoff of the order of the lattice spacing, to distinguish the two and neglect the contribution from the core as we are interested in the overall behaviour:

$$
\begin{aligned}
E_v &= J \int_{r_0} (\nabla \theta_{\mathbf{r}})^2 d^2\mathbf{r} \\
&= 2\pi J \int_{r_0}^{L} \left(\frac{q}{r}\right)^2 r dr \\
&= 2\pi J q^2 \ln\left(\frac{L}{r_0}\right)
\end{aligned}
$$

for L being the linear dimension of the system. Thus we see, that the energy diverges in the thermodynamic limit. Now we can conclude that single vortices can not spontaneously formate. The configurational entropy of a single vortex is given by $S = 2k_B \ln(L/r_0))$ as there are $L^2/{r_0}^2$ possibilities to locate a vortex in a domain of area L^2. Therefore the change in free energy due to the formation of a vortex is just

$$
\Delta F = \left(2\pi J q^2 - 2k_B T\right) \ln\left(\frac{L}{r_0}\right).
$$

Not only the entropy but also the energy grows as $\ln L$. Hence, at low temperatures, the energy term dominates and configurations with single vortices vanish, whereas at high temperatures the entropy dominates and is large enough to favour the spontaneous formation of vortices. Therefore we can consider the case of vortices with a topological charge equal $q = \pm 1$ being clearly the energetically "cheapest" case and get for the critical temperature:

$$
T_{BKT} = \frac{\pi J}{k_B}.
$$

It is important to bear in mind that this estimate for the critical temperature is an upper bound because at lower temperatures the formation of vortex-antivortex pairs is favourable as we will show next (cf. [9]). We consider a vortex-antivortex pair separated by a distance d and investigate the distortions far away from the dipole center, $r \gg d$. This case can be considered similar to the case of a dipole in an electric field, therefore we expect now that $|\nabla \theta| \propto \frac{d}{r^2}$. Calculating the energy leads to

$$
E_{v,a} \propto 2\pi J \int_a^L \frac{d^2}{r^3} dr
$$

which is converging in the thermodynamic limit, thus causing a finite energy. Looking at these results, it becomes clear that at low temperatures there can be vortex-antivortex pairs and at high temperatures above T_{BKT} free vortices and antivortices. As a result T_{BKT} marks the critical temperature at which, starting at the low-temperature phase, the unbinding of vortex-antivortex pairs takes place.

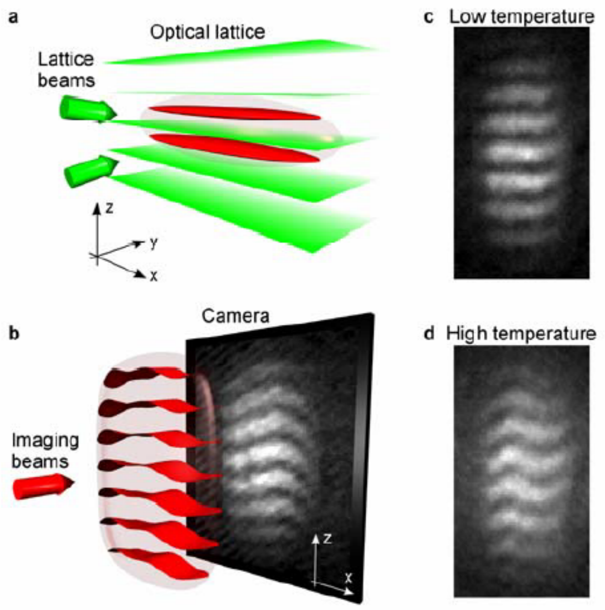

Figure 2: Sketch to the experimental setup [3].

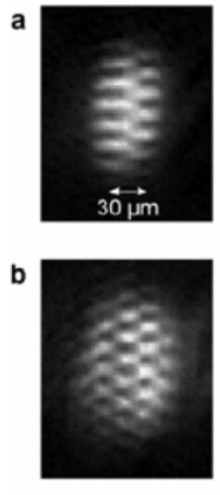

Figure 3: Proliferation of free vortices [3].

4. Experimental Realisation

As mentioned above the Berezinskii-Kosterlitz-Thouless (BKT) transition had a wide impact on future research in general and therefore was also reason to more than 500 experimental articles touching this theory [8]. Due to the concepts of universality the BKT theory is applicable to a wide variety of two-dimensional phenomena. One example which we will consider in the following are superfluids. The condensate wave function of a superfluid is given by

$$\psi(\mathbf{r}) = |\psi(\mathbf{r})|e^{i\theta(\mathbf{r})},$$

(cf. [8]). Hence the important thermal fluctuations are only in the phase θ such that the order parameter can be described by a single angle just as in the case of the XY model. Now we can conclude that the critical behaviour of two-dimensional superfluids can be described by the same effective theory as in the case of the two-dimensional XY model and we expect a BKT transition.

There is a noteworthy experiment providing direct experimental evidence for the microscopic mechanism underlying the BKT theory, which was carried out by Hadzibabic et. al. in 2006 [3]. Their work differs from previous ones by revealing the binding and unbinding of vortex-antivortex pairs by using a trapped quantum degenerate gas of rubidium ^{87}Rb atoms. According to the theory a uniform two-dimensional fluid of identical bosons, in contrast to the three-dimensional case, can not undergo Bose-Einstein condensation as shown by Hohenberg [4], but become superfluid below a finite critical temperature T_{BKT} due to the pairing of vortices and antivortices. Therefore first a quantum degenerate cloud of ^{87}Rb atoms is trapped in a two-dimensional optical lattice such that the three-dimensional gas is split into two independent clouds and compressed into the two-dimensional regime with about 10^5 atoms per plane, see figure (2a). These Bose-Einstein condensates are allowed to equilibrate independently and then the trapping potentials are turned off. The two clouds expand predominantly perpendicular to the planes, thus forming a three-dimensional matter wave interference pattern as they overlap which allows to get information about the correlation function and the microstructure. A jump between a quasi-LRO phase and a disordered phase could be identified as the waviness of the interference fringes due to phase fluctuations in the two planes increased for temperatures beyond $T_{BKT} = (290 \pm 40)$nK, see figure (2c) and (2d). Moreover, it was occasionally possible to observe a sudden onset of vortex proliferation with increasing temperature as in figure (3), in (a) the change in the interference pattern is attributed to the presence of a free vortex and in (b) to several ones. The critical temperature at which those vortices disappeared due to the pairing up of vortices and antivortices coincides with the loss of quasi-LRO indicating conclusive evidence for the observation of the BKT transition.

5. Summary and Outlook

The Berezinskii-Kosterlitz-Thouless transition solved the problem of a lack of explanation for phase transitions in two-dimensional systems which could not be explained by the conventional type of phase transitions due to the destruction of LRO with rising temperature. The theory of such topological phase transitions opened up many new areas of physics. Until 2013 the work of Kosterlitz and Thouless has been mentioned by nearly 2200 papers [10] and due to the wide impact their theory had, they got the Nobel Prize for physics in 2016. We already saw applications to magnetic and superfluid systems, another application is the theory of melting of two-dimensional crystals, although the situation there is much more complicated and therefore ”their physical ideas are correct but incomplete” ([8], p.21).

We considered the simplest model showing this new kind of phase transition in detail, namely the XY model, and were able to see that the behaviour of the spin-spin correlation function implicates a phase transition at some nonzero temperature. In the low temperature phase there is an algebraic fall off of correlations rather than an exponential one as in the case of a disordered, high-temperature phase, therefore the low-temperature phase can be identified to be quasi-ordered rather than disordered. The idea of Berezinskii, Kosterlitz and Thouless to explain the crossover by an unbinding process of vortices [1], [9], makes it accessible to consider the energy costs of creating single vortices and vortex-antivortex pairs. This leads to the derivation of a critical temperature which defines the temperature at which single vortices become energetically favourable. These heuristic arguments made it possible to get an insight into the processes behind topological phase transitions such as the experimental realisation of Hadzibabic et. al.

[3] which proved in a direct way the existence of those unbindings. Nevertheless one could argue that the spin wave approximation might be too inaccurate and therefore the concluded critical temperature a fallacy. Notwithstanding it was possible to verify the nature of this critical temperature by renormalisation group techniques, cf. [8] and references therein. Furthermore, it is also already shown in a rigorously manner by Fröhlich and Spencer that the Berezinskii-Kosterlitz-Thouless transition exists [2]. In contrast to that, it remains an unsolved problem to show that the Heisenberg model in two dimensions has no phase transition at nonzero temperatures, neither a conventional one nor a topological as expected from non-rigorous theoretical physics literature [14]. From the experimental point of view there are also still many improvements to be done. For example, in the above mentioned direct experiment it was expected to reach a pure, fully coherent Bose-Einstein condensate at extremely low temperatures which could not be achieved due to residual heating.

A. Appendix

A.1. Gaussian Distributions

If $\mathbf{X}$ with components $X_1, ..., X_N$ is a set of Gaussian distributed variables, then the expectation value of an exponential formed from a linear combination of these variables is an exponential of a quadratic form in the coefficients, i.e., the generating function $\langle \exp(i\mathbf{q} \cdot \mathbf{X}) \rangle$ for $\mathbf{q} \in \mathbb{R}^N$ being an n-component vector is given by

$$\langle \exp(i\mathbf{q} \cdot \mathbf{X}) \rangle = \exp\Big(i\mathbf{q} \cdot \langle \mathbf{X} \rangle - \mathbf{q} \cdot G \cdot \frac{\mathbf{q}}{2} \Big) \tag{2}$$

where G is related to the correlation matrix. To motivate this result one can look at the case of a single random variable X with variance σ^2 and considering the generating function one obtains

$$\begin{aligned}
\langle \exp(iqX) \rangle &= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(-\frac{(x - \langle X \rangle)^2}{2\sigma^2} \right) \exp(iqx) dx \\
&= \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} \exp\left(\frac{-(x - (\langle X \rangle + iq\sigma^2))^2}{2\sigma^2} \right) \exp\Big(iq\langle X \rangle - \frac{q^2\sigma^2}{2} \Big) dx \\
&= \exp\Big(iq\langle X \rangle - \frac{q^2\sigma^2}{2} \Big).
\end{aligned}$$

Therefore (2) is just the case for having a set of Gaussian variables. We will not go into greater detail, some of these steps and more about Gaussian distributions can be found in [5] and one can get the same result as in (2) by considering cumulants, see for example [6]. Using cumulants it becomes clear that $\mathbf{q} \cdot G \cdot \mathbf{q} = \langle X^2 \rangle - \langle X \rangle^2$ for sets of Gaussian distributed variables.

A.2. Logarithmic Decrease of Gaussian Variables in Two Dimensions

We want to calculate $\langle e^{i(\theta_{\mathbf{0}}-\theta_{\mathbf{r}})}\rangle$ and we do this according to [6]. The probability of a particular configuration is given by

$$\mathcal{P}(\theta_{\mathbf{r}}) \propto \exp\left(-\frac{J}{k_B T}\int (\nabla\theta(\mathbf{r}))^2 d\mathbf{r}\right)$$

and in terms of Fourier components,

$$\mathcal{P}(\theta_{\mathbf{k}}) \propto \exp\left(-\frac{J}{k_B T}\sum_{\mathbf{k}} k^2 |\nabla\theta(\mathbf{k})|^2\right). \tag{3}$$

Each mode $\theta_{\mathbf{k}}$ is an independent random variable with Gaussian distribution of zero mean, and with

$$\langle\theta_{\mathbf{k}}\theta_{\mathbf{k}'}\rangle = \frac{k_B T \delta_{\mathbf{k},-\mathbf{k}'}}{2Jk^2} \tag{4}$$

as we can read off from (3) the variance of these Gaussian fluctuations to be equal to $\frac{k_B T}{2Jk^2}$ if $\mathbf{k} = -\mathbf{k}'$, and vanishing else. Using this we can calculate the correlations in the phase $\theta_{\mathbf{r}}$ in real space. Clearly, $\langle\theta_{\mathbf{r}}\rangle = 0$ by symmetry, while with (4)

$$\begin{aligned}
\langle\theta_{\mathbf{r}}\theta_{\mathbf{r}'}\rangle &= \frac{1}{a^2}\sum_{\mathbf{k},\mathbf{k}'} e^{i\mathbf{k}\cdot\mathbf{r}+i\mathbf{k}'\cdot\mathbf{r}'}\langle\theta_{\mathbf{k}}\theta_{-\mathbf{k}'}\rangle \\
&= \frac{1}{a^2}\sum_{\mathbf{k}} \frac{k_B T e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{2Jk^2} \\
&\to \int \frac{k_B T e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}}{(2\pi)^2 2Jk^2} d\mathbf{k} \\
&= -\frac{k_B T C_2(\mathbf{r}-\mathbf{r}')}{2J} \quad \text{with } C_2(\mathbf{r}) := -\int \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi k)^2} d\mathbf{k}.
\end{aligned}$$

The function C_2 is just the Coulomb potential due to a unit charge at the origin in a two-dimensional space, since it is the solution to

$$\begin{aligned}
\nabla^2 C_2(\mathbf{r}) &= \int \frac{k^2 e^{i\mathbf{k}\cdot\mathbf{r}}}{(2\pi k)^2} \\
&= \delta^2(\mathbf{k}).
\end{aligned}$$

Using Gauss' theorem one gets

$$\int d^2x \nabla^2 C_2 = \oint dS \cdot \nabla C_2,$$

and for a spherically symmetric solution, $\nabla C_2 = \frac{dC_2}{dx}\hat{e}_x$, therefore

$$\begin{aligned} 1 &= 2\pi|\mathbf{r}|\frac{dC_2}{dr} \\ \Rightarrow \frac{dC_2}{dr} &= \frac{1}{2\pi|\mathbf{r}|} \\ \Rightarrow C_2 &= \frac{\ln(|\mathbf{r}|/a)}{2\pi}, \end{aligned}$$

where we introduced a short-distance cutoff a which is in the order of the lattice spacing. As by symmetry the mean values are vanishing, we get

$$\frac{1}{2}\langle(\theta_{\mathbf{0}} - \theta_{\mathbf{r}})^2\rangle = \langle\theta_{\mathbf{0}}^2\rangle - \langle\theta_{\mathbf{0}}\theta_{\mathbf{r}}\rangle = \frac{\ln(|\mathbf{r}|/a)k_B T}{4\pi J} \tag{5}$$

References

[1] V. Berezinskiĭ. Destruction of Long-range Order in One-dimensional and Two-dimensional Systems Possessing a Continuous Symmetry Group. II. Quantum Systems. *Soviet Journal of Experimental and Theoretical Physics*, 34(3):610, 1972.

[2] J. Fröhlich and T. Spencer. The Kosterlitz-Thouless Transition in Two-Dimensional Abelian Spin Systems and the Coulomb Gas. *Communications in Mathematical Physics*, 81(4):527–602, 1981.

[3] Z. Hadzibabic, P. Krüger, M. Cheneau, B. Battelier, and J. Dalibard. Berezinskii-Kosterlitz-Thouless Crossover in a Trapped Atomic Gas. *Nature*, 441(7097):1118–1121, 2006.

[4] P. C. Hohenberg. Existence of Long-Range Order in One and Two Dimensions. *Physical Review*, 158(2):383–386, 1967.

[5] L. P. Kadanoff. *Statistical Physics: Statics, Dynamics and Renormalization.* World Scientific Publishing Company, 2000.

[6] M. Kardar. *Statistical Physics of Fields.* Cambridge University Press, 2007.

[7] J. M. Kosterlitz. The Critical Properties of the Two-Dimensional XY Model. *Journal of Physics C: Solid State Physics*, 7(6):1046–1060, 1974.

[8] J. M. Kosterlitz. Kosterlitz-Thouless Physics: A Review of Key Issues. *Reports on Progress in Physics*, 79(2):26001, 2016.

[9] J. M. Kosterlitz and D. J. Thouless. Ordering, Metastability and Phase Transitions in Two-Dimensional Systems. *Journal of Physics C: Solid State Physics*, 6(7):1181–1203, 1973.

[10] J. M. Kosterlitz and D. J. Thouless. Early Work on Defect Driven Phase Transitions. *International Journal of Modern Physics B*, 30(30):1–67, 2016.

[11] N. D. Mermin and H. Wagner. Absence of Ferromagnetism or Antiferromagnetism in One- or Two-Dimensional Isotropic Heisenberg Models. *Physical Review Letters*, 17(22):1133–1136, 1966.

[12] M. Plischke and B. Bergersen. *Equilibrium Statistical Physics.* World Scientific Publishing Company, 1994.

[13] N. Provatas and K. Elder. Phase-Field Methods in Materials Science and Engineering. *Phase-Field Methods in Materials Science and Engineering*, 2010.

[14] B. Simon. Fifteen Problems in Mathematical Physics. *Perspectives in mathematics, Birkhäuser, Basel*, 423, 1984.