Berezinskii-Kosterlitz-Thouless Transition in a Trapped Rubidium Gas

Jimmy Yuan

Abstract

The BKT transition is a topological phase transition that arises naturally from the XY spin model, a common toy model that describes a variety of 2D systems. We derive the behavior of the two-point correlation function via low-temperature expansions, and we explore the critical behavior using the renormalization group. It can be shown that that above the critical temperature for the BKT transition, but not too much higher, defects in the form of topologically-charged vortex pairs spontaneously are created, giving rise to quasi-long-range order. Experimental evidence has been found for this in an optically trapped rubidium gas.

Introduction

The Berezinski-Kosterlitz-Thouless (BKT) transition is a phase transition that occurs in many two-dimensional systems such as nematic liquid crystals, superconducting arrays, superfluid helium films, etc. The BKT transition is unique in that the long-range behavior of the system is encoded into the topology of the system. As such the BKT transition is often classified as a topological phase transition. One of the main results of undergoing such a transition is the emergence of topological defects, such as a topological charge excitation known as a vortex. Experimental evidence for the BKT transition is quite strong, as several experiments have confirmed aspects of the theory such as the existence of topological defects, and the critical values from renormalization group (RG) analyses.

2D Classical XY Model [3][4]

The simplest toy model that exhibits the BKT transition is the XY model which is a spin model where spins are localized onto lattice points in two dimensions and their interaction length is restricted only to nearest-neighbor interactions. The spins are allowed to point in any direction within the XY plane, hence the name XY model. The Hamiltonian, $\mathcal{H}$ of such a system with no external field can be written as

$$\mathcal{H} = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \tag{1}$$

where J refers to the coupling constant of any particular spin and θ_i refers to the angle a spin points at lattice point i. Implicitly we assumed that the magnitude of each of the spins is unity. For low temperatures, one can see from the Hamiltonian that the nearest-neighbor spins would prefer to point in the same direction, making changes in angle small. Thus in this limit, one can Taylor expand about the minimum energy configuration and take the continuum limit.

$$\mathcal{H} \approx \frac{J}{2} \sum_{\langle ij \rangle} (\theta_i - \theta_j)^2 = \int \frac{J}{2} \left(\nabla\theta(\mathbf{r})\right)^2 dr \tag{2}$$

One quantity of interest is the two-point correlation function $\langle \mathbf{S}(0)\mathbf{S}(\mathbf{r}) \rangle$, which reveals how ordered the system is.

$$\langle \mathbf{S}(0)\mathbf{S}(\mathbf{r})\rangle = \mathrm{Re}\langle e^{i\theta(0)-\theta(\mathbf{r})}\rangle \tag{3}$$

$$\sim \mathrm{Re}\left(\int \frac{d^2\theta}{(2\pi)^2} e^{(i[\theta(0)-\theta(\mathbf{r})])\left[\frac{J}{2}\nabla\theta^2\right]}\right) \tag{4}$$

One can calculate this correlation function by Fourier transforming to momentum space and taking the small k limit.

$$\theta(\mathbf{r}) = \int \frac{d\mathbf{k}}{(2\pi)^2}\theta(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{r}} \tag{5}$$

$$\theta(\mathbf{r}) - \theta(0) = \int \frac{d\mathbf{k}}{(2\pi)^2}\theta(\mathbf{k})\left[1-\cos\left(\mathbf{k}\cdot\mathbf{r}\right)\right] \tag{6}$$

Substituting these values into the original Hamiltonian and then completing the square inside the integral part of the correlation function, one finds that

$$\langle \mathbf{S}(0)\mathbf{S}(\mathbf{r})\rangle \sim \exp\left[-\int^{|\mathbf{r}|^{-1}} \frac{d^2k}{(2\pi)^2}\frac{1-\cos(\mathbf{k}\cdot\mathbf{r})}{\beta J k^2}\right] \tag{7}$$

Only the first term survives because one of the dimensions in d^2k is implicitly integrating over the angles. One thus can obtain a correlation function that scales in the following way:

$$\langle \mathbf{S}(0)\mathbf{S}(\mathbf{r})\rangle \sim \left(\frac{1}{|\mathbf{r}|}\right)^{T/2\pi J} \tag{8}$$

Since the scaling relation above shows that the two-point correlation function decays with distance, there should be no long-range order. However, one should also note that this function decays algebraically, not exponentially like the Ising model above the critical temperature (no long range order in that scenario). One can interpret these findings as the following: for the low temperature approximation there is a phase transition, now known as the BKT transition, that has occurred, but that BKT phase transition is somewhat different from that of the Ising magnetic transition. As such, it is commonly said that the low-temperature phase transition of the 2D XY model gives rise to a phase that possesses quasi-long range order.

When calculating the two-point correlation function in the high-temperature limit, one cannot use the same approximations as the low-temperature limit. The Boltzmann factors for this limit are $\exp\left[\beta J \cos(\theta_i - \theta_j)\right]$. From the functional form of this Boltzmann factor, one can interpret the high-temperature limit as also being the small J limit, and as such one can expand the Boltzmann factor about small J to lowest non-trivial order. The two-point correlation function (excluding trivial constant values of energies) will be

$$\begin{aligned}
\langle \mathbf{S}(0)\mathbf{S}(\mathbf{r})\rangle &\sim \int \frac{d^2\theta}{2\pi} \cos(\theta_0 - \theta_r) \prod_{ij} J \cos(\theta_i - \theta_j) && (9)\\
&\sim \left[\int \frac{d^2\theta}{2\pi} J \cos^2(\theta_0 - \theta_r)\right]^{|\mathbf{r}|} && (10)\\
&\sim \exp\left(\frac{|\mathbf{r}|}{\ln(J/2)}\right) && (11)
\end{aligned}$$

This correlation function gives an exponential decay for high temperature spin systems as expected, and as such in this regime, the system has true long-range order. One can conclude that the 2D XY model has two phase transitions: one at low temperatures that gives rise to quasi-long-range order, and one at high temperatures that gives rise to true long-range order.

Topological Phase Transition [3][4]

For low temperatures, one can minimize the Hamiltonian with respect to the functional $\theta(\mathbf{r})$ to get Laplace's equation.

$$\nabla^2 \theta(\mathbf{r}) = 0 \tag{12}$$

The solutions to this equation, other than the trivial linear and constant solutions, give rise fields that can be thought of as emanating from a charge (or defect) of some kind. One of the boundary conditions for this field comes from looking at the continuum limit of the change in the $\theta(\mathbf{r})$ functional.

$$\Delta\theta = \int \nabla\theta(\mathbf{r}) d\mathbf{r} \tag{13}$$

If one integrates over a closed curve, one must get $2\pi q$, where q is an integer, and can be thought of as the "charge" that gives rise to the field that solves equation (12). From this analysis, one can see that the "charge" gives rise to vortices which cannot be continuously

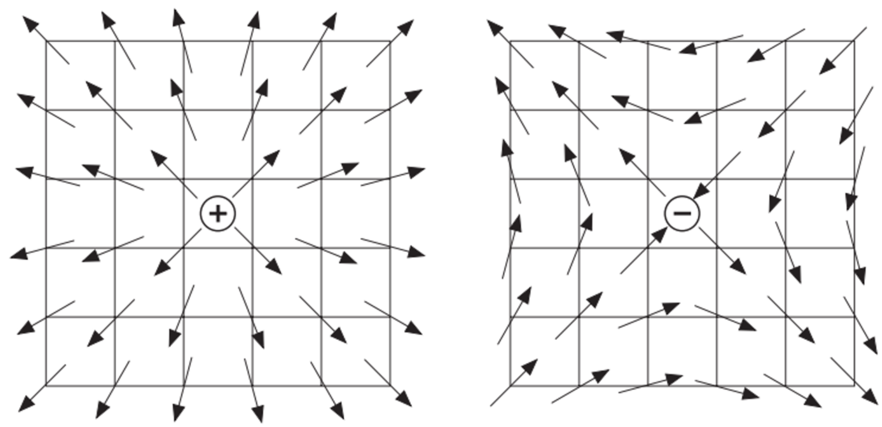

Figure 1: The positively and negatively charged vortices that come about above T_c for the BKT transition. Each of the arrows represents the order parameter.

deformed to the uniform spin state which represents $q = 0$. As such, one can interpret this vortex to be topological in nature, with the topological charge being the mathematical winding number. Due to the integer property of winding number, one can see that $\nabla\theta(\mathbf{r})$ scales inversely with distance. Using this fact, one can find from the 2D continuum form of equation (2), that the energy of this topological defect with system size L that circulates with radius a is

$$E_{\text{vortex}} = E_{\text{core}} + \int_0^{2\pi}\int_a^L \frac{J}{2}\left(\nabla\theta(\mathbf{r})\right)^2 dr d\phi \tag{14}$$

$$= E_{\text{core}} + \pi J q^2 \ln\left(\frac{L}{a}\right) \tag{15}$$

The second term, which represents the energy of distortions away from the core can also be thought of as the energy for vortices to spontaneously exist. To investigate the phase transition, one can look at the partition function excluding the constant of the core energy.

$$Z \approx \left(\frac{L}{a}\right)^2 e^{-\beta\pi J\ln\left(\frac{L}{a}\right)} \tag{16}$$

This factor of $\left(\frac{L}{a}\right)^2$ comes from the multiplicity, or entropy, of different configurations that a vortex of area a^2 can take in a system of size L^2 in 2D. The free energy is then

$$F \approx \pi J - 2T \ln\left(\frac{L}{a}\right) \tag{17}$$

where the first term is the energetic contribution to the free energy which acts to suppress vortex formation, while the second term is the entropic contribution, which acts to promote vortex formation.

At low enough temperatures, one can see that vortex formation is not spontaneous, but at higher temperatures, [but still low enough to use the approximation in equation (2)] one can see that vortices will form. The critical temperature, at which this will take place is where the free energy vanishes, which is at $T_c = \frac{\pi J}{2}$, and its critical coupling constant will be $J_c = \frac{2}{\pi}$. However, not all kinds of vortices can spontaneously exist as the energy of the vortex diverges as the system approaches the thermodynamic limit of $L \to \infty$. It is only when a vortex couples with another vortex with a topological charge of the opposite sign can one remove the L dependence in the energy and thus allow the energy to be finite. The low-temperature result above T_c of the BKT transition can thus be summarized as the spontaneous formation of a gas of topological "dipoles," sometimes referred to as a Coulomb gas. It is through this result that shows how the XY model can attain quasi-long range order.

Rescaling and Renormalization [1]

While the previous argument for the topological phase transition does provide much of the correct phenomenology, the argument is not exactly correct since it does not account for any interaction energies between vortices once the system has reach the critical temperature. The partition function for such a system will be the same partition function in equation (16), (defined now as Z_{sw}) except now multiplied by the partition function for the interactions (defined now as Z_{int}). Z_{sw} is analytic everywhere so by that fact alone, it would initially seem as though there would be no phase BKT transition for low temperatures given the argument from the previous section. However one ultimately finds that Z_{int} may become non-analytic at certain temperatures, which implies reconciles the phenomenology with the formulation. The partition function for the interactions can be found by considering a vortex with vorticity and by using several vector calculus identities, giving an expected result: an exponential of a 2D Coulombic Hamiltonian that is non-analytic at $r = 0$.

$$Z_{\text{int}} = e^{-\beta \sum E_{\text{core}} - 4\pi^2 J \sum \frac{q_i}{q_j} \ln |\mathbf{r}|} \tag{18}$$

However, if one considers the model where there are multiple topological dipoles, there will be multiple kinds of interactions between multiple sets of dipoles. If one takes a coarse-grained view of the system, one can think of one set of the net interaction can be thought of as shielding another set of dipoles from the potential from the rest of the dipoles. This would mean that the coupling constant, J would rescale into J_{eff}, which incorporates the shielding effect. One can obtain the interaction energy using various lowest-order perturbation theory calculations and the result that one gets will be

$$J_{\text{eff}}^{-1} = \left[J - 4\pi^3 J^2 y_0^2 \int_1^\infty x^{3-2\pi J} dx \right]^{-1} \tag{19}$$

$$\approx J^{-1} + 4\pi y_0^2 \int_1^\infty x^{3-2\pi J} dx \tag{20}$$

where y_0 comes from the terms involving the core energy and can be thought of as the fugacity, and x is now the variable used to rescale r for short distance 2D Coulombic potential divergences. To get a recursion relation from this integral, one can use a renormalization procedure of breaking the integral up into two integrals: one that represents large (convergent) length scales and that represents small (divergent) length scales. One can then rescale the coupling constant J to incorporate the divergent part of the integral.

$$J_{\text{eff}}^{-1} = \tilde{J}^{-1} + 4\pi^3 y_0^2 \int_{e^\ell}^\infty x^{3-2\pi \tilde{J}} dx \tag{21}$$

The term e^ℓ is the arbitrary length cutoff that separates the short length scales and the long length scales. To get this previous integral into the original form of equation (20), one can rescale y_0 to be $y_0 = e^{(2-\pi J)\ell} y_0$ such that all length scales x become $\frac{x}{e^\ell}$.

$$J_{\text{eff}}^{-1} = \tilde{J}^{-1} + 4\pi^3 \tilde{y}_0^2 \int_1^\infty x^{3-2\pi \tilde{J}} dx \tag{22}$$

One can take several infinitesimal iterations of renormalization such that $e^\ell \approx 1 + \ell$. Then one can formulate an explicit recursion relation in terms of two differential equations to lowest non-trivial order.

$$\frac{dJ_{\text{eff}}^{-1}}{d\ell} = 4\pi^3 \tilde{y}_0^2 \tag{23}$$

$$\frac{d\tilde{y}_0}{d\ell} = (2 - \pi J) y_0 \tag{24}$$

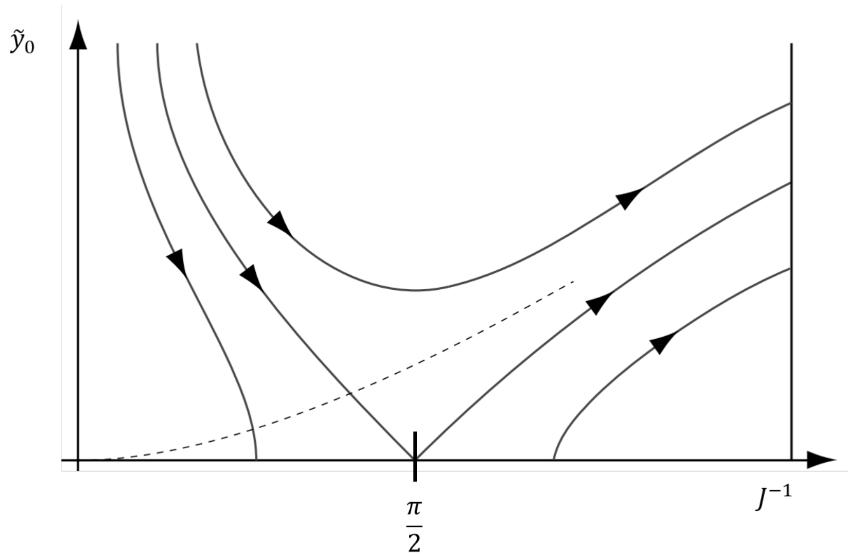

Figure 2: The RG flow diagram for the XY model (far from the critical point)

From equation (24) one can see that the critical value $J_c = \frac{2}{\pi}$ is consistent with the renormalization analysis and thus must be a fixed point on the RG flow diagram. One can also see that for small (large) J the slope of the flows for y_0 are negative (positive), which implies that the y_0 in that region is relevant (irrelevant). Flows for J^{-1} will always tend towards ∞ and thus are irrelevant. A summary of the results is described in the following RG flow diagram in Figure 2. To observe the behavior near the critical point, one can find three differential equations for the point $t = J_{\text{eff}}^{-1} - \frac{\pi}{2}$ and for the value of $c = t^2 - \pi^4 y_0^2$.

$$\frac{dt}{d\ell} = 4\pi^3 y_0^2 \tag{25}$$

$$\frac{d\tilde{y}_0}{d\ell} = \frac{4}{\pi} t y_0 \tag{26}$$

$$\frac{dc}{d\ell} = 2t\frac{dt}{d\ell} - 2\pi^4\frac{dy_0}{d\ell} = 0 \tag{27}$$

From these equations, one can show that c is a conserved value near the critical point on one side, and from Figure 2 one can see that it changes sign but not magnitude as one flows across the critical point. The point where that crossover occurs is at where $c = 0$ or when $t_c = -\pi^2 y_c$ where t_c and y_c are other critical values. This suggests that the value of y_c (which if one recalls is related to the core energy) shifts the value of of the critical coupling constant by

$$J^{-1} = \frac{\pi}{2} - \pi^2 y_c \tag{28}$$

The temperature dependence of c close to the critical point can be argued to be $c = a^2(T - T_c)$ since the value vanishes at T_c and increases (decreases) as one moves away from the critical point in the positive (negative) direction. One can then find the functional form of the critical behavior of the coupling constants for the BKT transition.

$$J_{\text{eff}} \sim \sqrt{T_c - T} \tag{29}$$

Rubidium Gas Experiments [2][5]

In 2006, Hadzibabic et. al experimentally tested the value of the critical exponent of the two-point correlation function and tested the prediction of topologically charged vortex pairs. The experiments used a cold bosonic gas of rubidium atoms that were known to undergo a superfluid phase transition that could be explained using the XY model and the BKT transition. For the superfluid transition, the critical exponents have already been determined theoretically to be 1/4 below the transition and 1/2 above the transition.

The goal of the experiments was to try to get an interference pattern which will indirectly give information about the correlation functions. It can be shown that interference fringes with the greatest amount of interference, and thus the greatest contrast, consist of waves (in this case atoms) that have the greatest coherence, which in the optical case means that the waves are closest to the "ideal" system of having the same wavelength but different phases. A system that is more coherent can be thought as being more correlated, and it can be shown that the correlation function $g(\mathbf{r}, 0) = \langle S(\mathbf{r}), S(0)\rangle$ is related to coherence via an equation for the contrast in the interference fringe

$$\langle C^2(L_x)\rangle = \frac{1}{L_x}\int_0^{L_x} g^2(r, 0)\; dx \sim \left(\frac{1}{L_x}\right)^{2\alpha} \tag{30}$$

where C is a measure of the full contrast, and L_x is the length scale of the system along the $\hat{x}$ direction. One can obtain the full contrast by averaging out all of the locals contrasts, $c(x)$ weighted by their phase, $\varphi(x)$, where both values can be directly measured.

$$C(L_x) = \frac{1}{L_x}\int_{-L_x/2}^{L_x/2} c(x)e^{i\varphi(x)}\; dx \tag{31}$$

The experimental setup first included rubidium atoms that were first brought to the gas phase using radiation. The gas was first split and then trapped into two different clouds

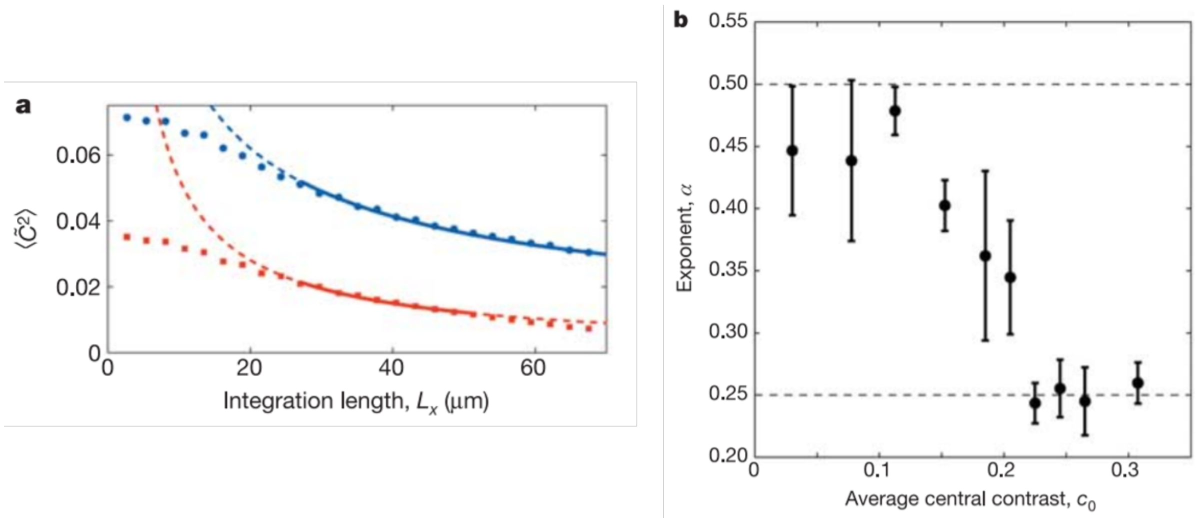

Figure 3: a) The graph of the functional form of the correlation function. The blue section corresponds to temperatures above T_c and the orange corresponds to temperatures below T_c. The dashed lines correspond to the theoretical result. b) Value of the critical exponent α, where the dashed lines refer to the theoretical predictions

via a 1D optical lattice. After the gases reached thermal equilibrium from Bose-Einstein condensation, the lattice potential was quickly turned off such that the rubidium atoms were now allowed to tunnel through to the other atom cloud and thus interfere in the xy plane with atoms in the other cloud. Hadzibabic et. al raised the temperature by tuning the frequency of the radiation and observed the interference pattern with a CCD detector.

The results for the behavior of the correlation function are presented in Figure 3. The average of the full contrast squared looks as if it fits well with the theoretical value, but the critical exponent above T_c had much more noise. There are also larger error bars around where one achieves a higher temperature, and nontrivial ones in below T_c. One issue noted by Hadzibabic et. al is that for very low temperatures, the critical exponent should be 0 due to Bose-Einstein condensation, but this is not observed. Their explanation for this is due to crossover phenomena from residual heating of the apparatus, but if that were not the case, then the accuracy of the entire experiment would be in question. The result of the vortex experiment came from the shape of the interference pattern. From an earlier paper by Stock et. al, it was shown that topological defects in 2D Bose-Einstein condensates formed dislocations [6]. The interference that Hadzibabic et. al found is shown in Figure 4, which clearly shows dislocations, and thus they concluded that topological defects were formed. They were able to resolve a single vortex as long as it was located close to the center of the gas cloud. They were not able resolve the charge of the vortex which means that they could not yet prove that the topological defects had to have come in pairs.

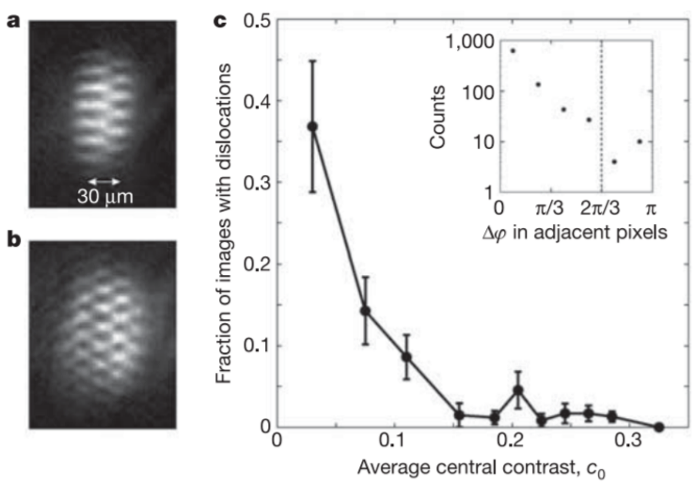

Figure 4: a) The functional form of the correlation function. The blue section corresponds to temperatures above T_c and the orange corresponds to temperatures below T_c. The dashed lines correspond to the theoretical result. b) Value of the critical exponent α, where the dashed lines refer to the theoretical predictions

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