Studying the Kosterlitz-Thouless Phase Transition in the 2D XY Model

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Abstract

In this paper, we study the Kosterlitz-Thouless Phase Transition (BKT Transition) in the 2D XY Model. Implementing the Metropolis-Hastings algorithm using python, we study the behaviour of energy, magnetization, and formation of vortex and anti-vortex in the XY model to approximate the critical temperature at which the transition occurs.

1 Introduction

A phase of states of matter and thermodynamic systems has uniform physical properties. When changes occur in this uniformity, a new state is formed and we refer to this process as phase transition. Like a liquid water becoming a gas upon heating to its boiling point, we can also see phase transitions in magnetic materials. In this paper, we'll use the 2D XY model as a reference to study the Berezinskii-Kosterlitz-Thouless (BKT) transition.

1.1 The XY Model

The Ising model in statistical mechanics can be used to describe phenomena such as magnets, liquid/gas coexistence, and alloys of two metals. In such models, two spins, ± 1 are used to describe the system: where the spins can represent a magnet pointing up or down, an atom of metal A or B, etc. The XY model can be regarded as a generalization of the Ising model, now that the spins can point in any direction instead of being a binary up or down. The XY model consists of planar rotors of unit length arranged on a two dimensional square lattice. The Hamiltonian of the system with no external field can be written as,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \mathbf{s}_i \cdot \mathbf{s}_j \tag{1}$$

Here, $\langle i, j \rangle$ represents the sum over all nearest neighbours in the lattice, and θ_i denotes the angle of the vector on site i with respect to some polar direction in the two dimensional vector space containing the rotors and J quantifies the interaction between the neighbouring rotors. We can write the normalized spins vectors $\mathbf{s}_i = (\cos\theta_i, \sin\theta_i)$ and $\mathbf{s}_j = (\cos\theta_j, \sin\theta_j)$. Then, the Hamiltonian transforms as,

$$\begin{aligned} \mathcal{H} &= -J \sum_{\langle i,j \rangle} \cos\theta_i \cos\theta_j + \sin\theta_i \sin\theta_j \\ &= -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j) \end{aligned} \tag{2}$$

Each state of the system occurs with probability given by the Boltzmann factor,

$$P = \frac{1}{Z} \exp\left(-\frac{\mathcal{H}}{k_B T}\right) \tag{3}$$

Here, T is the temperature, k_B is the Boltzmann constant, and Z is a normalization factor. We also see that the energy is invariant under a global continuous rotation of spins - it has continuous global symmetry.

1.2 The BKT Phase Transition

The BKT transition occurs in many two-dimensional systems such as nematic liquid crystals, superconducting arrays, superfluid helium films, etc. As the long range behaviour of the system is encoded in the topology of the system, the BKT transition is classified as a topological phase transition. It is the transition from bound vortex-antivortex pairs at low temperatures to unpaired vortices and anti-vortices at some critical temperature. To understand this transition, we take the XY model and look at what (anti)vortex represent physically.

If we assume that the direction of the rotors varies smoothly from site to site, we can expand the cosine in the Hamiltonian using Taylor expansion and get,

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \left[1 - \frac{1}{2} (\theta_i - \theta_j)^2 + \mathcal{O} (\theta_i - \theta_j)^4 \right] \quad (4)$$

This sum over the nearest neighbours corresponds to discrete Laplace operator, which we can express in terms of partial derivatives through $\theta_i - \theta_j = \partial_x \theta$ [8]. So, we can write the continuum Hamiltonian as,

$$\mathcal{H} \simeq E_0 + \frac{J}{2} \int d^2r |\boldsymbol{\nabla}\theta(\mathbf{r})|^2 \quad (5)$$

Here, the scalar field $\theta(\mathbf{r})$ represents the angle of rotors at each point in the plane, and $E_0 = -2JN$ is the energy of the system when all N rotors are aligned. Let us define,

$$\mathcal{H}[\theta] = \frac{J}{2} \int d^2r |\boldsymbol{\nabla}\theta(\mathbf{r})|^2 \quad (6)$$

Then, the field configurations corresponding to the local minima of $\mathcal{H}$ are the solutions to the extremal condition,

$$\frac{\delta \mathcal{H}[\theta]}{\delta \theta(\mathbf{r})} = 0 \implies \nabla^2 \theta(\mathbf{r}) = 0 \quad (7)$$

The above equation has two types of solutions. The first consists of the ground state $\theta(\mathbf{r}) = \texttt{constant}$, which is the configuration of all rotors pointing in all direction, with energy E_0. The second solution corresponds to topological defects such as vortices and anti-vortices.

Vortex and Anti-vortex

The vortices and antivortices can not be reached by simple perturbations of the ground state, instead they correspond to non-pertubative solutions. These are obtained by computing the circulation integral of $\theta(\mathbf{r})$:

$$\Gamma[\theta] = \oint_\gamma \boldsymbol{\nabla}\theta(\mathbf{r}) \cdot d\mathbf{l} = 2\pi n \quad (8)$$

Here, γ is the curve over which we find the integral, and n is an integer which corresponds to the total charge of vortices enclosed by this curve. The charge gives rise to vortices which can not be continuously deformed to the uniform spin state which represents $n = 0$. This way, one can interpret vortex to be topological in nature, with the topological charge being the mathematical winding number. For a single charged vortex and anti-vortex, $\oint_\gamma \boldsymbol{\nabla}\theta \cdot d\mathbf{l} = 2\pi$ and $\oint_\gamma \boldsymbol{\nabla}\theta \cdot d\mathbf{l} = -2\pi$ respectively. If we choose a path large enough to enclose both vortex and anti-vortex, then the circulation will be zero.

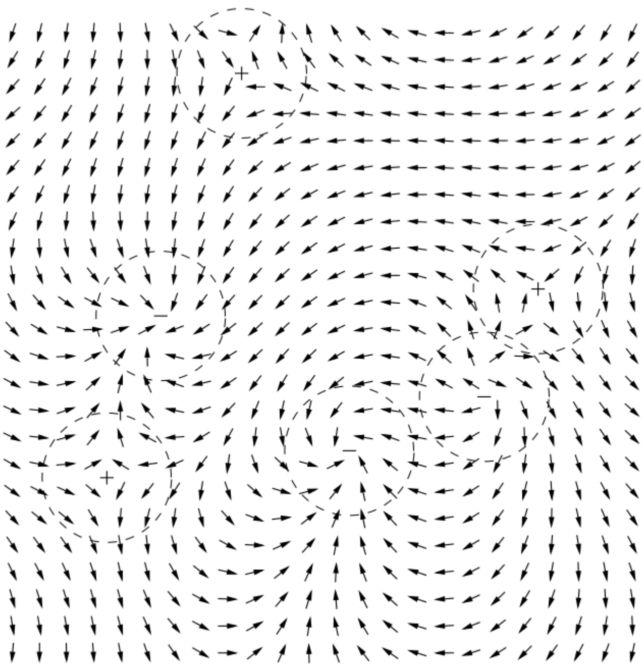

Figure 1: Arrows representing vortex (+) and antivortex (-) in the 2D XY model. [5]

The vortex solutions exhibit rotational symmetry ($\boldsymbol{\nabla}\theta(\mathbf{r}) = \boldsymbol{\nabla}\theta(r)$), so the circulation integral along the circle with radius r becomes,

$$\Gamma[\theta] = 2\pi r |\boldsymbol{\nabla}\theta(\mathbf{r})| \implies |\boldsymbol{\nabla}\theta(r)| = n/r \quad (9)$$

Let L be the size of the lattice and a be the lattice spacing. Then, equation 5 can be written for a single vortex as,

$$\begin{aligned} E_{\text{vor}} &= E_0 + \frac{J}{2} \int_a^L dr 2\pi r \frac{n^2}{r^2} \\ &= E_0 + \pi n^2 J \ln\left(\frac{L}{a}\right) \end{aligned} \quad (10)$$

For vortex-antivortex pair separated by distance R, the energy can be written as,

$$E_{\text{2vor}} = E_0 + 2E_c + E_1 \ln\left(\frac{R}{a}\right) \quad (11)$$

Here, E_c is the energy of individual vertex core and E_1 is a constant proportional to J. We also infer that vortex-antivortex pair have significant impact to the system if their separation is large.

To look at the phase transition, we look at the partition function excluding the constant E_0 in equation 10. The partition function is,

$$Z \approx \left(\frac{L}{a}\right)^2 e^{-\pi J \ln(L/a)/T} \tag{12}$$

The factor $(L/a)^2$ comes from the multiplicity of different configurations that a vortex of area a^2 can take in a system of size L^2 in 2D (see appendix A). We can then write the change in free energy as,

$$\Delta F = (\pi J - 2T) \ln\left(\frac{L}{a}\right) \tag{13}$$

The free energy diverges in the limit $L \to \infty$, however, we also notice it's sign depends on the temperature, given by the critical limit $T_c = \pi J/2$. Above T_c, the vortex formation becomes a spontaneous process, through which the system can reduce its free energy. If we are in dimensions $d \neq 2$, the vortex energy would not combine with the change in entropy to cause a phase transition. At very low temperatures, below T_c, only vortex-antivortex pairs are important due to their finite energy. As temperature increases, the average separation of the pairs increase until they unbind at T_c. After the unbinding, there are free vortices in the system, which disorders the system enough to break down the low temperature approximation. Hence, in 2D, we a phase transition at T_c.

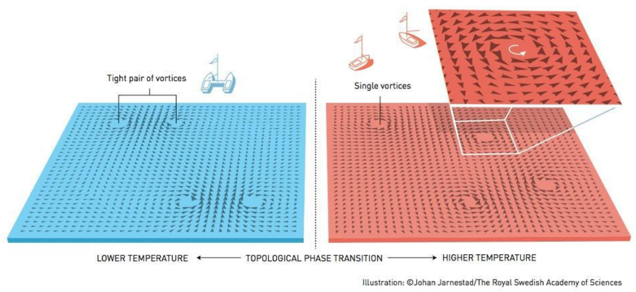

Figure 2: Schematics of a BKT phase transition. We see free vortices after the critical temperature. [4]

This simple approximation of vortex unbinding is a good enough estimate. The value of Kosterlitz-Thouless temperature at which the vortex pairs unbind differs from one system to another. In the 2D XY model, this critical temperature is $T_c \simeq 0.893J$ [6].

2 Computational XY Model

Now that we have explained the XY model and how BKT transition takes place in it, we will look into a computational model to understand the system in more details. The core of the model lies in the Metropolis-Hastings algorithm, which updates the spin values in the lattice and energy of the system after each Monte-Carlo sweep. The code for the model is listed in appendix B.

2.1 The Metropolis-Hastings Algorithm

The Metropolis algorithm is a Markov chain Monte Carlo method for choosing a sequence of random sample of states from a sequence of such steps. In the case of simulation of XY model, the general approach of the implementation of the algorithm is as below.

a. Input initial lattice of size $L \times L$, energy E, temperature T, and interaction constant J.

b. Choose a random point (x, y) in the lattice, call the spin s_o.

c. Make a trial change in the spin, call it s_n.

d. Constraint $-\pi < s_n < \pi$.

e. Calculate the nearest-neighbour old energy E_{Old} using s_o and the new energy E_{New} using s_n.

f. Calculate change in energy $\Delta E = E_{\text{New}} - E_{\text{Old}}$

g. Find the Boltzmann factor $w = e^{-\Delta E/T}$ and generate a random number $r \in (0, 1)$.

h. If $\Delta E \leq 0$ or $r < w$, accept the change: $s_o = s_n$ and $E = E + \Delta E$. Else, retain the previous microstate.

i. Return the energy and lattice.

In our model, using the equation 2, we calculate the energy of the nearest neighbours. The function `metropolis` implements the Metropolis algorithm in our model. To simulate the system over n Monte-Carlo (MC) sweeps, we use the `simulate` function.

2.2 Finding vortices and anti-vortices

An important part of our model is studying the BKT phase transition. At low temperatures, the vortex and anti-vortex exist in pairs and thus their number are equal. After the critical temperature, we see a phase transition and free vortex exist in the system. To see this behaviour, we implement a `vortex` function in our model, which returns if we have a vortex around a point in the lattice. The basic implementation of the function is as below.

a. Input the lattice of size $L \times L$.

b. Loop over all the sites (i, j) in the lattice.

c. Choose a block of size 2×2 around a spin $\theta_1 = s_{i,j}$. We choose spins $\theta_2 = s_{i+1,j}$, $\theta_3 = s_{i+1,j+1}$, $\theta_4 = s_{i,j+1}$.

d. Find the difference in angles $\delta\theta$. For a 2×2 block, $\delta\theta_1 = \theta_2 - \theta_1$, $\delta\theta_2 = \theta_3 - \theta_2$, $\delta\theta_3 = \theta_4 - \theta_3$, and $\delta\theta_4 = \theta_1 - \theta_4$.

e. Check if $\delta\theta \in (-\pi, \pi)$. If yes, no change in $\delta\theta$.

f. If $\delta\theta \geq \pi$, update $\delta\theta = \delta\theta - 2\pi$.

g. If $\delta\theta \leq -\pi$, update $\delta\theta = \delta\theta + 2\pi$.

h. Find $a = \sum \delta\theta_i$.

i. If $a = 2\pi$, increase vortex count. If $a = -2\pi$, increase anti-vortex count.

After setting up the vortex and anti-vortex count, we use the function `BKT` to look at the vortex-antivortex pairing across temperatures. This function calculates the average difference between vortex and anti-vortex at a particular state of the system.

2.3 Results

2.3.1 System parameters

To understand how the system is evolving with temperature, we look at several properties that a system possesses. We have already looked into how the energy of the system looks as we evolve in temperature. For our model, we take the interaction constant to be $J = 1$. Above the critical temperature, as we get free vortices, the energy of the system should increase.

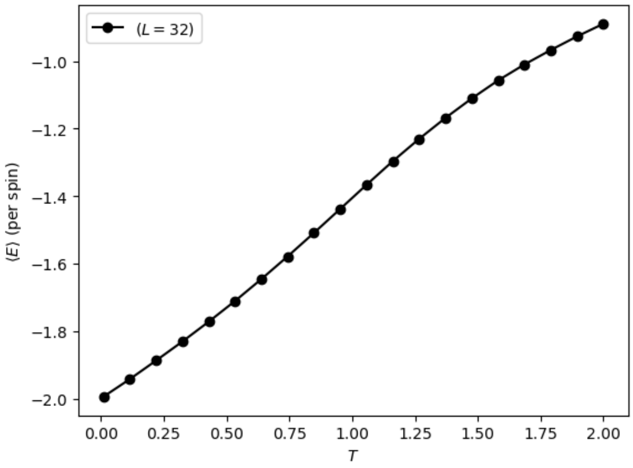

Figure 3: Energy per spin against Temperature for 100000 MC sweeps, Lattice size = 32×32.

We see that the average energy per spin increases as we increase the temperature, which is expected. We then look at the specific heat per spin for the system, which is a response parameter of the system. The Kosterlitz-Thouless theory tells that the specific heat does not peak at T_{KT}, the phase transition temperature. It can also be seen from the graph as we don't get a peak around 0.893, but a temperature value higher than it.

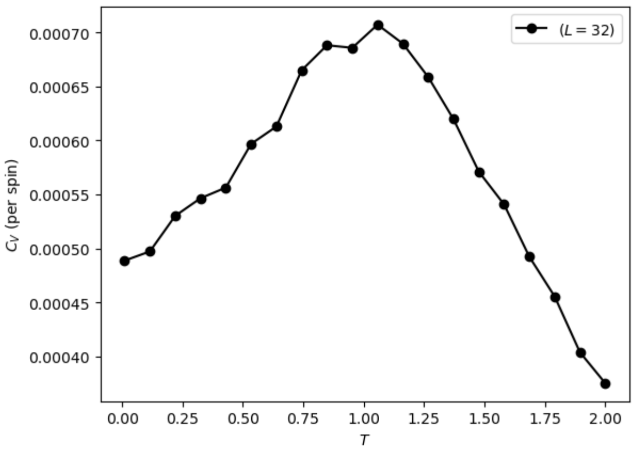

Figure 4: Specific heat against Temperature for 100000 MC sweeps, Lattice size = 32×32.

The average magnetization for the XY model vanishes after we reach around the critical temperature. While the average magnetization $\langle M \rangle$ vanishes for all temperatures, we don't see this behaviour in our system. The average magnetization per spin seems to be around the vicinity of zero after $T = 0.75$.

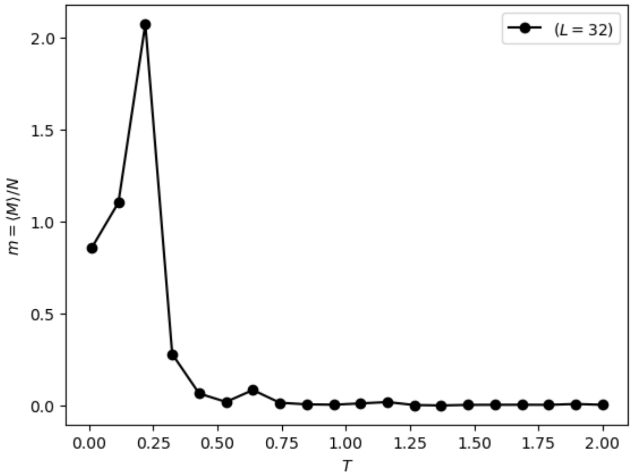

Figure 5: Magnetization per spin against Temperature for 100000 MC sweeps, Lattice size $= 32 \times 32$.

2.3.2 Visualizing vortices and antivortices

Using the `vortex` function, we also find the coordinates where the vortices and anti-vortices lie in the lattice. We then visualize the lattice by drawing a circle around the points where they appear.

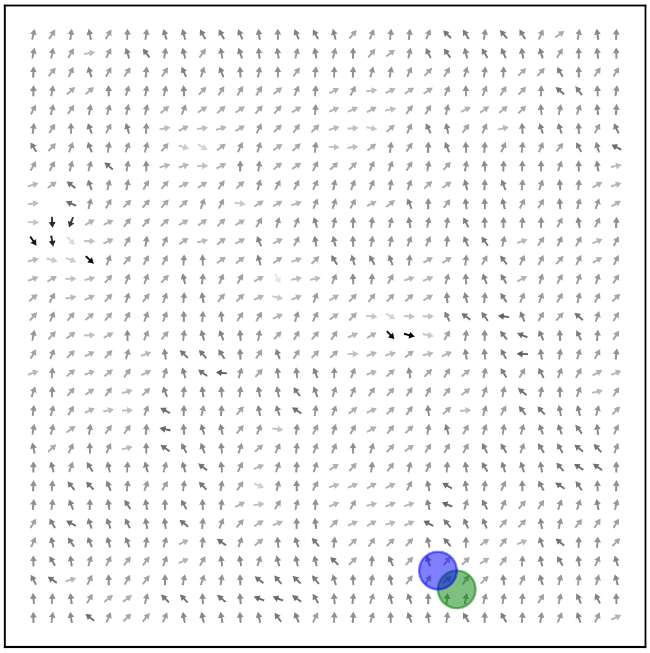

Figure 6: Visualizing the system at temperature $T = 0.5$ with one vortex-antivortex pair. The green circle represents a vortex and blue circle represents anti-vortex.

The snapshots of the lattice at a particular state after equilibrium at different temperatures can be seen in figures 6, 7, and 8 to see how the vortices and anti-vortices evolve in our model (For animation, see appendix B which has the code link.)

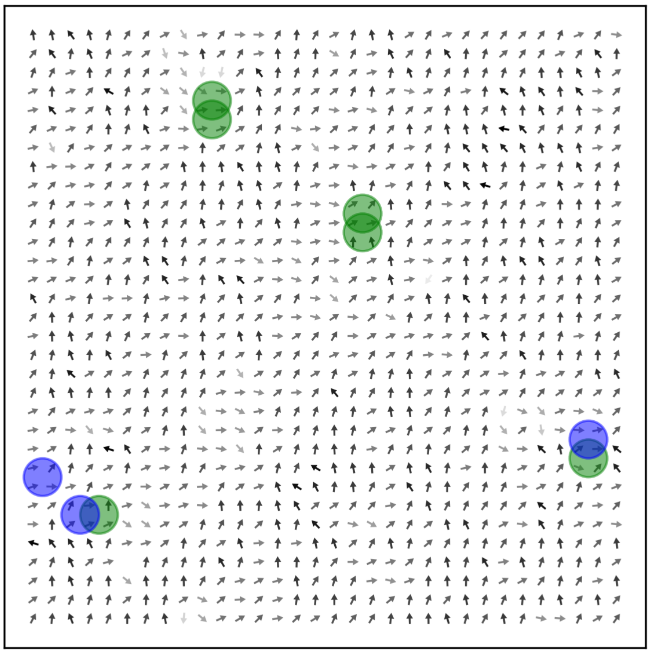

Figure 7: Visualizing the system at temperature $T = 0.9$ with two vortex-antivortex pairs, four free vortices (green) and one free anti-vortex (blue).

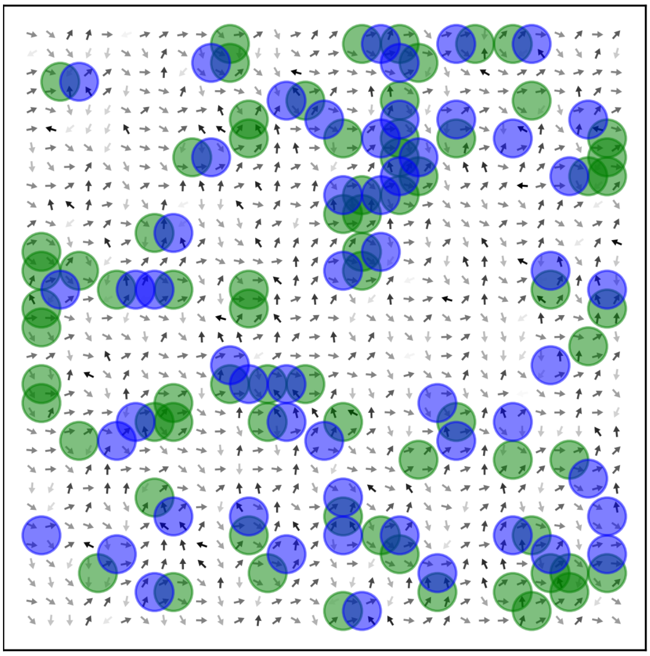

Figure 8: Visualizing the system at temperature $T = 3$ with many paired and free vortices and anti-vortices. Green circle represents vortex and blue circle represents anti-vortex.

We see that at low temperatures, the spins are more ordered and the density of vortex-antivortex is low (see Figure 6). As we increase the temperature and go above the critical temperature, we begin to see free vortices in the system (see Figure 7). As we further increase the temperature, the density of the vortex-antivortex pairs increases, and we begin to see more free vortices and anti-vortices (see Figure 8). This in fact shows the phenomenon of BKT phase transition. As we increase temperature, the vortex-antivortex pairs suddenly unbind and break apart. At these temperatures, the density of the vortex-antivortex pairs is so high, and they bump into each other a lot since these vortex and anti-vortex act like particles appearing and disappearing in the 2D lattice. So, it is hard to distinguish which vortex is the partner of which antivortex, and are left with a soup of vortices and antivortices. We now look at the difference in number of vortices and antivortices.

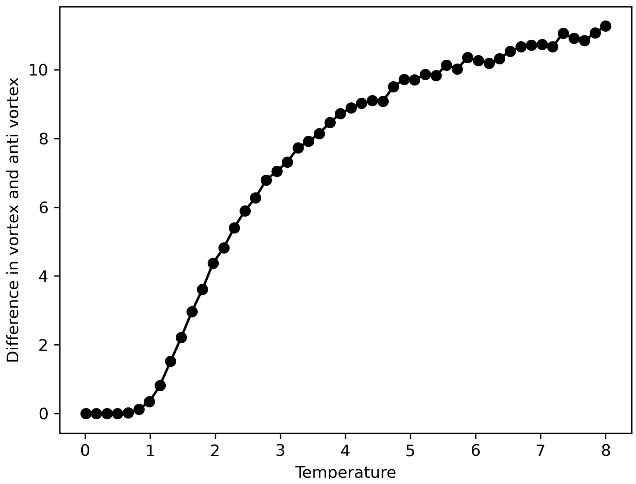

Figure 9: Difference in number of vortices and anti-vortices against temperature.

As we discussed, the vortices and anti-vortices always exist in pairs below the critical temperature. This implies that the difference in their number should be zero. As we increase the temperature and go above the critical temperature, free vortices and anti-vortices appear in the system and we see that there are more vortices than anti-vortices. The critical temperature can be seen to lie below $T = 1$, which is close to the temperature $T_{KT} = 0.893$. In our model, we have counted the vortices and anti-vortices over a 2×2 block, which implies that in a random change of spin, vortex and anti-vortex might appear in the system. We do see Kosterlitz-Thouless phase transition in our model, where the sudden unbinding of vortex-antivortex pairs near the critical temperature T_{KT} happens as we heat up our 2D lattice model.

3 Conclusion

In this paper, we have built a computational model to study Kosterlitz-Thouless phase transition (BKT transition) in the 2D XY model. The topological vortex and anti-vortex show if the system is ordered or disordered. At low temperatures, the XY model is in an ordered state, with the energy being finite as the vortex-antivortex exist in pairs. However, as we go above the phase transition temperature, we go towards a disordered state as the density of the vortex-antivortex pairs increases and we begin to see free vortices and anti-vortices, which contribute large amount of energy (see section 1.2). The phase transition happens when these paired vortex-antivortex unbind suddenly to form free vortices and anti-vortices, and the critical temperature at which it happens is $T_{KT} = 0.893J$. The critical temperatures from the graphs in our model are close to this value, implying that it is a good enough simulation of the 2D XY model.

4 Discussions

While the model is close to the theoretical predictions, several improvements can be done to get better results. One behaviour is to study the vanishing of the magnetization at all temperatures, which happens only after certain temperature in our model. We could run the simulation for more number of MC sweeps to get a better result. Studying correlation length in the 2D XY model would give more information about the critical temperature and phase transition than just the energy, magnetization, and the specific heat. This is an improvement to the model which we can implement further. The model is based on a random choice of spins and changing the configuration of the system. This implies that at any instance, there might be a change in spin of the lattice, which can cause random appearance of vortices and anti-vortices. Thus a better way to visualize them would be to take a larger block of spins, and see if they are stable enough to represent the behaviour of the system.

The BKT phase transition can be seen in systems like superfluid films, 2D crystals, superconductors, etc. Our 2D spin model to study BKT transition also gives insight into how these systems behave as we change their temperature. Like in superfluids, there is possibility of formation of quantized vortices, which have logarithmic dependence on the energy.

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5 Appendix

A Calculation of the Free energy

We'll use another approach to see how we get the expression for free energy in equation 13. Assuming system size and temperature are constant, we can write the free energy of adding a charge +1 vortex to the system as,

$$\Delta F = \Delta U - T\Delta S \tag{14}$$

The internal energy is just the energy of the vortex E_{vor}. The change in entropy will be the Boltzmann entropy, written as,

$$\Delta S = \ln(\Omega) = \ln\left(\frac{L^2}{a^2}\right) \tag{15}$$

The number of microstates Ω is given by the total number of sites by requiring the vortex to be centered at a lattice site. Hence, using these, we get the change in free energy as,

$$\Delta F = (\pi J - 2K)\ln\left(\frac{L}{a}\right) \tag{16}$$

B Code

The code to simulate the 2D XY model and study the BKT phase transition is accessible in the github repository below: BKT Phase Transition Github Link