

Simulating the Two Dimensional XY Model

Project Report

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1 Introduction

The 2D XY Model[1] represents a lattice of spins confined to a plane, with each spin characterized by an angle, rather than a binary state as in the more famous Ising Model. These spins interact via a continuous, short-range potential, reflecting the tendency of neighboring spins to align. While seemingly straightforward, the model exhibits rich dynamics, including the celebrated Kosterlitz-Thouless (KT) phase transition, which elucidates the emergence of long-range order in two dimensions.

Consider a 2D square lattice with N^2 lattice points. A configuration s is a set of unit-length vectors $s_j = (\cos \theta_j, \sin \theta_j)$ at each site. The Hamiltonian is:

$$H(\mathbf{s}) = -J \sum_{i \sim j} \cos(\theta_j - \theta_i) \quad (1)$$

The probability of each configuration is given as:

$$P(s) = \frac{1}{Z} e^{-\beta H(s)}, \beta = \frac{1}{T} \quad (2)$$

2 Numerical Method Used:

The 2D XY model can be studied in great detail using Monte Carlo simulations, for example with the Metropolis algorithm. These can be used to compute thermodynamic quantities like the system energy, specific heat, magnetization, etc., over a range of temperatures and time-scales. The algorithm goes as follows:

- Choose a lattice site at random.
- Choose a new angle value for the chosen site.
- Calculate the total energy of the system.
- If $\Delta E < 0$, accept the change.
- If $\Delta E > 0$, then:
 1. Select a uniform random number $u \in [0, 1]$.
 2. If $u \leq e^{-\beta \Delta E}$, then accept the new configuration.
 3. If $u > e^{-\beta \Delta E}$, then reject the new configuration and start over again with the previous one.
- Repeat these steps as many times as needed for the system to equilibrate.

Thermodynamic quantities can then be calculated by computing the average of the values for each Monte Carlo iteration (a single iteration corresponds to N^2 spin angle changes). As sample size increases, the value of the average converges to the thermodynamic value of the system.

3 Results

3.1 Simulations at low Temperature:

The energy values at each spin angle changes are calculated using the formula

$$E = - \sum_{i \sim j} \cos(\theta_j - \theta_i) \quad (3)$$

At low temperature, the energy seems to have equilibrated at around 750 steps with very less fluctuations (Figure 1).

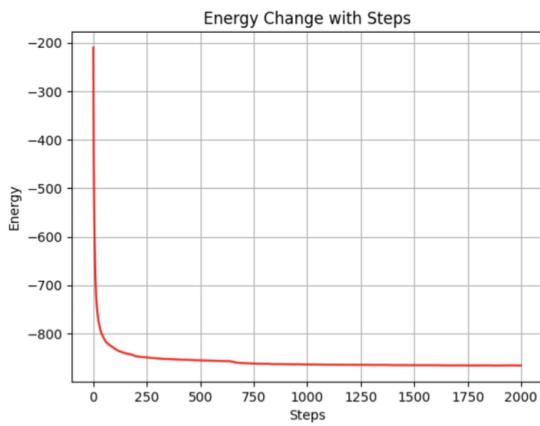


Figure 1: Energy change with Metropolis steps

Simulations of a 40x40 lattice at temperature $T = 0.01$ ($J = 1$) (Figure 2) show formation of spin vortices and antivortices at low temperature which are attracted by each other and destroyed while undergoing equilibration. Large areas of the lattice show spins directed in a certain direction.

Simulations of a 250x250 lattice at temperature $T = 0.01$ (Figure 3) show the formation of domain structures by destruction of vortex-antivortex pairs. There is no complete symmetry breaking as per the Mermin-Wagner theorem.

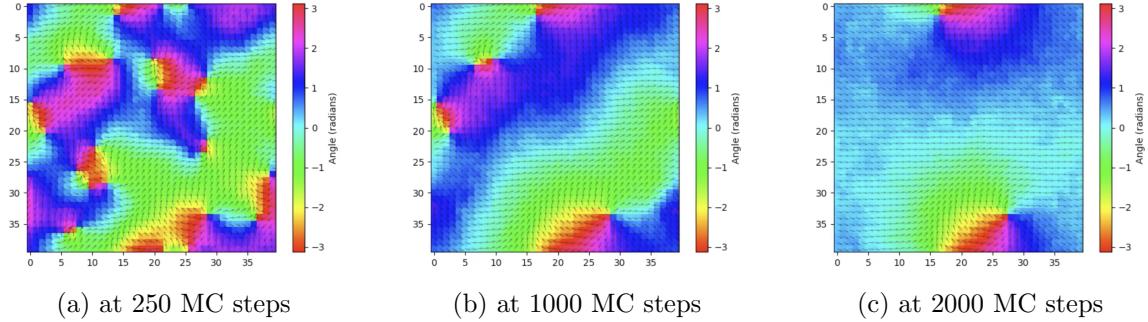


Figure 2: Simulation of a 40×40 lattice at $T=0.01$

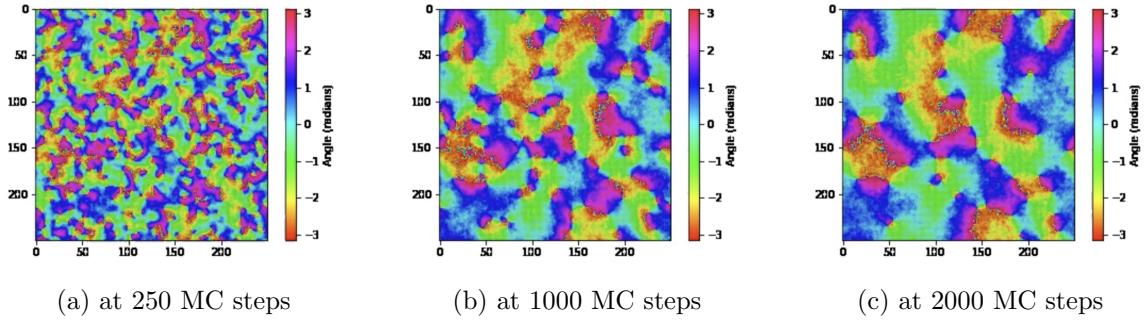


Figure 3: Simulation of a 250×250 lattice at $T=0.01$

3.2 Simulations at high Temperature:

At high temperature, the energy seems to have equilibrated at around 100 steps with some fluctuations throughout (Figure 4).

Simulations of a 40×40 lattice (Figure 5) and a 250×250 (Figure 6) lattice at temperature $T = 1.5$ ($J = 1$) show disorder where spins align in random directions.

3.3 Plots of Thermodynamic quantities:

Thermodynamic quantities are calculated by averaging from the sample of iterations of Metropolis algorithm for different temperatures and then plotted (Figure 7). The peak in the specific heat plot is of similar orders with increase in system size and hence, does not depict a phase transition.

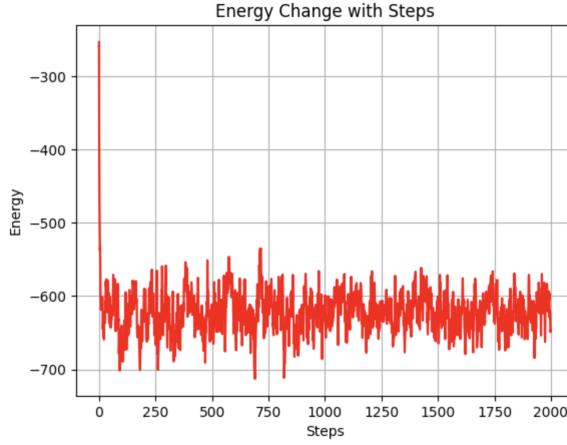


Figure 4: Energy change with Metropolis steps

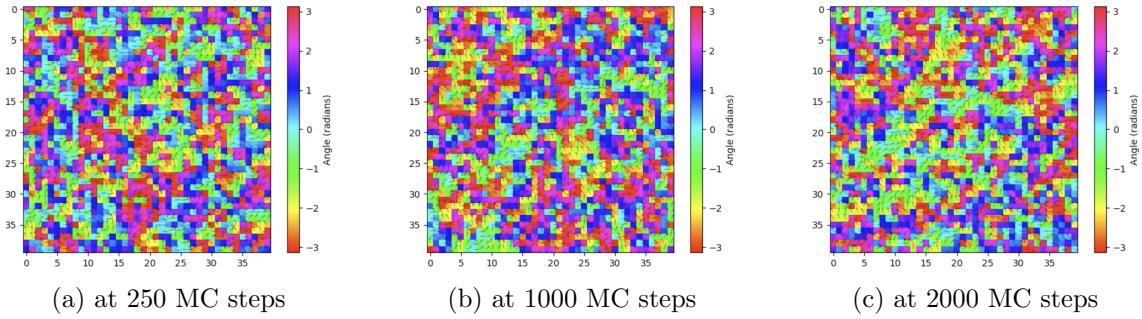


Figure 5: Simulation of a 40x40 lattice at $T=1.5$

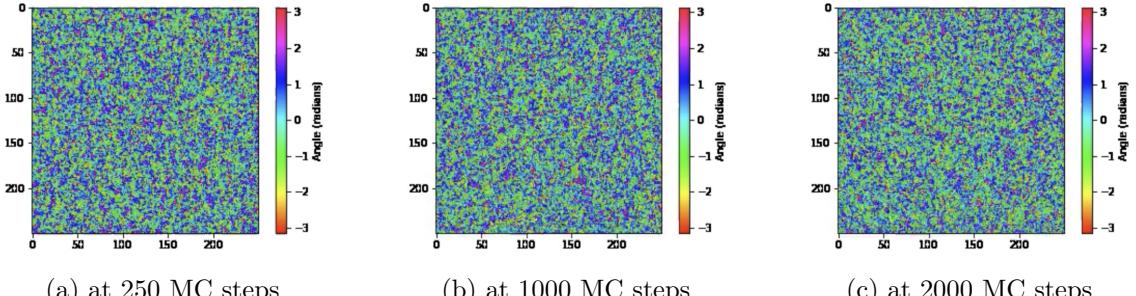
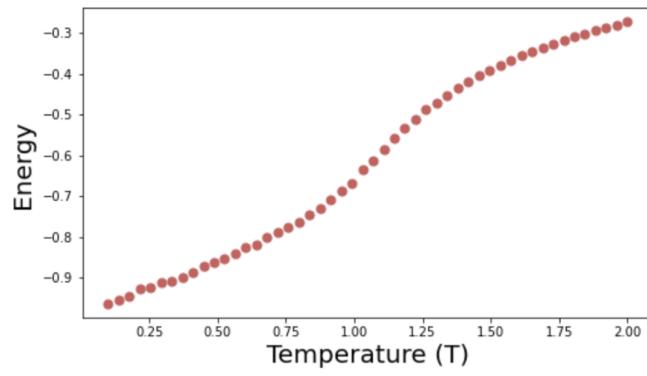


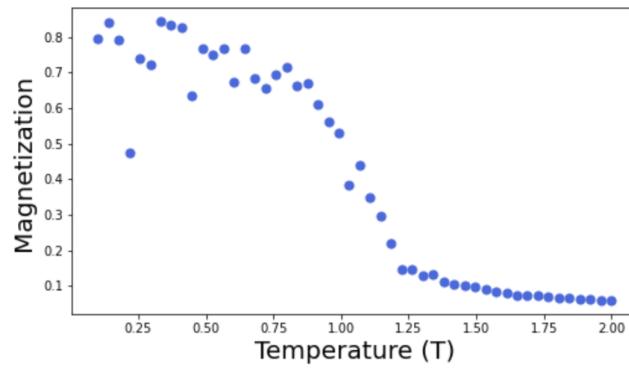
Figure 6: Simulation of a 250x250 lattice at $T=1.5$

3.4 Simulation of Annealing:

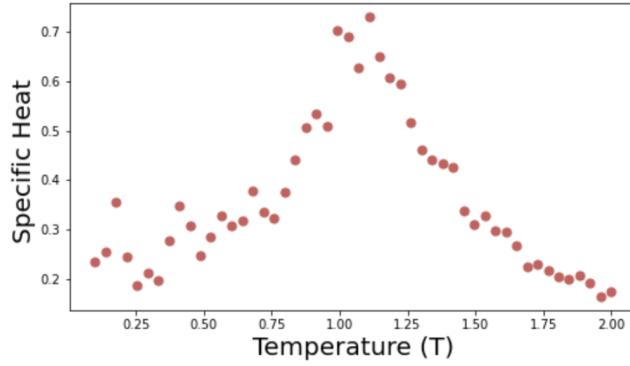
The Metropolis Algorithm is then applied with varying temperatures after each iteration to see how the spins change when the system is quasistatically heated (Figure 8).



(a) Energy vs Temperature



(b) Specific Heat vs Temperature



(c) Magnetisation vs temperature

Figure 7: Plots of Thermodynamic Features of the 2D XY Model

The simulation shows the domains getting destroyed slowly as the system is heated and as disorder sinks in.

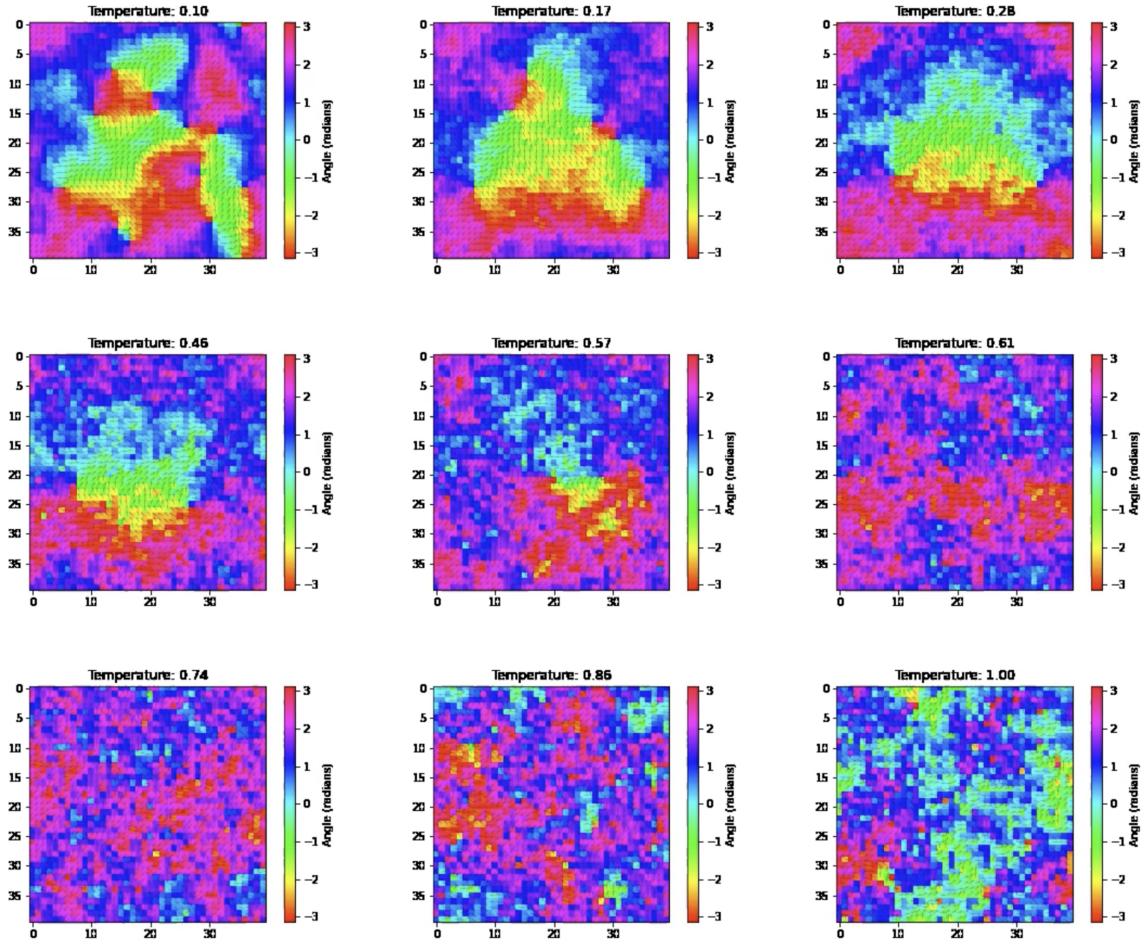


Figure 8: Simulation of Annealing

4 Conclusion

: The simulations show the system transitioning from some ordered to some disordered state at some critical temperature. Although the Mermin Wagner theorem doesn't allow any symmetry breaking, the system undergoes a infinite order phase transition called the Berezinskii–Kosterlitz–Thouless (BKT) transition. The BKT transition is a transition from bound vortex-antivortex pairs at low temperatures to unpaired vortices and anti-vortices at some critical temperature. In the 2-D XY model, vortices are topologically stable configurations. It is found that the high-temperature disordered phase with exponential correlation decay is a result of the formation of vortices. Vortex generation becomes thermodynamically favorable at the critical temperature

T_C of the BKT transition. At temperatures below this, vortex generation has a power law correlation. BKT transition is thus described as a dissociation of bound vortex pairs with opposite circulations, called vortex–antivortex pairs.

References

- [1] Wikipedia. *Classical XY model*. https://en.wikipedia.org/wiki/Classical_XY_model. [Online; accessed 13-May-2024].