Jesse Antinoja 29.5.2024
Classical simulation methods in physics

2D Simulation of Ferromagnetism using Classical XY Model

The goal of the project was to simulate ferromagnetism in a 2D lattice using classical XY model, in which classical spins are represented as 2-component unit-length vectors on 2D lattice vertices. This was done using Metropolis Monte Carlo algorithm.

1 Theory

1.1 XY Model

The XY model is a specialization of n-vector model where n=2. In it, each lattice point is seen as two dimensional vector. The total energy of XY model is [1]

$$E_{\mathrm{XY}} = -\sum J_{\mathrm{i,j}}\ \hat{s}_{\mathrm{i}} \cdot \hat{s}_{\mathrm{j}} \tag{1}$$

As the vectors are unit length, their dot product becomes

$$E_{\mathrm{XY}} = -\sum J_{\mathrm{i,j}}\ \cos\left(\theta_{\mathrm{i}} - \theta_{\mathrm{j}}\right) \tag{2}$$

I decided to implement the simplest case, so called nearest neighbour case where $J_{\mathrm{i,j}} = 1$ for ij neighbours and zero for all else.

The magnetic dipole moment of a classical electron may be described with equation (3):

$$\vec{\mu} = -g_{\mathrm{s}}\frac{e}{2m_{\mathrm{e}}}\ \vec{s} \tag{3}$$

By choosing unitless scale, we get $-g_{\mathrm{s}}\frac{e}{2m_{\mathrm{e}}} = 1$ and our magnetic dipole moment is just the spin vector. The total magnetization of the system may be calculated as magnitude of average magnetization components in each direction [2]:

$$|M| = \frac{1}{N}|\sqrt{M_x^2 + M_y^2}| \tag{4}$$

$$= \frac{1}{N} \left| \sqrt{(\sum_{i=0}^{L} s_x)^2 + (\sum_{i=0}^{L} s_y)^2} \right|$$
$$= \frac{1}{N} \left| \sqrt{(\sum_{i=0}^{L} \cos\theta_i)^2 + (\sum_{i=0}^{L} \sin\theta_i)^2} \right|$$

1.2 BKT Transition

The phase transition happening in the 2D XY model is the Berezinskii-Kosterlitz-Thouless transition or sometimes just Kosterlitz-Thouless transition. It's a phase transition going from bound vortex-antivortex pairs to unpaired vortices and antivortices at some temperature T_{BKT} [1]. The exact solution is still not found, but over the decades researchers have came up with better and better approximations on the transition temperature, the latest being $T_{\mathrm{BKT}} \approx 0.8935$ [3]. Examples of vortices shown in figures 1 and 2.

1.3 Metropolis Algorithm

The metropolis Monte Carlo algorithm is a type of mcmc where the system's future depends only on it's current state. In it, the system's future steps are decided with some probability distribution f. The algorithm draws samples from the distribution and tries to move about in the sample space. The acceptance rate of the algorithm is dependent on the probability distribution, temperature and the chosen method of changing the sample state. The distribution used in the XY model is the Boltzmann distribution:

$$P = e^{\frac{-\Delta E}{k_{\mathrm{B}} T}} \tag{5}$$

Here ΔE is the system's would be energy change going from state $i \to i+1$, k_{B} is the Boltzman constant and T the temperature. Again, the unitless scale is used and Boltzmann constant $k_{\mathrm{B}} = 1$. The algorithm steps are:

1. Start with some initial system configuration. This can be random or specific initial condition.
2. Pick a random sample and choose a new state for it randomly.
3. Calculate energy change ΔE.

4. If the energy change is $\Delta E < 0$, accept the change as new state for the sample.

5. If energy change is $\Delta E > 0$, accept the change with chosen probability distribution, here the Boltzmann distribution.

6. Iterate previous steps for large number of times to ensure proper sampling of the state space - here chosen the total number of spins.

2 Simulation Methodology

At the heart of the algorithm are the spin vector creation, rotation and energy calculation. I created a lattice as LxL grid, where each vertice is an angle ϕ chosen randomly between interval [0,2π]. Another important parameter is the change of angle in each metropolis step, $\Delta\phi$. The choice of right $\Delta\phi$ is crucial for good acceptance rate. After some tries I arbitrarily chose to create each test angle as a random number between $[\frac{-\pi}{20}, \frac{\pi}{20}]$. If the change of angle is accepted, $\Delta\phi$ is added to the current angle and then taken modulo 2π to normalize angle to the interval [0,2π]. Other possible topics for study would be alternative methods for the decision of $\Delta\phi$, such as sampling from normal distribution with some standard deviation such as $\frac{\pi}{20}$. Energy change calculation was done using equation (2) where energy change is calculated over all four closest neighbours [(1+i,j),(i-1,j),(i,j+1),(i,j-1)]:

$$\Delta E_{\text{neighbours}} = -J(\cos(\phi + \Delta\phi - \phi_{\text{neighbours}}) - \cos(\phi - \phi_{\text{neighbours}}))$$

The inherent flaw of the Metropolis algorithm is the sample autocorrelation. To combat this, I decided to calculate magnetic moments only for one in every ten samples.

3 Results

I studied the magnetization model in two ways. First by running single Metropolis algorithms and inspecting model animations as well as magnetizations as functions of simulation steps. Secondly I ran temperature series over some range of temperatures and tried to spot any signs of phase transition in the magnetization curves.

3.1 Single Temperature

When the temperature is set low, the acceptance rate is high and the spins adjust fast to form uniform magnetization in the lattice. In figure 1 shown a snapshot of the beginning of vector animation with low temperature. Here large parts of grid have already adjusted to uniform direction while some big vortices still present. In figure 2 shown snapshot of similar animation but with T= 0.9, slightly greater than the transition temperature. Here the snapshot is taken long after the initial configuration but still the system is mostly composed of small unpaired vortices.

In figure 3 plotted the total magnetization of a 20x20 lattice as a function of simulation steps. Here the total simulation steps were 5000 with 4000 steps thermalization. With adjusted to autocorrelation, in total 100 sample points were collected. One can see that in fig. 3a with temperature 0.1 the system stays in uniform total magnetization with minimal fluctuation. As the temperature is risen, magnetization fluctuation increases. Notably in fig. 3c on the verge of critical temperature, the fluctuation is still quite small, approximately 0.09 but in 3d fluctuation has increased to about 0.14.

3.2 Temperature Series

My goal was to find some correlation with the theoretical critical temperature associated with the model, T_{BKT}. In figures 4 and 5 shown time series simulations with 20x20 and 30x30 lattices respectfully. The temperature range was [0.1,1.0] in both. In the $L = 20$ case one can see a quite uniform slope in magnetization decrease until the critical temperature at about $T = 0{,}9$. In the L = 30 case the slope isn't so defined but a great drop in magnetization value is noticeable. These temperature series observations as well as visual observations from figures 1 and 2 go quite well with the literature value for phase transition, $T_{\mathrm{BKT}} = 0{,}8935$.

Lastly, in figure 6 is shown an attempt at a multiple lattice size temperature series simulation. The data isn't ideal but one can see a drop in magnetizations at around 0.9 for lattice sizes L = 20 & 30 but for some reason fail to do so as clearly for the L= 40 case.

4 Discussion

The findings are supported by literature to some extent. They're somewhat hindered by the available computation power but are close enough for the scope of this study. I would've liked to get better results especially with the multiple lattices simulation in figure 6 but due to time constraints I couldn't dive deeper into that. This project and the course as a whole were demanding but still interesting, fun and rewarding.

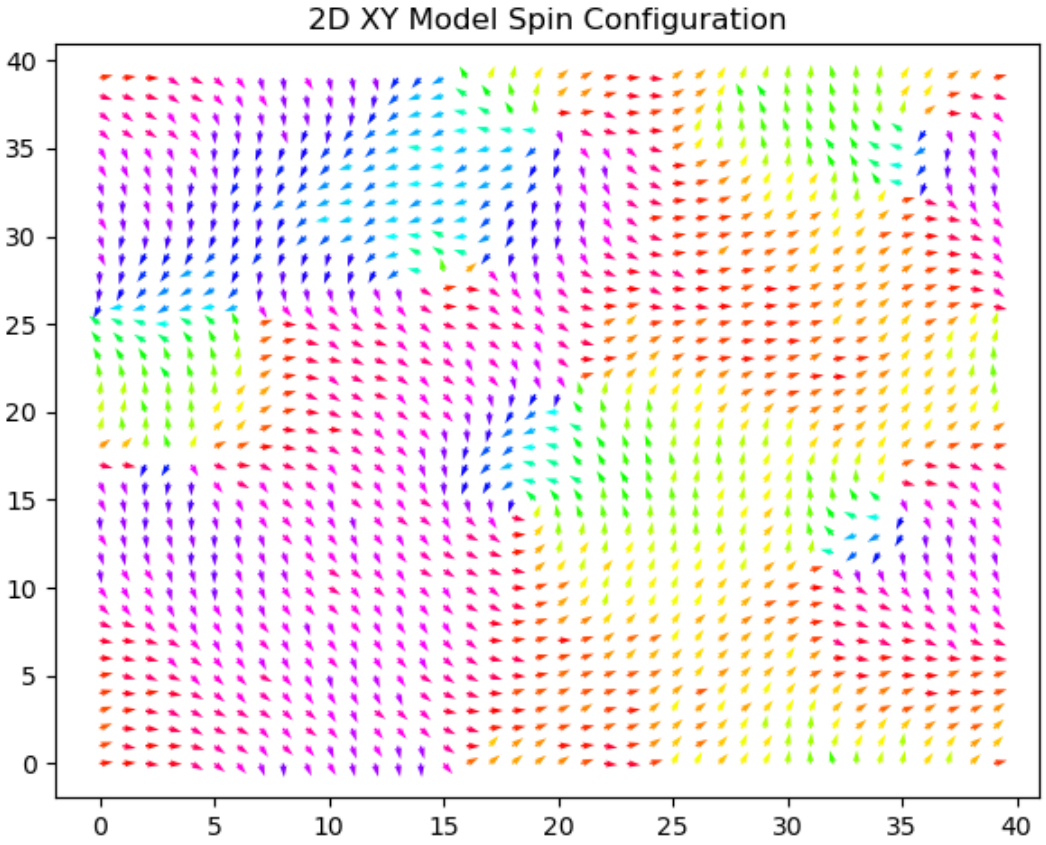


Figure 1: Vector animation snapshot with 40x40 lattice and T = 0.1.

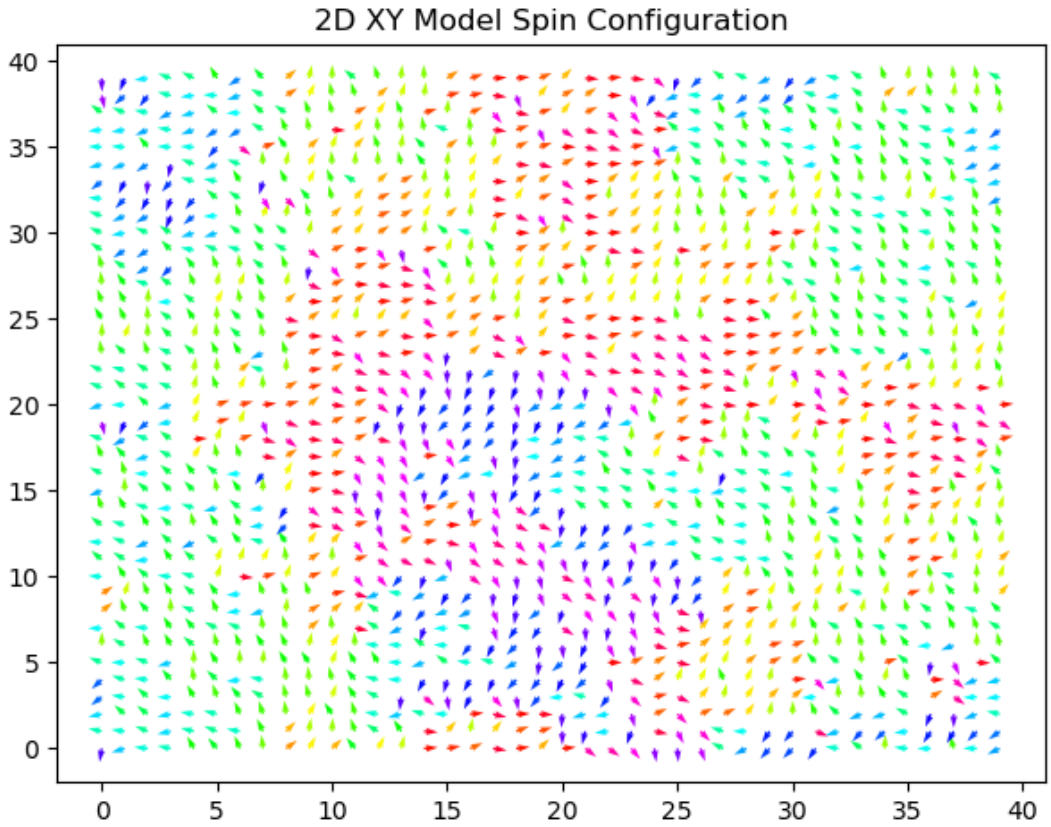
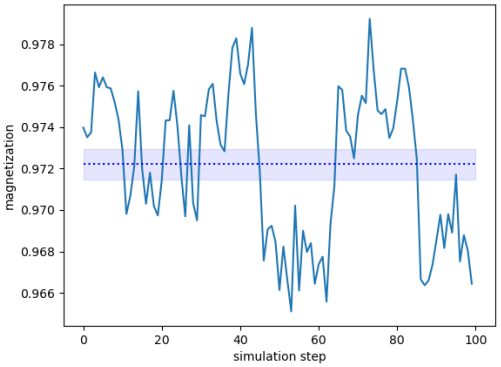
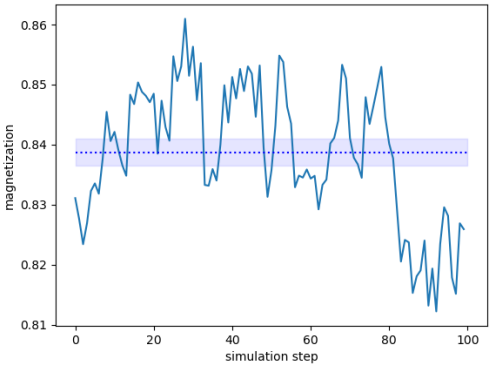


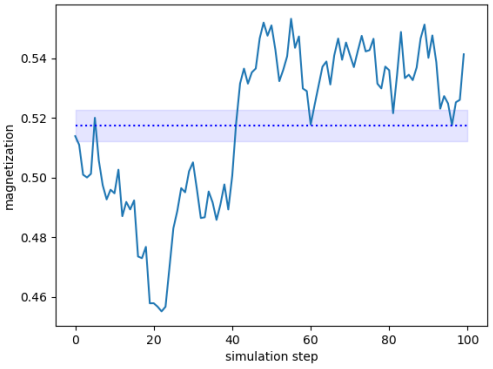
Figure 2: Vector animation snapshot with 40x40 lattice and T = 0.9.



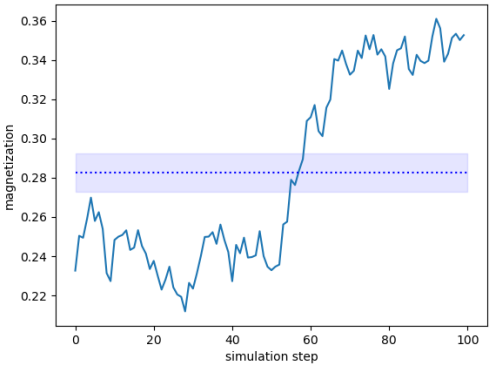
(a) T= 0.1



(b) T= 0.5



(c) T= 0.89



(d) T= 1.0

Figure 3: Magnetizations with 20x20 lattice and 5000 steps.

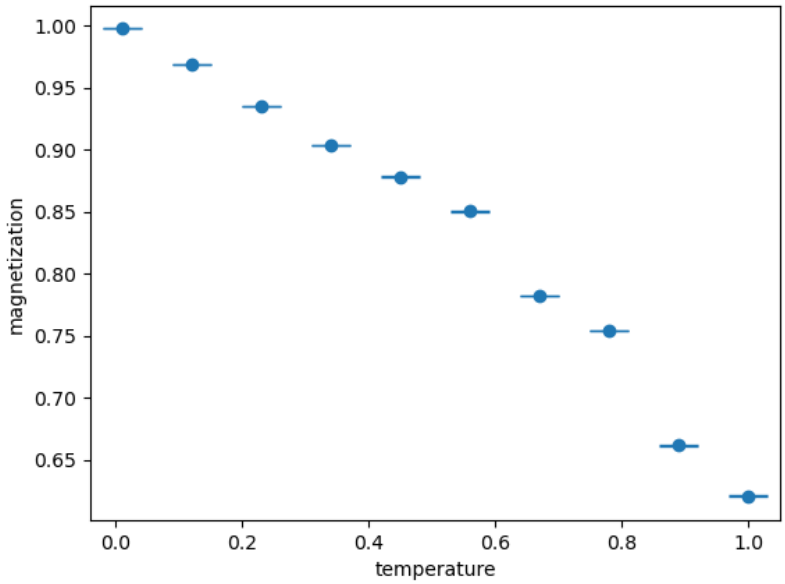


Figure 4: temperature series with 20x20 lattice, 10 000 steps and T= [0.1,1.0].

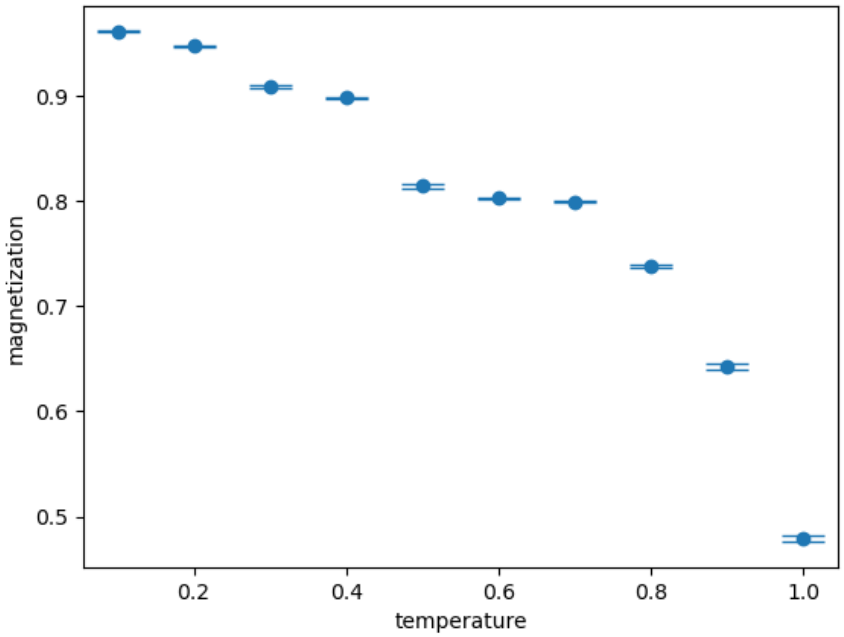


Figure 5: temperature series with 30x30 lattice, 5000 steps and T = [0.1,1.0]

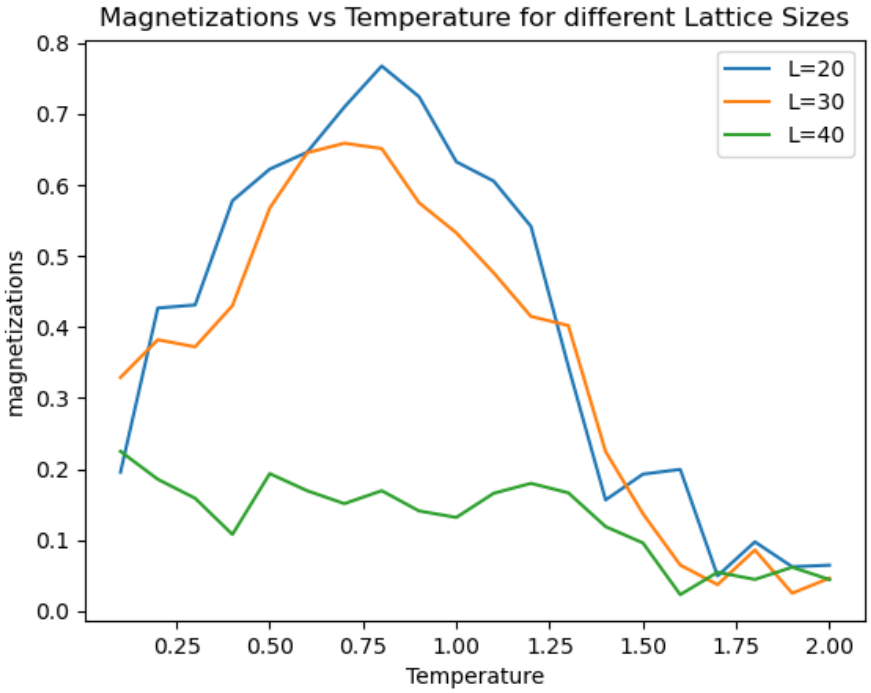


Figure 6: Temperature series with 3 lattice sizes, 1000 steps and T = [0.1,2.0].

References

[1] Ahamed, S., Cooper, S., Pathak, V., & Reeves, W. *The Berezinskii-Kosterlitz-Thouless Transition.*
Dept. of Physics Astronomy, University of British Columbia, Canada.
<https://phas.ubc.ca/~berciu/TEACHING/PHYS502/PROJECTS/18BKT.pdf>
(29.5.24)

[2] Banerjee, N (2023) *Simulation of Kosterlitz-Thouless (KT) Transition with Classical Monte-Carlo Simulation*
Department of Physics,University of Seoul,South Korea
<https://arxiv.org/pdf/2307.10310>
(28.5.24)

[3] Hsieh, Y. D., Kao, Y. J., & Sandvik, A. W. (2013) *Finite-size scaling method for the Berezinskii-Kosterlitz-Thouless transition*
Arxiv
<https://arxiv.org/pdf/1302.2900>
(28.5.24)