Monte Carlo Simulations of the 2D XY Model using Markov-chains

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Introduction

The 2D XY model is a system that exhibits many interesting physical phenomena, for example phase transitions [2] which are studied in this task. These types of systems are studied with Monte Carlo simulations using the principles of the Metropolis algorithm, where Markov chains are used to generate spin configurations [1]. The focus was primarily on measuring the magnetization and energy as a function of temperature for the system and using the function called Binder cumulant to determine the critical temperature [1]. The 2D XY model is of special interest because of it's topological properties manifesting the Berezinski - Kosterlitz - Thouless (BKT) transition which exhibits similar characteristics found in for example liquid films and 2D superconductors.

Theory

The spins of the system is layered on a square lattice with nearest neighbour interactions and with periodic boundary conditions. The layout is illustrated in Figure (1) where each spin represented by a dot has two components S_x and S_y acting like a magnetic arrow.

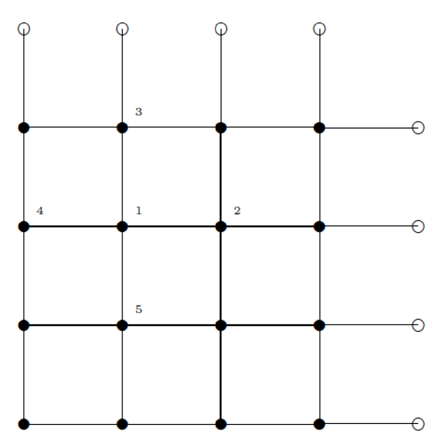

Fig. 1: Spins on a square lattice with nearest neighbour interaction.

This study uses an angular representation where each spin is assigned an angle $\theta \in [0, 2\pi]$ in the XY-plane. The 2D XY model can be described by the Hamiltonian given by

$$\mathcal{H} = -J \sum_{<i,j>} cos(\theta_i - \theta_j) + H \sum_i cos(\theta_i), \qquad (1)$$

where $< i, j >$ denotes summation over the nearest neighbours, H represents an external magnetic field (H = 0 is used) and the variable J represents the coupling constant ($J = 1$). Each new state is generated by changing the angle of one spin using a random walking algorithm to a new angle $\theta \in [0, 2\pi]$ randomly and calculating the energy difference $\Delta\mathcal{H} = \mathcal{H}_{new} - \mathcal{H}_{old}$. The value for $\Delta\mathcal{H}$ is then used with the Metropolis algorithm to determine if the new state is accepted or discarded. The system starts in a randomly generated state and is iterated on until the system is in equilibrium. Measurements of the magnetization and energy are done in the equilibrium state.

Method

The critical temperature (τ_c) is determined by measuring the Magnetic susceptibility (χ), Specific heat capacity (C_v) and the Binder cumulant (g) [3, 1] defined as

$$\chi = \frac{L^2(<M^2> - <M>^2)}{\tau} \quad (2), \quad C_v = \frac{<E^2> - <E>^2}{L^2\tau^2} \quad (3), \quad g = 1 - \frac{<M^4>}{3<M^2>^2} \quad (4) \quad ,$$

where L^2 denotes lattice size, τ is the fundamental temperature [2], $< M >$ and $< E >$ denotes the average magnetization and energy per spin.

The critical temperature is at the value τ where the Binder cumulant for different lattices sizes cross.
The critical exponents can be determined by using the finite size scaling relations according to [1]

$$g \sim \tilde{G}\left[L^{1/\nu}(\tau - \tau_c)\right] \quad (4), \quad \chi \sim L^{\gamma/\nu}\tilde{C}\left[L^{1/\nu}(\tau - \tau_c)\right] \quad (5)$$

where the values for the exponents ν and γ are correct when the magnetic susceptibility and Binder cumulant form a universal curve for different lattice sizes. However, due to the nature of the phase transition in the XY model, it is not possible to extract the exponents with the usual power laws and is consequently excluded from the analysis.

Results

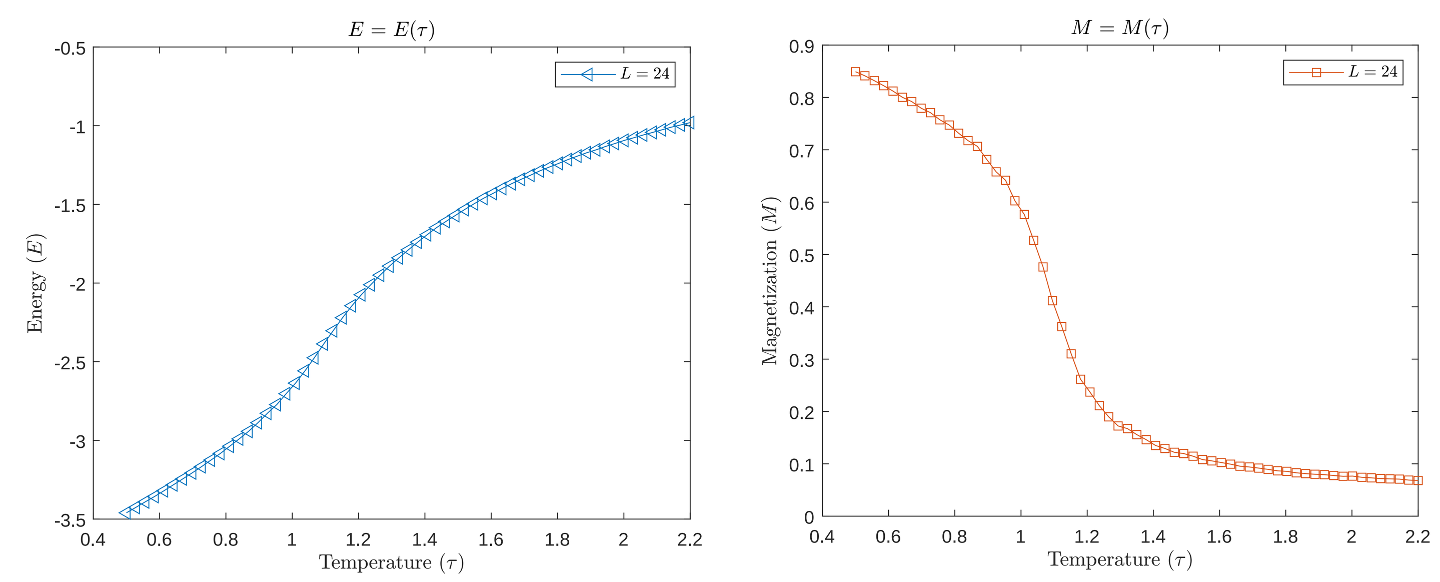

Fig. 2: **Left:** Average energy per spin as a function of temperature.
Right: Average magnetization per spin as a function of temperature.

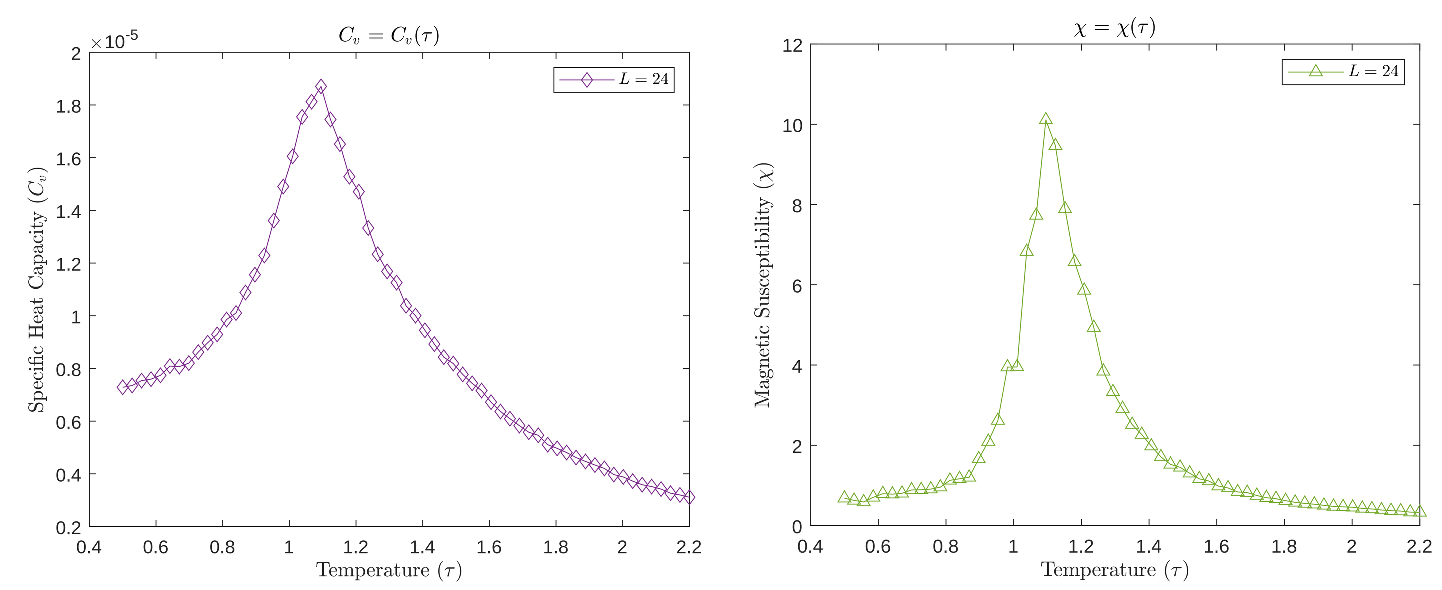

Fig. 3: **Left:** Average magnetic susceptibility per spin as a function of temperature.
Right: Average specific heat capacity per spin as a function of temperature.

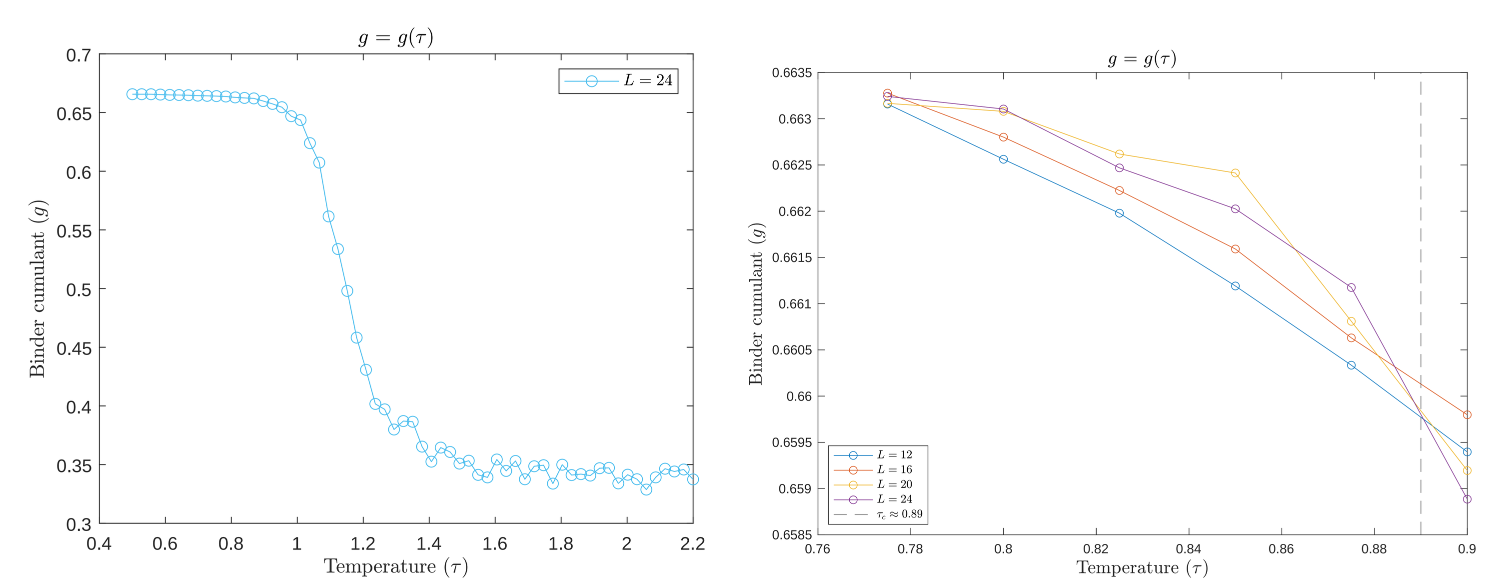

Fig. 4: **Left:** Binder cumulant as a function of temperature for lattice size L = 24.
Right: Binder cumulant as a function of temperature for lattice sizes L = 12 - 24. The crossing temperature show the critical temperature $\tau_c \approx 0.89$.

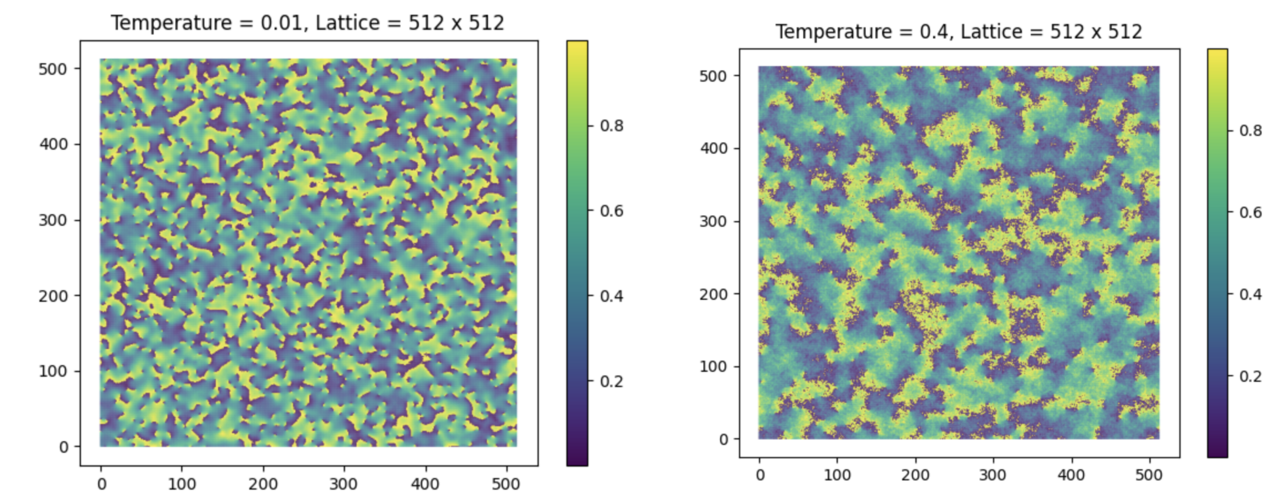

Fig. 5: The figures show the lattice with 512 x 512 spins. The colorbar represents the scaled angle for each spin. The fundamental temperature for the left figure is $\tau = 0.01$ and right figure $\tau = 0.4$.

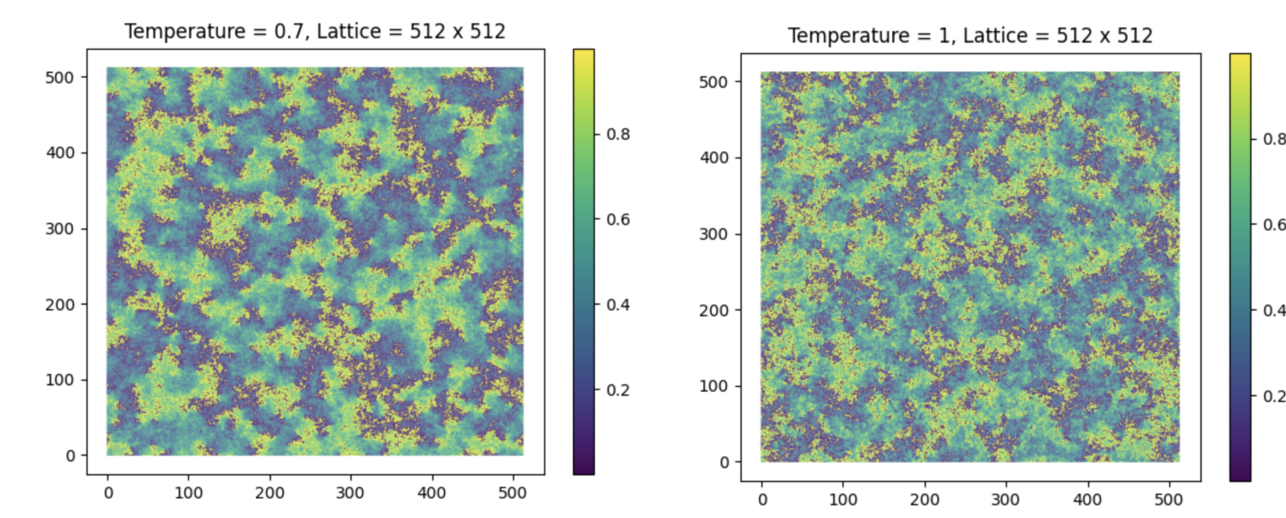

Fig. 6: The figures show the lattice with 512 x 512 spins. The colorbar represents the scaled angle for each spin. The fundamental temperature for the left figure is $\tau = 0.7$ and right figure $\tau = 1$.

Conclusions

The graph in Figure (4) shows the Binder cumulant for different lattice sizes in the range $L = 12 - 24$. The critical temperature in the thermodynamic limit is at the temperature where the Binder cumulant crosses for different lattice sizes, and was determined to be $\tau_c \approx 0.89$.

The Figures (5) and (6) shows the spins for a system size of 512×512 with colors representing the angle $\theta \in [-\pi, \pi]$ for each spin. The BKT transition is characterised by the binding and unbinding of topological defects in the form of vortices and anti-vortices. A vortex is characterised by spins whirling around a point, with the antivortex being the same but having the spin orientation in the opposite direction. At low temperatures the vortices are bound in pairs seen in Figure (5) and (6) leading to a "quasi-ordered" phase with long-range correlation in the orientations of the spins. At the critical temperature $\tau_c \approx 0.89$, a transition occurs where the vortex-antivortex pairs "unbind" leading to a disordered phase which destroys the long-range correlation.

The 2D XY model does not exhibit a normal second order transition leading to symmetry breaking, but instead undergoes a phase transition of infinite order entering a quasi-ordered state characterized by topological defects.

References

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[2] C. Kittel and H. Kroemer. *Thermal Physics.* W. H. Freeman and Company, 1980.

[3] M. E. J. Newman and G. T. Barkema. *Monte Carlo Methods in Statistical Physics.* Oxford University Press, 2001.