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

Kim-Jonas Ylivainio

Luleå University of Technology

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. The model is often studied in statistical physics and condensed matter physics due to these unique properties, which also has real-world analogues in various physical systems.

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 attempting to use the function called Binder cumulant to determine the critical temperature [1].

The 2D XY model holds special interest due to its topological properties, which give rise to the Berezinski - Kosterlitz - Thouless (BKT) transition. This transition exhibits characteristics similar to those found in certain real-world systems, including superfluid films and two-dimensional 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.

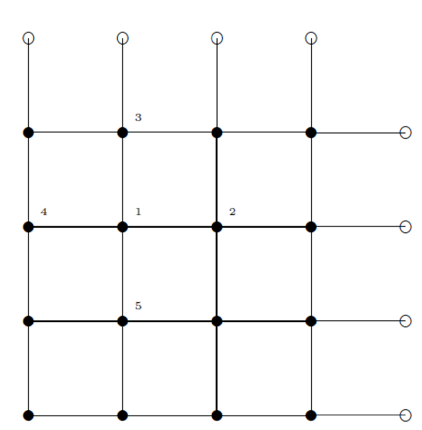

Fig. 1: Spins on a square lattice with nearest neighbour interaction.

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

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

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

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

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, specifically for systems which undergoes a first or second order phase transition.

The critical exponents can be determined by using the finite size scaling relations according to [1]

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

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 cumbersome to extract the exponents with the usual power laws and is consequently excluded from the analysis.

Results

This section presents the results from the simulations. The graphs in Figure 2 shows the measurements of the energy and magnetization, which where used to derive values for the magnetic susceptibility, the specific heat capacity and the binder cumulant seen in Figure 3 and 4. To study the topological properties, quiver graphs were created with the angle of each arrow represented by a color scale. These graphs can be found in Figure 5 and Figure 6.

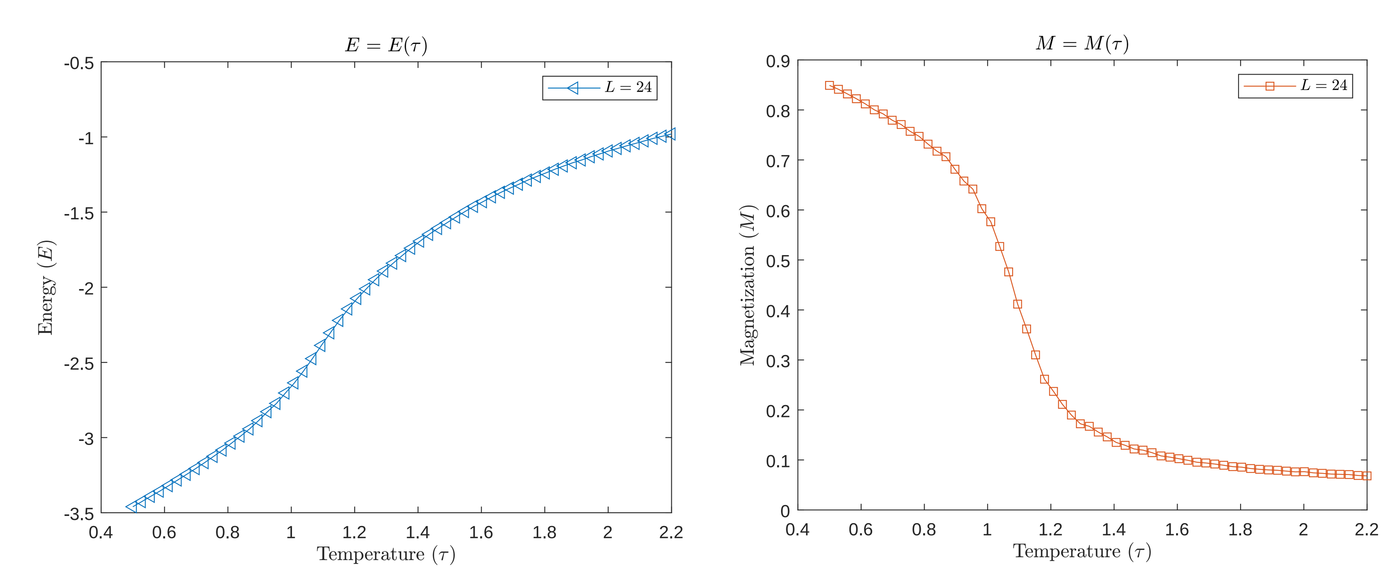

Fig. 2: **Left:** Average energy per spin $< E >$ as a function of temperature.
Right: Average magnetization per spin $< M >$ as a function of temperature.

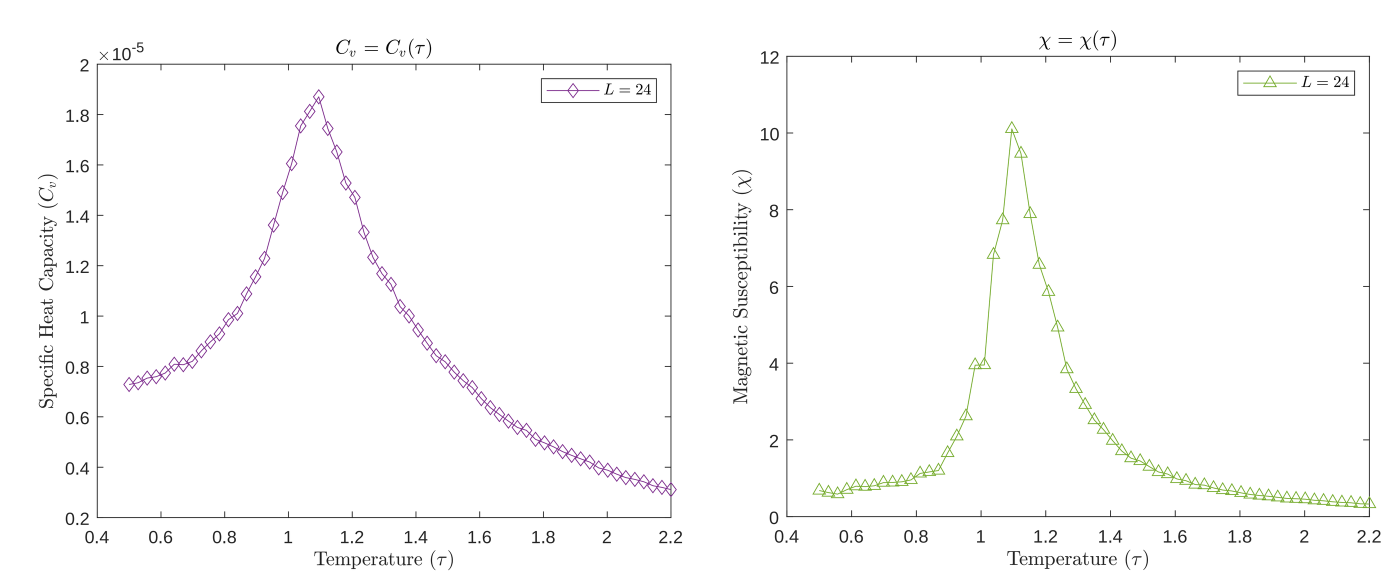

Fig. 3: **Left:** The graph shows the specific heat capacity (C_v) as a function of temperature.
Right: The graph shows magnetic susceptibility (χ) as a function of temperature.

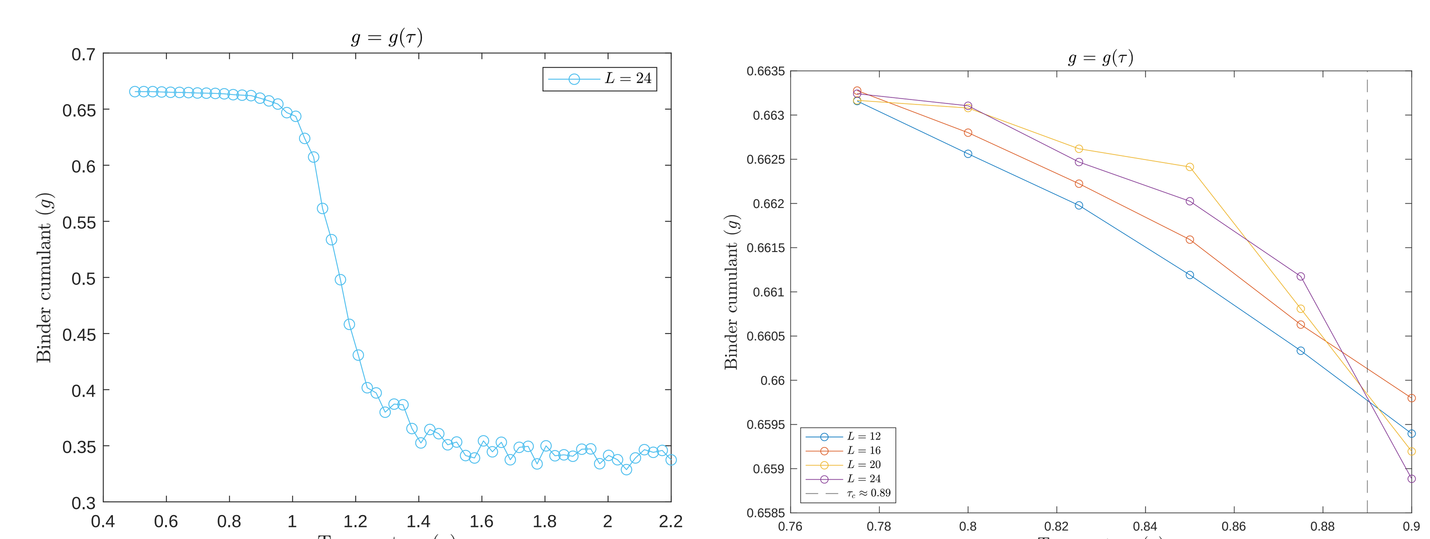

Fig. 4: **Left:** Binder cumulant as a function of temperature for lattice size $L = 24$.
Right: Binder cumulant as a function of temperature for lattice sizes $L = 12 - 24$. The crossing value show the critical temperature $\tau_c \approx 0.89$.

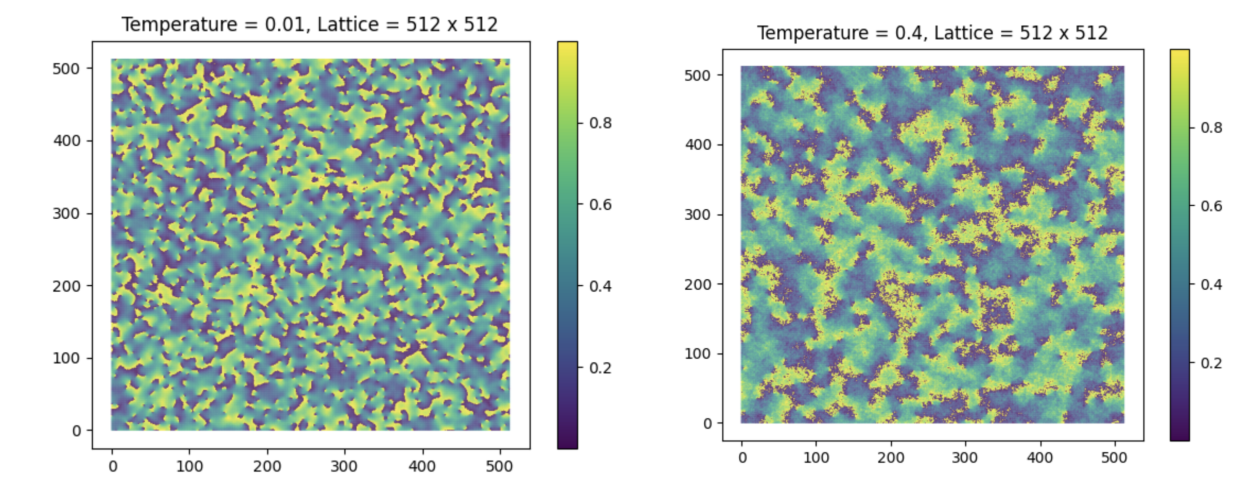

Fig. 5: The figures show the lattice with 512×512 spins. The colorbar represents the scaled angle for each spin. The fundamental temperature for the left figure is $\tau = 0.01$ and right figure $\tau = 0.4$. The Figures shows the topological characteristics when the systems is below the critical temperature τ_c.

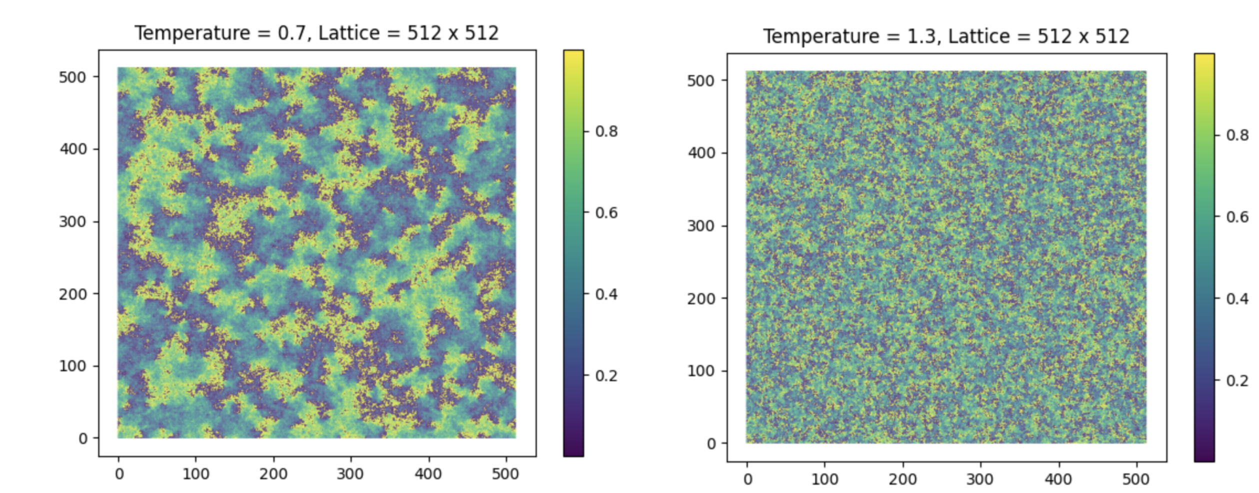

Fig. 6: The Figures show the lattice with 512×512 spins. The colorbar represents the scaled angle for each spin. The fundamental temperature for the left Figure is $\tau = 0.7$, which is below τ_c and right Figure $\tau = 1.3$, which is above τ_c, showing the topological characteristics before and after the phase transition.

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 value where the Binder cumulant crosses for different lattice sizes, which was determined to be $\tau_c \approx 0.89$. This value is in agreement with estimations of the critical temperature found in various sources, but the analysis is not complete and should be complemented with an analysis of the helicity modulus Υ.

The Figures 5 and 6 shows the spins for a system of size 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, with a vortex characterised by spins whirling around a point, and the antivortex being the same but having the spin orientation in the opposite direction. At low temperatures the vortices are bound in pairs leading to a "quasi-ordered" phase with long-range correlation of the spin orientations. At the critical temperature τ_c, a transition occurs where the vortex-antivortex pairs "unbind" leading to a disordered phase which destroys the long-range correlation. The results found from the simulations are presented in Figure 5 and 6, which show the topological characteristics of the system for temperatures under the critical temperature τ_c illustrating the "quasi-ordered" state, together with the topology of the disordered state after the phase transition.

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 from a quasi-ordered state characterized by topological defects.

The simulation was done in MATLAB and the source files can be found at `https://github.com/kimyliv`.

References

[1] Helmut G. Katzgraber. *Introduction to Monte Carlo Methods.* 2011.

[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