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. The critical temperature and the critical exponents where determined by using these measured physical quantities together with finite size scaling [1].

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.

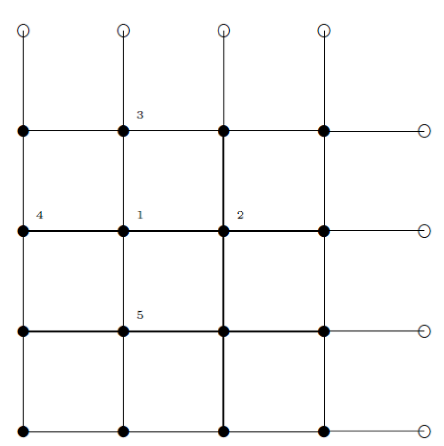

Fig. 1: Spins on a square lattice with nearest neighbour interaction.

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

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

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 are determined by using the finite size scaling relations [1].

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

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.

Results

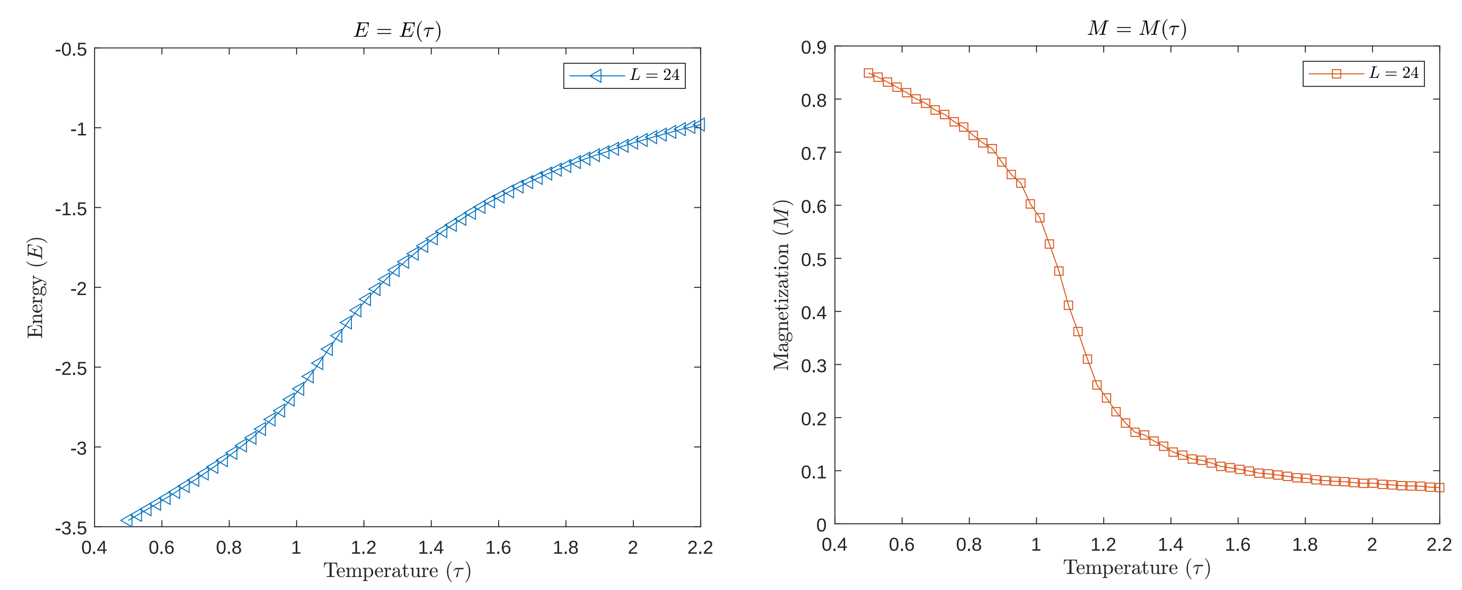

Fig. 2: **Left:** Average energy per spin as a function of temperature.
Right: Average magnetization per spin as a function of temperature.

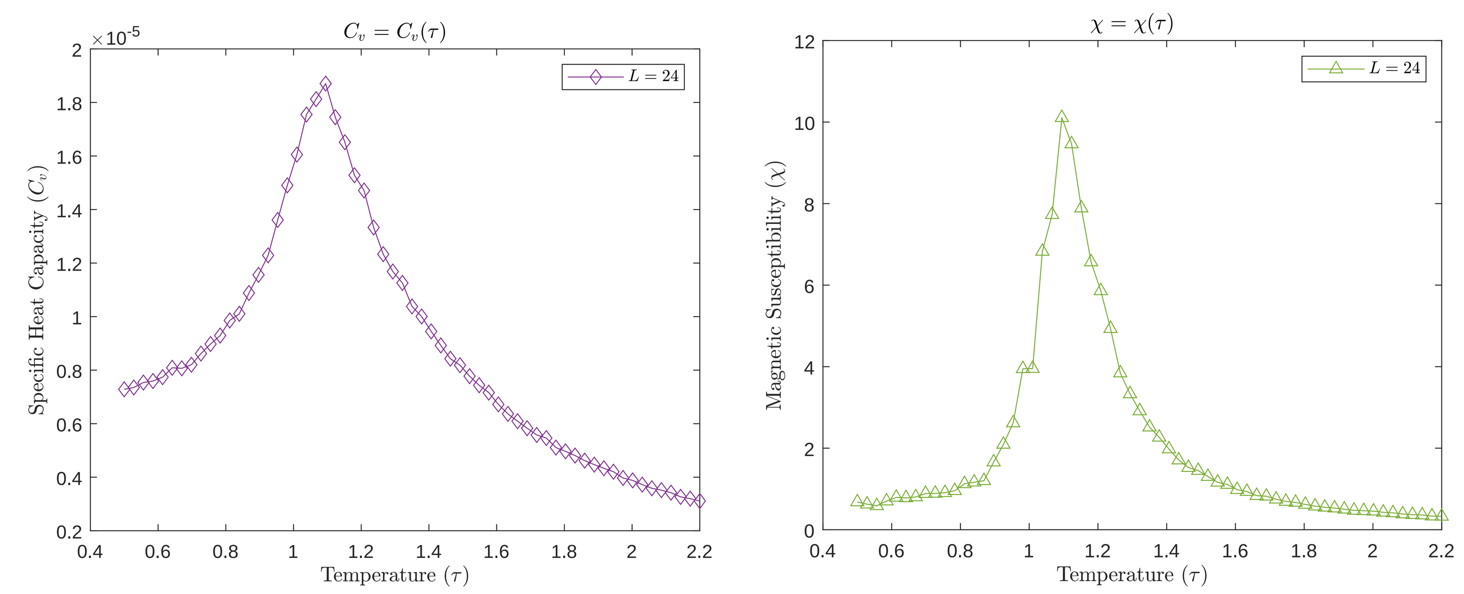

Fig. 3: **Left:** Average magnetic susceptibility per spin as a function of temperature.
Right: Average specific heat capacity per spin as a function of temperature.

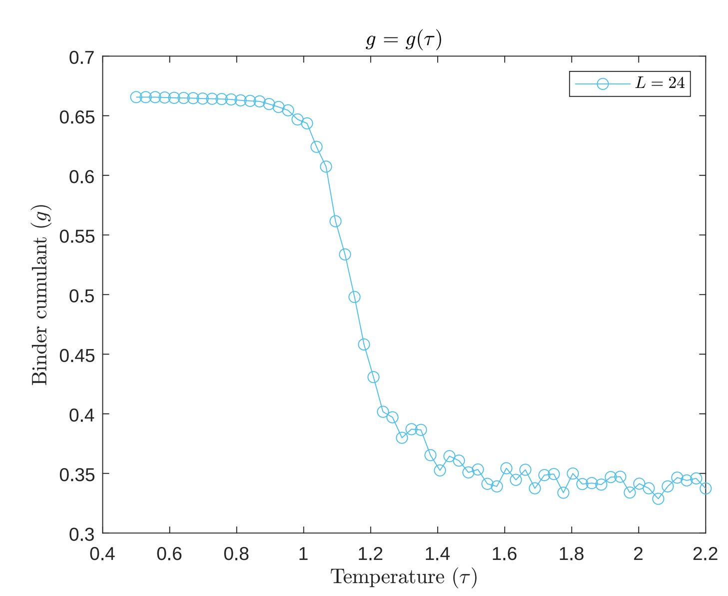

Fig. 4: Binder cumulant as a function of temperature

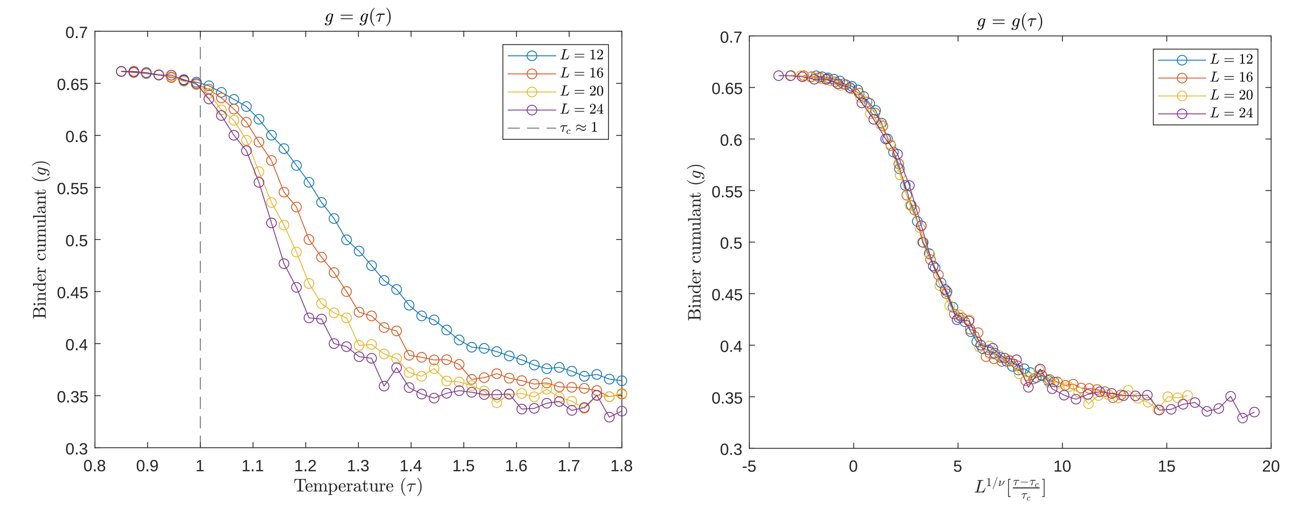

Fig. 5: **Left:** Binder cumulant as a function of temperature for lattice sizes L = 12 - 24. The crossing temperature show the critical temperature $\tau_c \approx 1$.
Right: Binder cumulant finite size scaled with Equation (4). Critical exponent value used is $\nu = 1$.

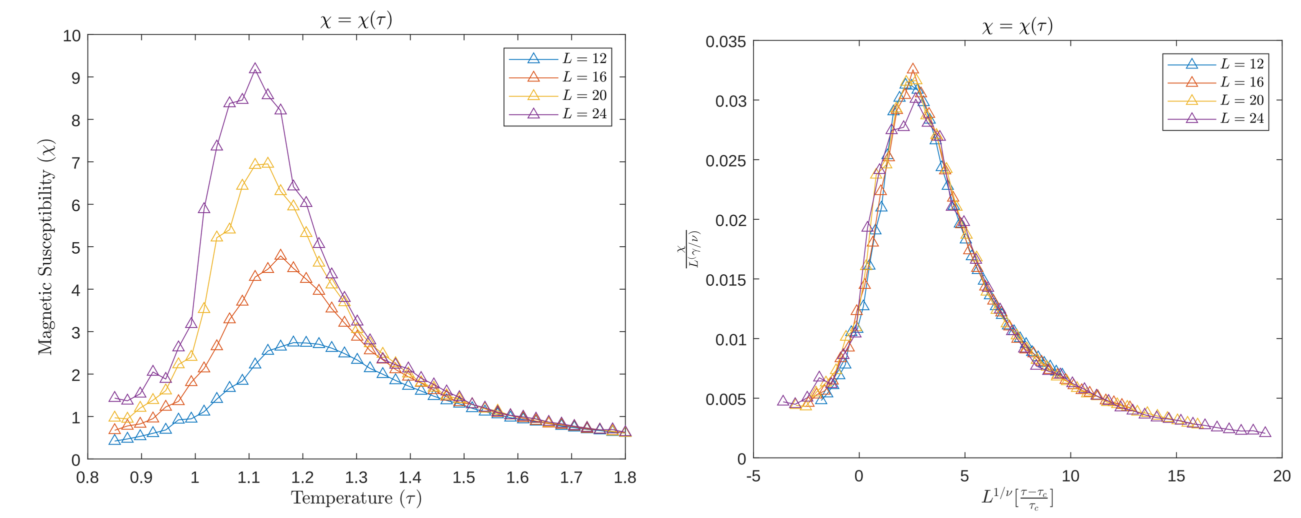

Fig. 6: **Left:** Magnetic susceptibility as a function of temperature for lattice sizes L = 12 - 24.
Right: Magnetic susceptibility finite size scaled with Equation (5). Critical exponent values used are $\nu = 1$ and $\gamma = 1.8$.

Conclusions

The plot in Figure (5) shows the Binder cumulant for different lattice sizes. 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 $\tau_c \approx 1$.

Measurements of the magnetic susceptibility and Binder cumulant can be seen in Figure (5) and Figure (6). By using the finite size scaling relations in Equations (4) and (5) together with the critical exponents $\nu = 1$ and $\gamma = 1.8$ shows that the quantities fall on to a universal curve for different lattice sizes. This is an indication that the values for critical temperature τ_c and the critical exponents ν and γ are close to the exact values.

The phase transition studied here can be classified as a second order transition. This is because of the smooth transition at the critical temperature seen in Figure (2) for the measurements of the average energy and magnetization per spin.

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 University Press, 2001.