The KT phase transition and the XY model

physics760 - Computational physics

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1 Introduction

The perhaps most well known model for the magnetization of lattice structures is the Ising spin model. It describes the total magnetization of a lattice as the superposition of all spins $\sigma_i = \pm 1$ on the lattice.

XY model One can now go and generalize the problem from a $\mathbb{Z}_2$ symmetry to a continous $U(2)$ symmetry. This model is called the XY model and describes the spins as two dimensional vectors on the unit circle

$$\sigma_i = \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix} \tag{1}$$

parametrized by the angle $\theta_i \in [0, 2\pi)$. The Hamiltonian for this system is thus given as

$$H = -J \sum_{\langle i,j \rangle} s_i \cdot s_j = -J \sum_{\langle i,j \rangle} \cos(\Delta\theta) \tag{2}$$

where $\Delta\theta = \theta_i - \theta_j$ is the angle between two spins and J the interaction strength. The $\langle i, j\rangle$ notation is used to indicate a nearest neighbour approximation. The partition sum for such a system is given by

$$Z = \sum \exp(-\beta H) \tag{3}$$

where $\beta = \frac{1}{k_B T}$. The constants β and J will from now on, be merged into β so that the temperature T is in units of $\frac{k_B}{\beta}$.

KT phase transition Unlike the Ising model, the XY model does not have a 2nd order phase transition.

2 Numerical Methods

2.1 Monte Carlo Metropolis-Hastings Algorithm

1. Calculate E and M for the initial lattice configuration.
2. Perform a lattice sweep by iterating over all lattice sites. For every site i do:
   a) Propose a new angle $\theta_i \in [0, 2\pi)$ from a uniform distribution.
   b) Calculate $\Delta H = \Delta E$ and ΔM for the proposed new state.
   c) Accept or reject state with propability $P = \min(1, \exp(-\beta\Delta H))$
3. Update the observables $E \mathrel{+}= \Delta E$ and $M \mathrel{+}= \Delta M$ and add them to the result set.
4. Repeat from 2. for a total of N sweeps.

2.2 Bootstrap Analysis

Since the Metropolis-Hastings algorithm scales with the number of lattices sites, it is computationally impractical to run the Metropolis-Hastings algorithm for very long times. To resolve this, one might use bootstrap sampling to obtain more measurements than were simulated.

2.3 Implementation

3 Results

The following results were obtained for a run on the JUSUF cluster with 2 nodes and 4 tasks per node. The simulation ran for $N = 1\,200\,000$ sweeps and the bootstrap parameter were $A = N$ and $B = 200\,000$.

3.1 Energy per Spin

As the total energy of the system as defined in eq. (1) scales with the number of lattice sites, it is often more insightful to observe the energy per spin

$$E = -\frac{\beta}{L^2} \sum_{\langle i,j \rangle} \cos(\Delta\theta) \tag{4}$$

which has been plotted in fig. 1.

For low temperatures we have a quasi-ordered state where the spins mostly align. Just like in the Ising model the energy per spin is -2.0 when extrapolating to $T = 0$. With increasing temperature the energy slowly vanishes until it asymptotically aproaches 0 for big T.

3.2 Magnetization per Spin

The absolute total magnetization per spin for the system is given by

$$|M|^2 = \frac{1}{L^2} \left(\left(\sum \cos\theta_i \right)^2 + \left(\sum \sin\theta_i \right) \right) \tag{5}$$

and has been plotted in fig. 2.

For low temperature the magnetzation tends to 1 which confirms the existance of a quasi-ordered low temperature state. With increasing temperature the

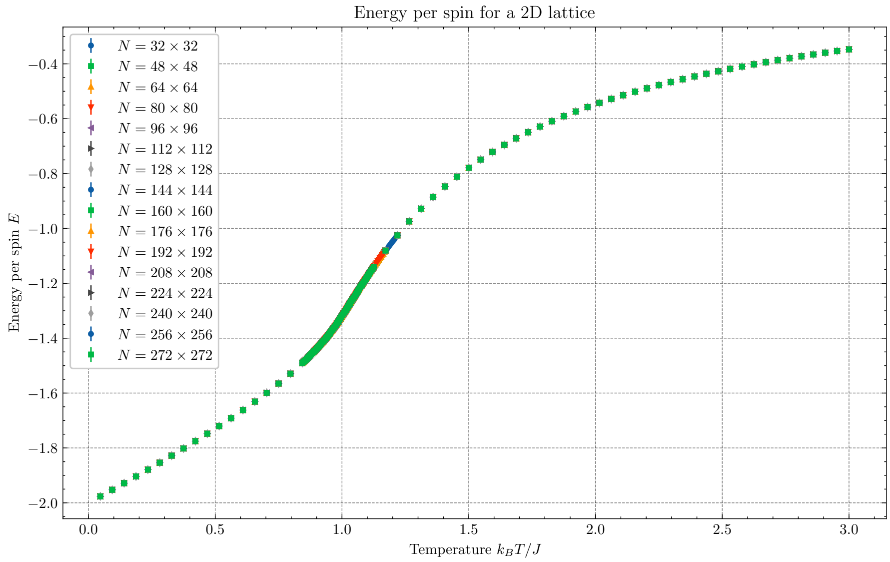


Figure 1: Plot of the temperature dependence of the energy per spin E (eq. (4)) for lattice sizes $L \in \{32, 48, \ldots, 272\}$. For small T the energy tends to -2 while for big temperatures the energy asymptotically aproaches 0.

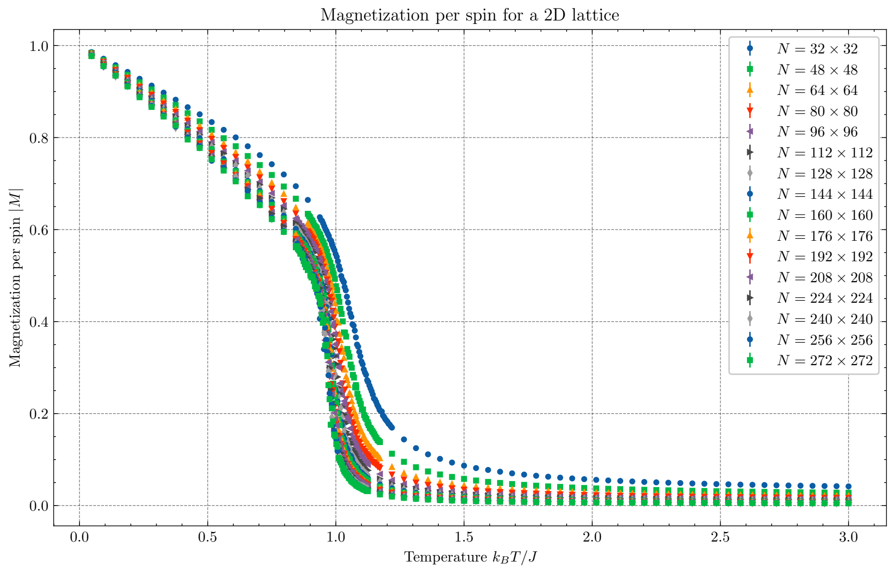
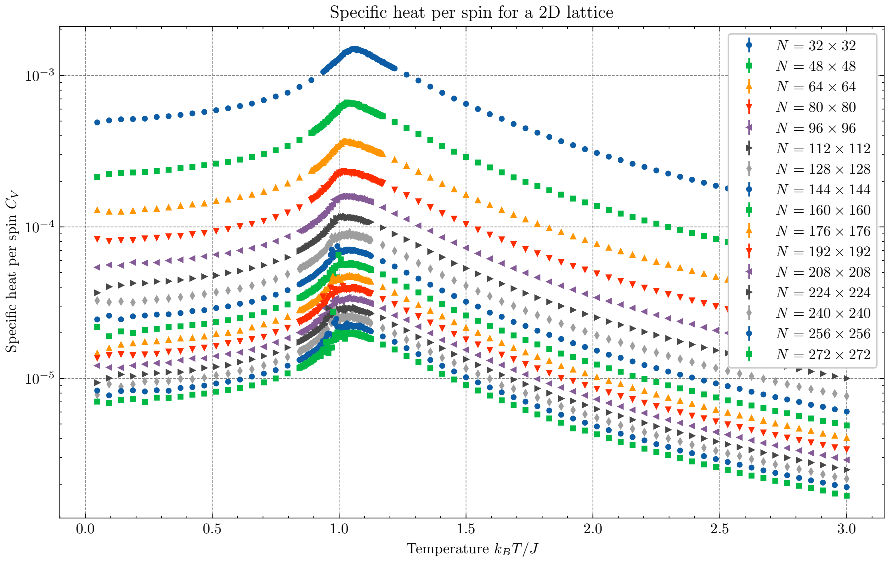
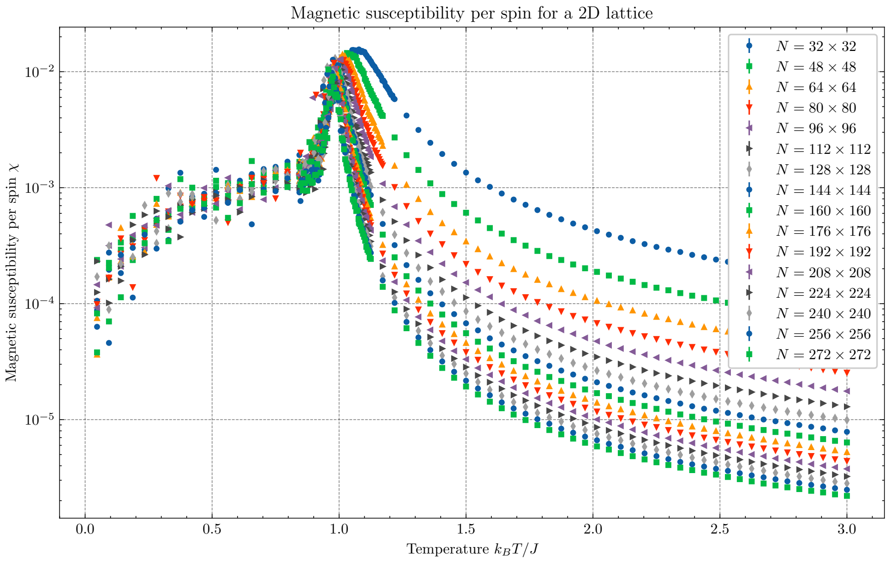


Figure 2: Plot of the temperature dependence of the magnetization per spin $|M|^2$ (eq. (5)) for lattice sizes $L \in \{32, 48, \ldots, 272\}$

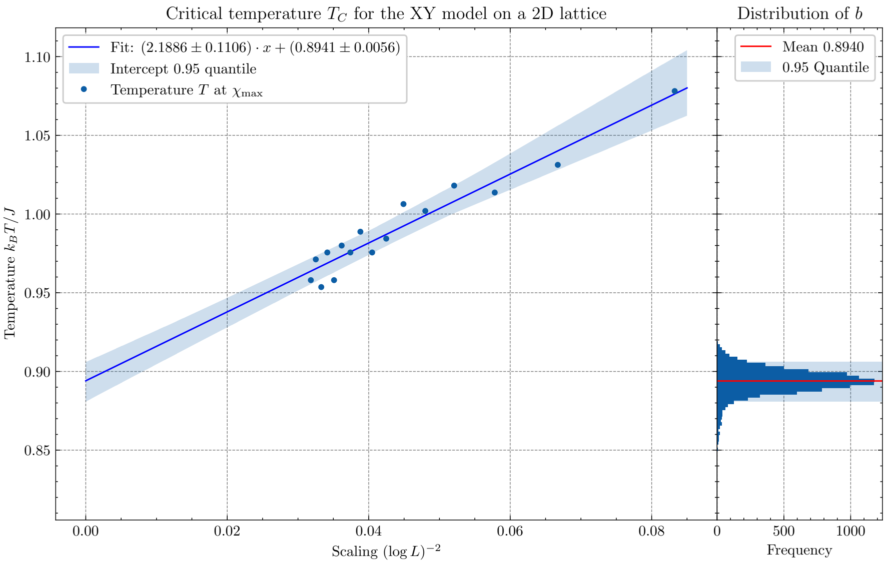
3.3 Specific Heat per Spin



3.4 Magnetic Susceptibility per Spin



3.5 Critical Temperature T_C



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