The KT phase transition and the XY model

physics760 - Computation 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 the spins $\sigma_i = \pm 1$ on the lattice.

One can now go and generalize the problem not only to a $\mathbb{Z}_2$ symmetry but 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

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

where $\Delta\theta = \theta_i - \theta_j$ is the angle between two spins. The partition sum for such a system is given by

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

where $\beta = \frac{1}{k_B T}$.

2 Numerical Methods

2.1 Monte Carlo Metropolis-Hastings Algorithm

1. Calculate E and M for the initial lattice configuration where $\theta_i = 0$ at every site.
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 $P = \min(1, \exp(-J\Delta H))$
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.

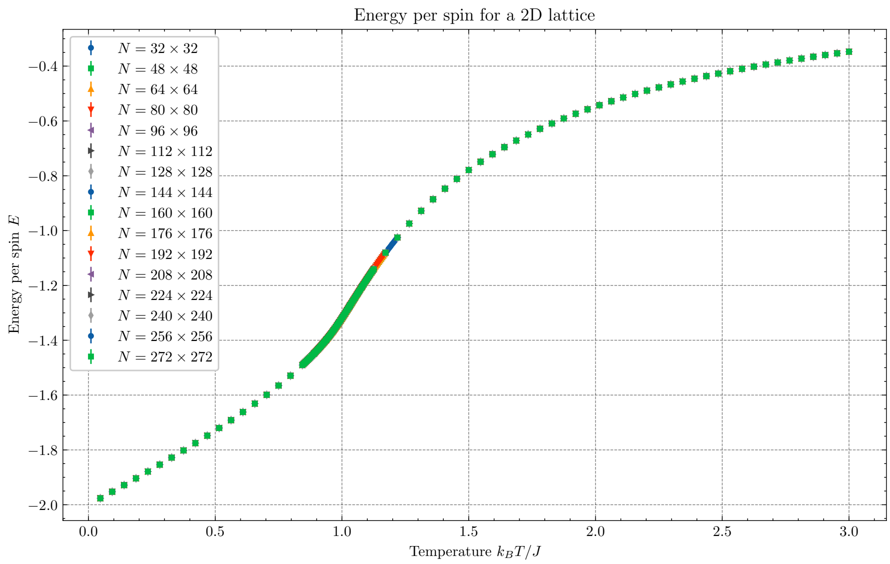
2.2 Bootstrap Analysis

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.

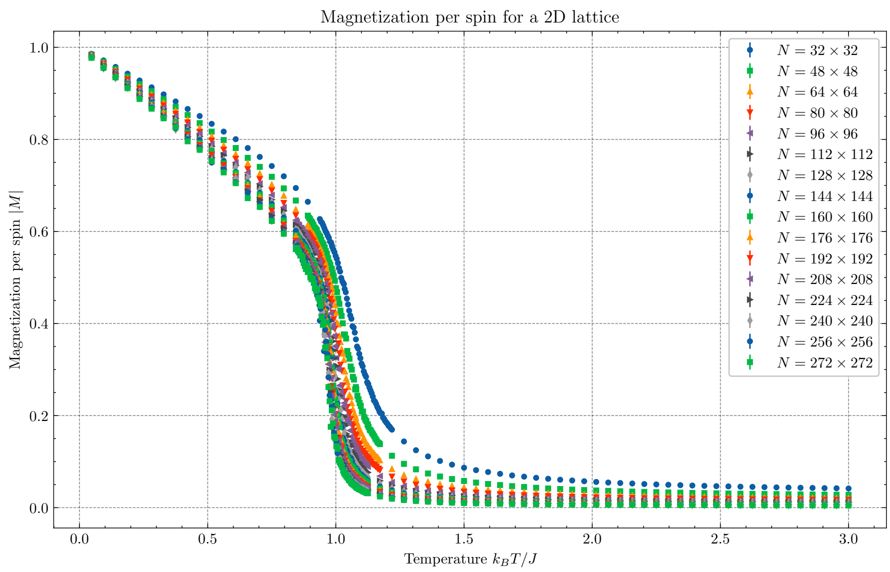
2.3 Implementation

3 Results

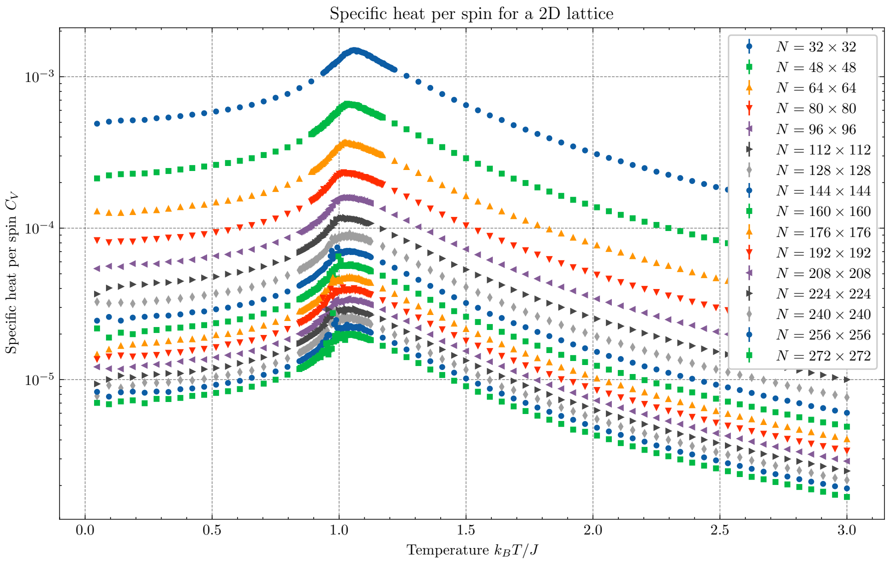
3.1 Energy per Spin



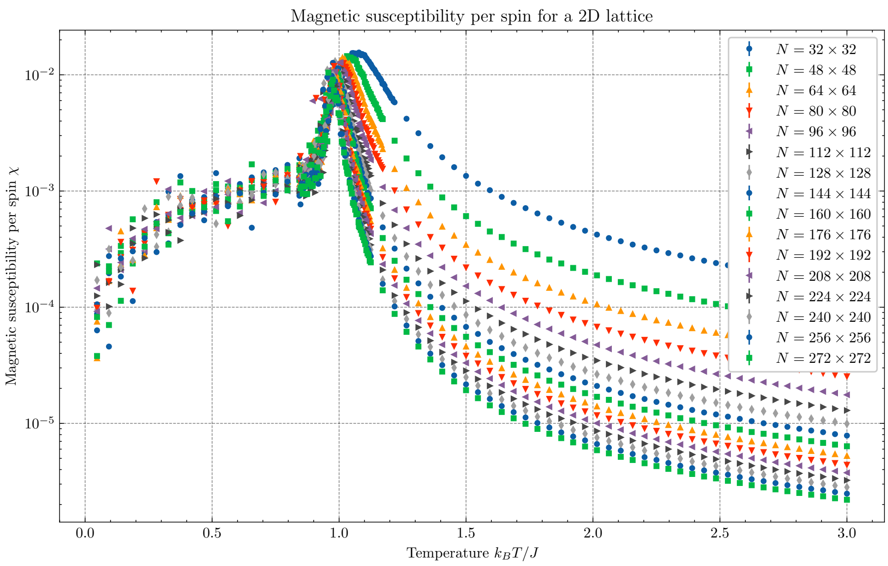
3.2 Magnetization per Spin



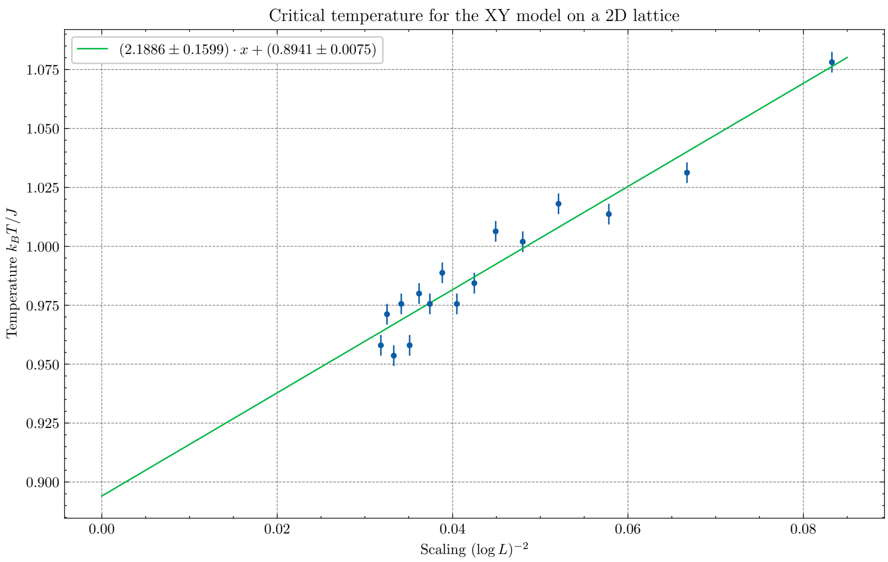
3.3 Specific Heat per Spin



3.4 Magnetic Susceptibility per Spin



3.5 Critical Temperature T_C



3.6 Vortices

4 Conclusion