Monte Carlo Study of the Ising Model

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Abstract

This project used the Metropolis Monte Carlo Method to study the Ising Model through various simulations. First, the basic Ising model was simulated. Next, several variations were examined, including variation in coupling strength, the variations with homogeneous external fields projected onto the lattice, 1D Ising chain, and examination of the critical temperature of the Ising Model phase transition. The study has let us gain a better understanding of ferromagnetic behaviour in lattices.

Background

$$H = -\sum_{\langle i,j \rangle} J_{ij} S_i S_j - \sum_i B_i S_i$$

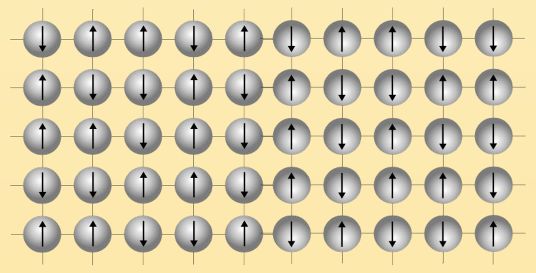

Figure 1: Ising Model Hamiltonian (left) and magnetic spins inhabiting a 2D lattice (right), from Eastman, Peter. *6.3 Phase Transitions: The Ising Model*.

The generalized **Ising Model** Hamiltonian is written above in Fig. 1. S_i, S_j signify the magnetic spins at lattice site i,j (-1 or +1 as their values); J_ij the coupling interaction between lattice site i,j; B_i the external magnetic field at lattice site i; and <i,j> mean to take the sum over the nearest neighbors j of lattice site i. The lattice is taken to have periodic boundary conditions, meaning for a 2D planar lattice, the shape will actually be of a torus. There are many variants of the Ising Model that yield interesting phase transition behavior when simulated, some of which are investigated in our work. The simulations were ran with implementations of the **Metropolis Monte Carlo Method**.

Basic Ising Model (J=1,B=0)

$$H = -\sum_{\langle i,j \rangle} S_i S_j$$

The basic Ising Model results shown below are based on a simulation of a 30x30 lattice with 1000 stabilizing MC steps and 200 measurement MC steps. There is a clear phase transition behavior with the drop off in <E> and |<M>| values at around a critical point Tc.

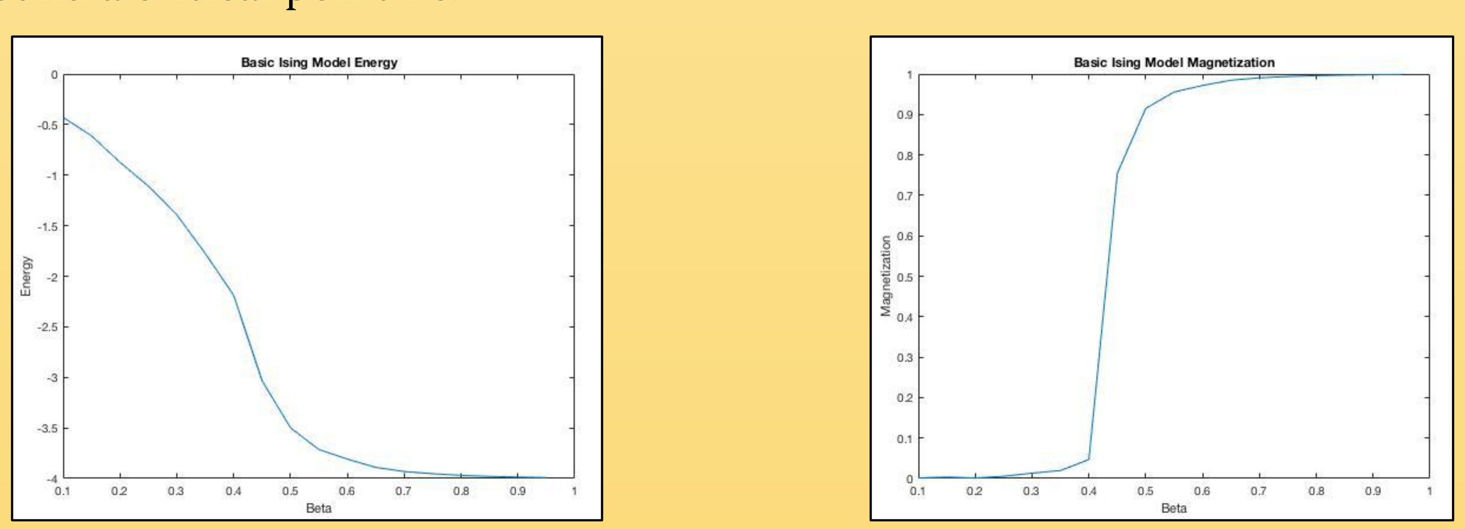

Figure 2: Average Energy <E> (left) and Average Magnetization |<M>| (right)

Variation in Coupling Strength J

$$H = -J\sum_{\langle i,j \rangle} S_i S_j$$

Stemming from the basic Ising Model, different bonding strengths within the lattice can be simulated by varying the coupling strength J in the Hamiltonian above. By increasing the value of J, it can be observed that the phase transition behavior is increasingly broken, and results in new behavior.

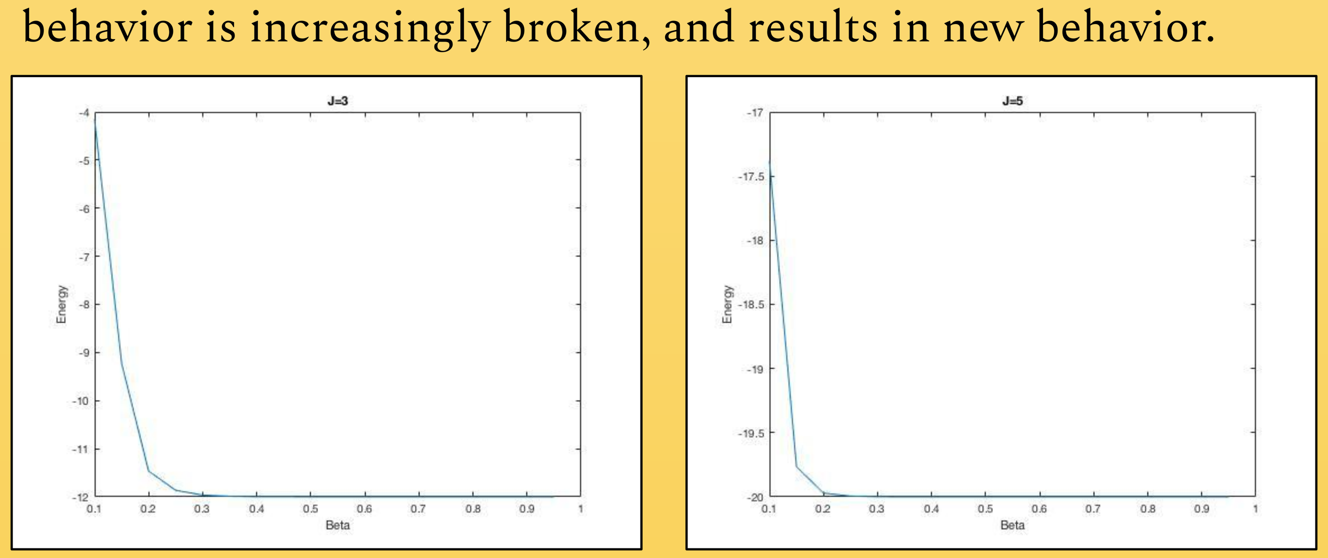

Figure 3: <E> for J=3 (left) and J=6 (right)

Homogeneous Ext. Field

$$H = -\sum_{\langle i,j \rangle} S_i S_j - B\sum_i S_i$$

Under a sufficiently large magnetic field, the total susceptibility χ of a given lattice appears to be independent of its size, which signifies that the interaction contribution is negligible.

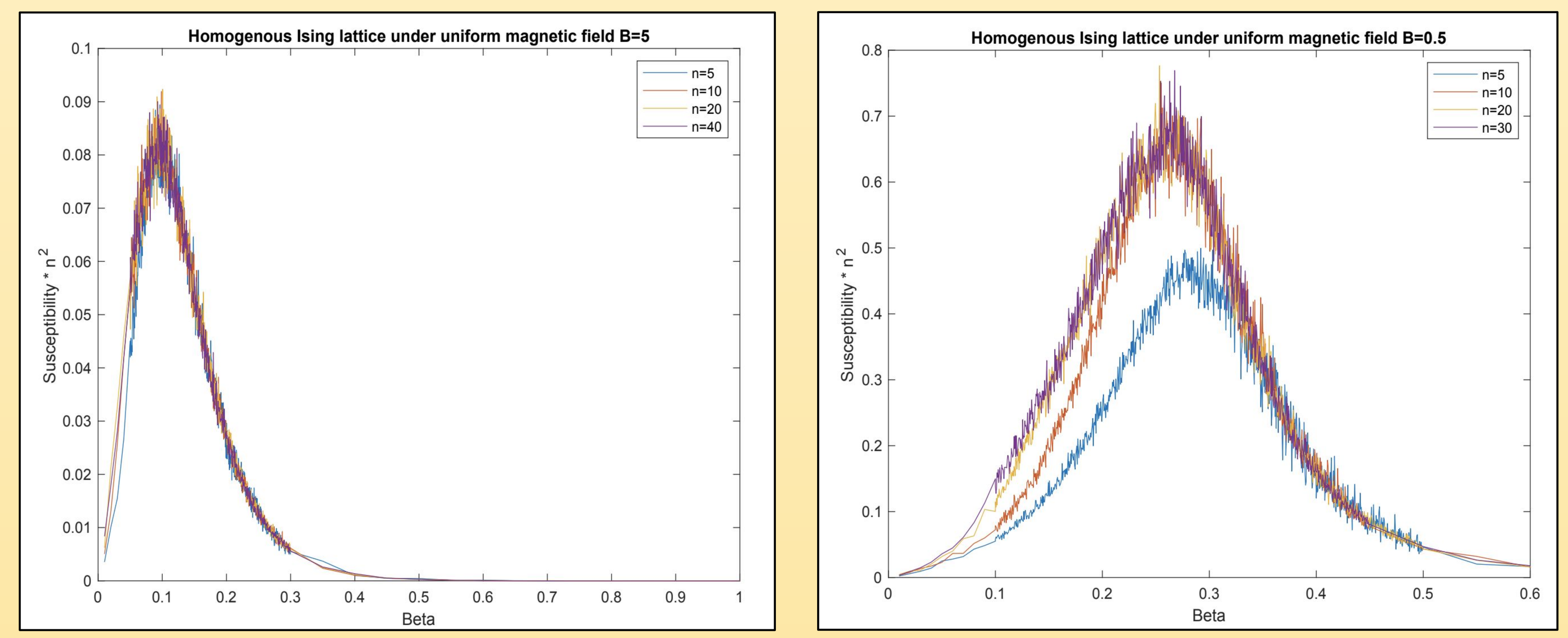

Figure 4: χ for B=5 (left) and B=0.5 (right)

Homogeneous Ext. Field on a ring of a 2D lattice

$$H = -\sum_{\langle i,j \rangle} S_i S_j - B\sum_{i_{\text{ring}}} S_i$$

After applying a large magnetic field on a specific ring of the torus, we notice that beside the trivial effect on the spins in that ring, there is a decaying tendency for parallel rings to align with the direction of magnetic field.

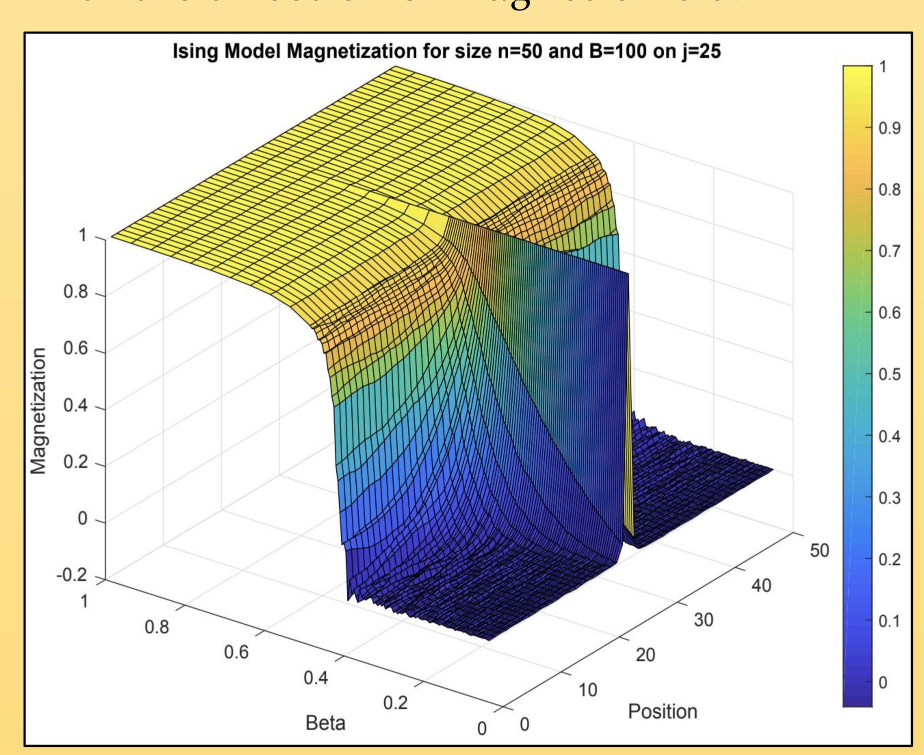

Figure 5: |<M>| for each ring with B=100 projected at the middle ring of the lattice

Phase transition in 1D Ising ring

$$H = -\sum J(d) S_i S_j$$

Per Dyson's paper, for an Ising ring with an interaction term of the form below, where d is the distance between ring indices i and j, a non-trivial phase transition is predicted as long as n is between 1 and 2. The plots below demonstrate the phase transition behavior.

$$J(d) = d^{-n}$$

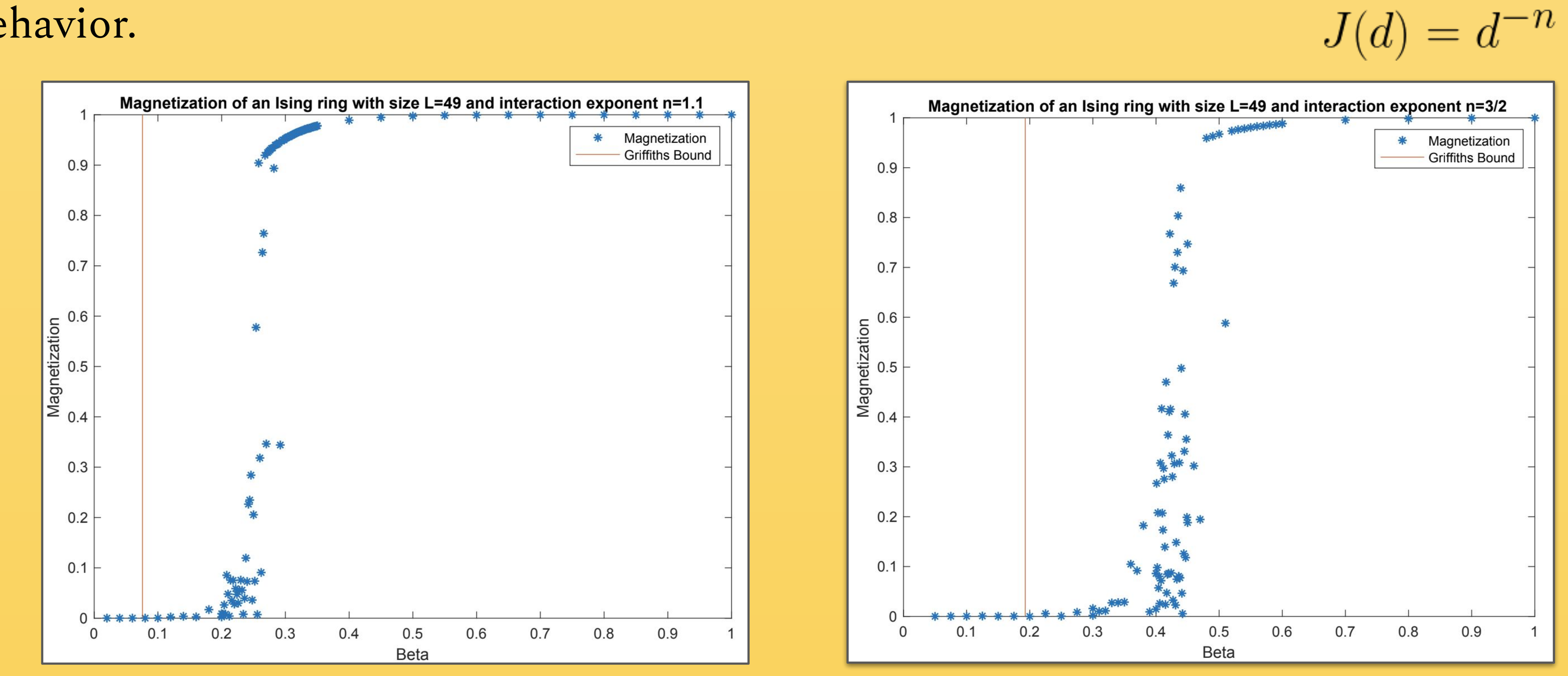

Figure 6: |<M>| for ring with n=1.1 (left) and n=1.5 (right)

Critical Temperature of Phase Transition

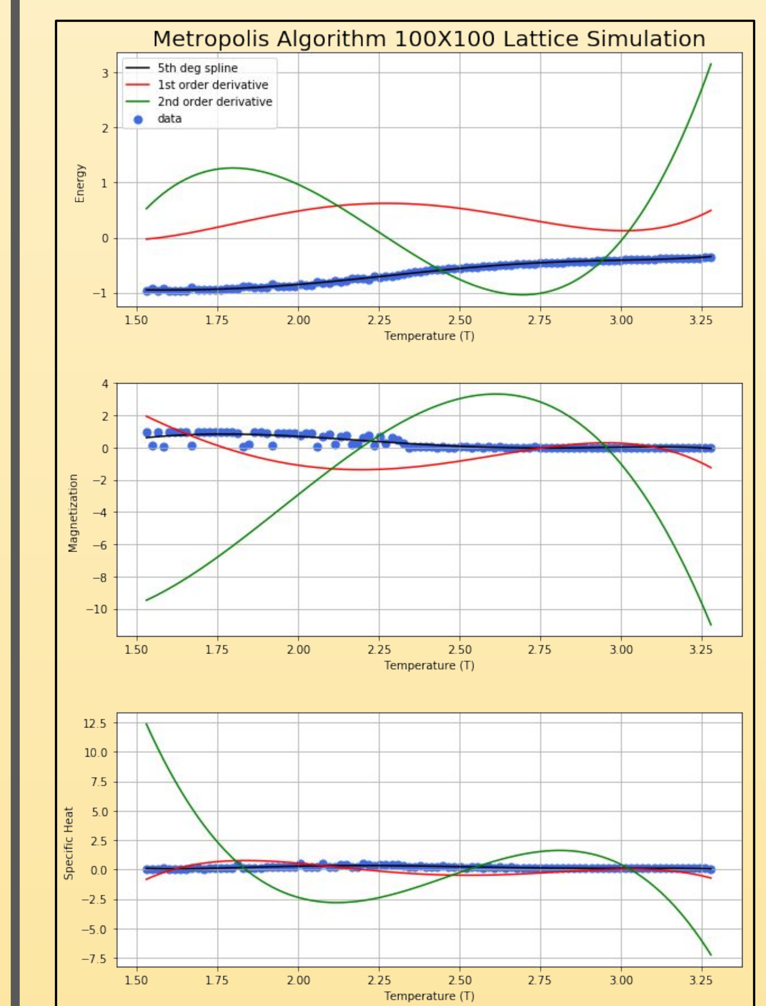

Figure 6: <E> (top), |<M>| (middle), C (bottom)

The critical temperature occurs when the lattice goes from a ferromagnetic (ordered) to a paramagnetic (disordered) state. The exact solution was given by Lars Onsager in 1944;

$$T_c = \frac{2J}{k\ln(1+\sqrt{2})}$$

Our simulation uses J=1, k=1. The formula then yields T=2.269.

Experimentally, this is found as the zero of the second derivative on the E/T and M/T graphs, and the local maximum on the C/T graph. The average value is found to be T=2.277.

The simulation is extremely accurate, yielding a percent error of just 0.353%, variant upon random error during each simulation run.

Future Work

An extension to this project will deal with further different variations of the Ising Model. Some of the variations could be: examining lattice impurities in the lattice such as having vacant spots on the lattice or in general having spins that interact with different coupling constants; studying antiferromagnetism by having alternative coupling constants; working on hexagonal shaped lattices such as graphene and investigating its magnetic properties; or expanding on Freeman's paper to 2D lattices and studying the phase transitions by varying the interaction exponent.

References

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