# The Ising Model

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**Abstract.** TODO

## Preface

Although the coursework was initially presented as a C++ project, I took the liberty of rewriting the Ising Model system in a programming language called Google Go (https://golang.org). The motivation for this is Go has been designed to accommodate systems with high concurrency. This means that instead of simulating 1 system at a time, 10,000 different systems can be simulated simultaneously in different threads. This greatly increases time efficiency and has allowed me to achieve a significant level of statistical significance in my ensemble averages. Furthermore, this has also allowed me to use ergodicity to calculate time averages for the same system with many different values of beta at the same time. The source code for my implementation is accessible on Github: `http://tiny.cc/brb75y`.

## 1. Introduction and Computational Method

Ferromagnetism is the property of a material to exhibit speontaneous magnetisation in the absence of an external magnetic field. The Ising Model is a mathematical model that uses the results of thermodynamics and statistical mechanics to describe how magnetic structure in some metals leads to ferromagnetism.

In the Ising Model presented in this paper, a magnetic material is modelled by a regular $L$ x $L$ dimensional square lattice $\Pi$. A given grid point on this lattice $\pi_{(i,j)} \in \Pi$ is indexed by cartesian coordinates $(i, j)$ where $i, j \in [0, L]$. These coordinates are not strictly unique as periodic boundary conditions are applied so that a closed system is modelled. This is to say the grid follows the mappings $(i+\Lambda_i D, j+\Lambda_j D) \to (i, j)$ for $\Lambda_i, \Lambda_j \in \mathbb{Z}$. Each grid point $\pi_{(i,j)} \in \Pi$ on this square lattice is assigned a discrete variable $s_{(i,j)} \in \{0, 1\}$ that corresponds to the spin of the grid point. The system is therefore composed of $N \equiv L^2$ spins. We arbitrarily define $s_{(i,j)} = 1$ to represent 'spin up' and $s_{(i,j)} = -1$ to represent 'spin down'.

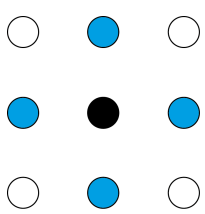


Figure 1: Each dot represents a grid point on the square lattice $\Pi$. The central black grid point represents the grid point $\pi_{(i,j)}$. The blue grid points represent the nearest neighbours of $\pi_{(i,j)}$. The white grid points represent points that are not considered nearest neighbours.

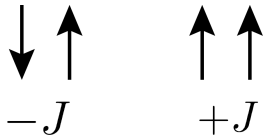



Figure 2: Two nearest neighbour spins on the grid have an interaction energy of $-J$ if they are aligned and $+J$ if they are not aligned.

For a given grid point $\pi_{(i,j)}$, the convention of nearest neighbours is defined as representing the grid points directly adjacent to the grid point, both vertically and horizontally, as shown in Figure 1. Using this convention, the energy of a given spin on the grid is defined by

$$E_{(i,j)} = -h_{(i,j)} s_{(i,j)} \tag{1}$$

where

$$h_{(i,j)} = \sum_{(\alpha,\beta) \text{ n.n. of } (i,j)} \left[ J s_{(\alpha,\beta)} \right] \tag{2}$$

Here "n.n" represents a sum over the nearest neighbours and $J$ is a positive real number with dimensions of energy that indicates the strength of the interactions between spins. Qualitatively this set of equations defines the energy of a given spin as the sum of the interaction energies between the spin and it's nearest neighbours, where the interaction energy between two nearest neighbour spins is defined to be $-J$ if the two spins are aligned and $+J$ if the two spins are antiparallel, as shown in Figure 2.

From this definition of the energy for a single spin in the system, the total energy for the system is defined as

$$E = \frac{1}{2} \sum_{i,j} E_{(i,j)} \tag{3}$$

where the summation simply runs over every grid point in the square lattice. Furthermore, the magnetisation (per spin) of the system is defined as

$$\mathcal{M} = \frac{1}{N} \sum_{i,j} s_{(i,j)} \tag{4}$$

As the number of spins in the system is fixed, a canonical thermodynamic ensemble is used. If we let a microstate $\mathcal{S}$ be defined by the instantaneous configuration of all the spins in the system, then the probability of finding the system in a microstate $S$ in thermal equilibrium at temperature $T$ is given by statistical mechanics as

$$p_{eq}(\mathcal{S}) = \frac{1}{Z(T)} e^{-E(S)/k_B T} \tag{5}$$

where $E(S)$ is the energy of microstate $S$ as given by equation (3). The canonical partition function $Z = Z(T)$ is used to enforce the normalisation condition $\sum_S p_{eq}(S) = 1$ which gives the expression for $Z$ as

$$Z(T) = \sum_S e^{-E(S)/k_B T} \tag{6}$$

where the summations here run over all $2^N$ possible microstates $S$ of the system.

In this paper, a Metropolis Monte Carlo method is used to investigate the properties $E$ and $\mathcal{M}$ of two dimensional Ising Model systems for different thermodynamic temperatures $T$.

## 2. Method

### *2.1. Calculating Equilibrium Averages*

Instead of calculating averages using an ensemble average as is conventional for statistical mechanical systems, it is in most cases also possible to calculate an average $\langle\Gamma\rangle$ for a quantity of interest $\Gamma$ by taking a time average of that value. For the case of a simulated Ising system, this means that average values can be determined by running a single simulation for a period of time as opposed to running many distinct simulation of that one system. In this way, the average value $\langle\Gamma\rangle$ is determined by taking $n$ samples of $\Gamma$ over a period of time $\{\Gamma_i\}_{i=1}^{n}$. The average value is then calculated by

$$\langle\Gamma\rangle = \frac{1}{n}\sum_{i=1}^{n}\Gamma_i \tag{7}$$

## 3. Results

### *3.1. Convergence to Equilibrium*

An Ising model simulation was prepared with all spins initially down. For different values of system temperature, as defined by the parameter $\beta$, the system was computationally simulated using the Metropolis Monte Carlo algorithm. The system's magnetisation per spin $\mathcal{M}$ and dimensionless energy $E/J$ were recorded as the number of Monte Carlo sweeps of the system was increased from 0 to 50. For each value of $\beta$, this simulation was run for an ensemble of $10,000$ independent sub-systems, each with different pseudo-random number generator seeds. The evolution of system magnetisation as the number of Monte Carlo sweeps completed increases is shown in Figure 3. Similarly, Figure 4 shows the evolution of the system's dimensionless energy $E/J$ as the number of Monte Carlo sweeps increases.

### *3.2. Measuring Equilibrium Averages*

Figure 5 shows averages of quantities of interest as a function of the parameter $\beta$ for an Ising system in thermal equilibrium. Figure 5 (a) shows the average magnetisation per spin as a function of $\beta$. Figure 5 (b) shows the average dimensionless energy per spin as a function of $\beta$. Figure 5 (c) shows the average of the absolute value of the magnetisation per spin as a function of $\beta$. For each of these graphs, the average value of interest is sampled over $\beta \in [0.25, 1]$ in discrete steps of $\Delta\beta = 0.001$.

## 4. Discussion

### *4.1. Determining the Fractal Dimension of DLA Aggregates where $p_{stick} = 1$*

### *4.2. Suggestions for Improvement*

## 5. Conclusion

## References

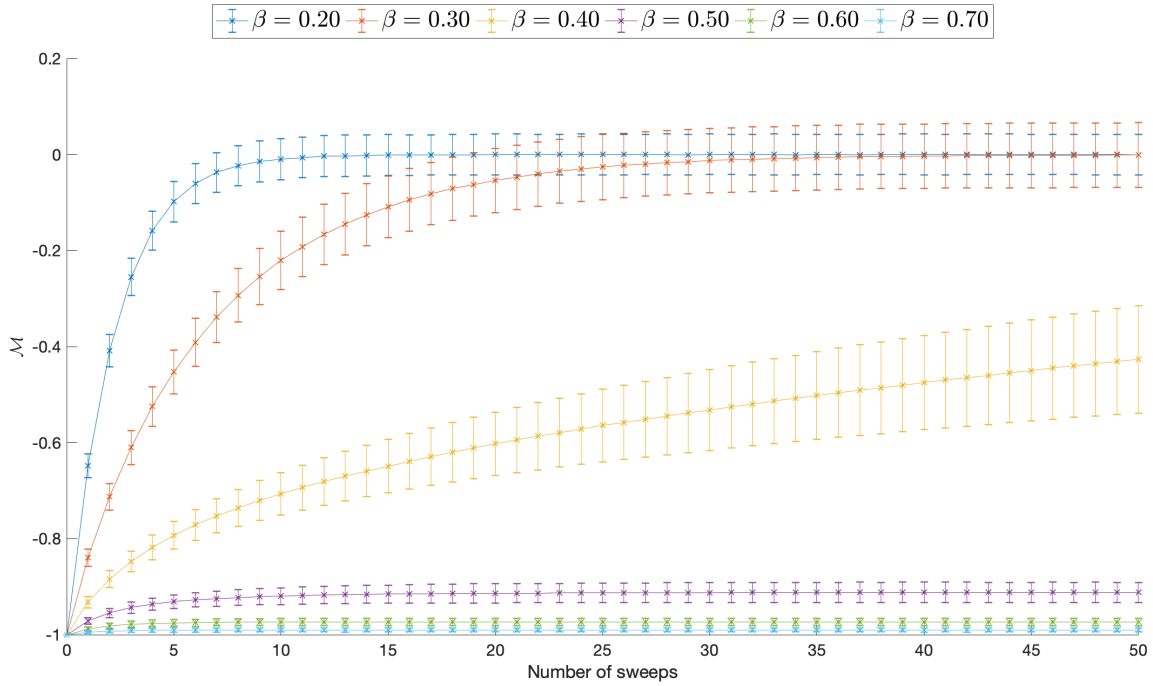



Figure 3: Evolution of system magnetisation per spin as a function of the number of Monte Carlo sweeps completed for a 2D Ising model simulation with all spins initially down. The simulation was ran for a set of systems with different thermodynamic temperatures, as defined by the parameter $\beta$. Each data point represents the ensemble average over $n = 10,000$ independent sub-systems, each initialised with different pesudo-random number generator seeds. Error bars represent the standard deviation in the values of $\mathcal{M}$ across the ensemble of systems.

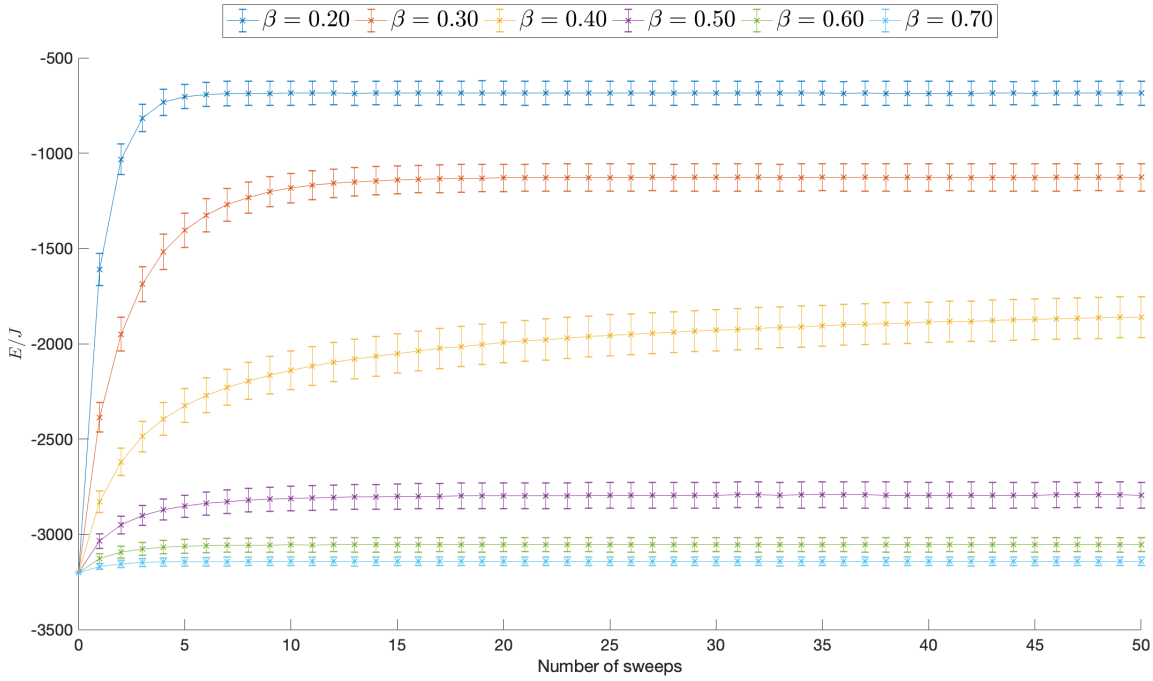
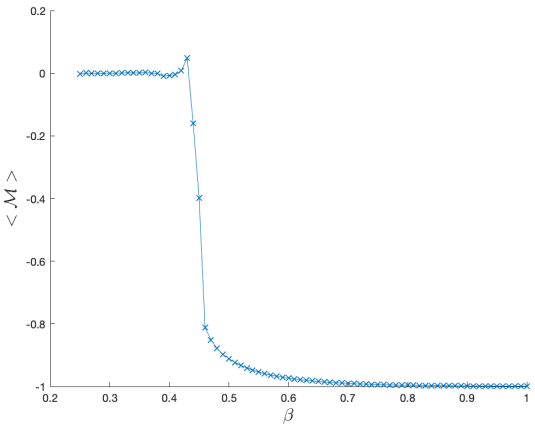
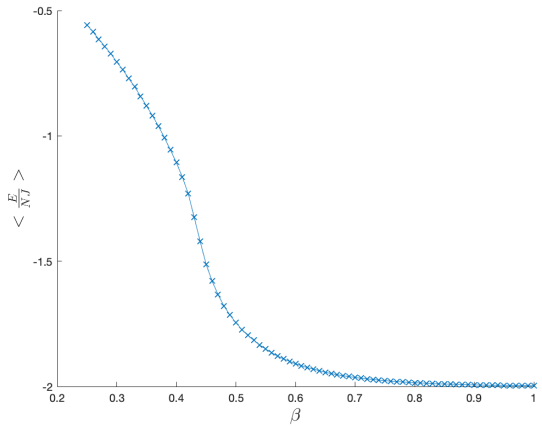



Figure 4: Evolution of dimensionless system energy as a function of the number of Monte Carlo sweeps completed for a 2D Ising model simulation with all spins initially down. The simulation was ran for a set of systems with different thermodynamic temperatures, as defined by the parameter $\beta$. Each data point represents the ensemble average over $n = 10,000$ independent sub-systems, each initialised with different pesudo-random number generator seeds. Error bars represent the standard deviation in the values for $E/J$ across the ensemble of systems.




(a) Average magnetisation per spin




(b) Average dimensionless energy per spin

Figure 5: Averages of quantities of interest as a function of $\beta$ for an Ising system in thermal equilibrium. (a) shows average magnetisation per spin $\langle \mathcal{M} \rangle$ vs $\beta$. (b) shows average dimensionless energy per spin $\langle \frac{E}{NJ} \rangle$ vs $\beta$. (c) shows average absolute magnetisation per spin $\langle |\mathcal{M}| \rangle$ vs $\beta$.