Monte Carlo Methods in an Ising Ferromagnet

Introduction

We utilized two Monte Carlo statistical methods (Metropolis-Hastings and Swendsen-Wang) to analyze the Ising model of ferromagnetism, a mathematical model involving a 2-D lattice of discrete magnetic dipole moments of either spin +1 or -1. Specifically, we investigated the time-evolution of the Hamiltonian (total energy) of the (anti)ferromagnet in accordance with a certain set of rules while varying environmental conditions (i.e temperature, external magnetic field). Under low-energy conditions, we found that sufficient spin-flip iterations would result in convergent behavior; systems having temperatures above a certain threshold would retain their initial randomness.

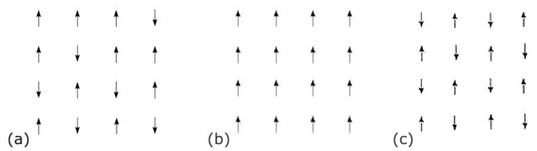

Figure 1. Two-dimensional lattice illustration of an Ising ferromagnet. The up and down arrows represent positive and a negative spins respectively.

- Fig. 1(a): Random orientations of magnetic dipoles in an ordinary material.
- Fig. 1(b): Fully upwards magnetic dipoles found in a ferromagnetic material.
- Fig. 1(c): Alternating magnetic dipole directions found in an antiferromagnetic material.

Background

In most ordinary materials, the constituent atoms' magnetic dipoles have random orientations. As a result, there is no overall macroscopic magnetic moment in the non-specific distribution. However, a magnetic moment can be produced as a result of alignment of the atomic spins in (anti)ferromagnetic materials, such as iron.

This phenomenon is based on two fundamental principles: energy minimization and entropy maximization. Temperature is the mediator between these opposing elements and ultimately determines which will be more dominant.

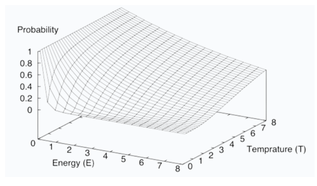

Figure 2. Boltzmann Probability Distribution vs Energy vs Temperature.

In the Ising model, the energy of the system depends on the arrangements of the spins and the interactions between neighboring spins. The Boltzmann distribution comes into play when considering the probability of the system being in a specific spin configuration with a specific energy at a specific temperature. We find based off of this distribution that decreasing a system's temperature will theoretically increase the likelihood of finding it at a lower energy state[1].

Methodology

The Hamiltonian of the Ising ferromagnet is given by the equation

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - h \sum_i \sigma_i$$

where $\sigma_i \in \{+1, -1\}$ corresponds to the spin of the ith dipole moment, J is the ferromagnetic coupling strength, and h is the magnetic field coupling constant.

Metropolis-Hastings

If the dipole moment at lattice coordinate (r, c) flips its spin, we find that final energy of the given moment and its local spins becomes

$$E_f = J[\sigma(r,c)\sigma(r,c+1)+\sigma(r,c)\sigma(r,c-1)+\sigma(r,c)\sigma(r+1,c)+\sigma(r,c)\sigma(r-1,c)]+h\sigma(r,c).$$

The initial energy of the dipole and its local spins is

$$E_i = -J[\sigma(r,c)\sigma(r,c+1)+\sigma(r,c)\sigma(r,c-1)+\sigma(r,c)\sigma(r+1,c)+\sigma(r,c)\sigma(r-1,c)]-h\sigma(r,c)$$

and thus

$$\delta E = 2J[\sigma(r,c)\sigma(r,c+1)+\sigma(r,c)\sigma(r,c-1)+\sigma(r,c)\sigma(r+1,c)+\sigma(r,c)\sigma(r-1,c)].$$

Accounting for over-counting, we find that the total energy of the system will change by the quantity ϵ given by the following equation:

$$\epsilon = 4J\sigma(r,c)[\sigma(r+1,c)+\sigma(r-1,c)+\sigma(r,c+1)+\sigma(r,c-1)]+2h\sigma(r,c).$$

Using this quantity, the Metropolis-Hastings algorithm updates individual dipole moments using the following rules:

1. If flipping the spin of the chosen dipole moment will lower the total energy of the system, then it will flip.
2. If flipping the spin of the chosen dipole moment will not lower the total energy of the system, then it will flip with probability $p = e^{\frac{-\epsilon}{T}}$, where T describes the temperature of the system[1].

Swendsen-Wang

Alternatively, we may implement the following algorithm:

1. For a ferromagnet (i.e. $J > 0$), a "bond" may form between any two parallel spins with probability $p = 1 - e^{-\frac{2J}{T}}$.
2. Dipole moments connected by bonds form "clusters," each of which flip with probability $\frac{1}{2}$. After all clusters have (or have not) flipped, the algorithm is reset.
3. In the presence of an external magnetic field, a "ghost spin" may be considered, whose spin is initially given by $\sigma_{ghost} = \operatorname{sign} h$. For $h > 0$, the "ghost spin" will form bonds with all magnetic dipoles with parallel spin in the lattice with probability $p = 1 - e^{-\frac{h}{T}}$ and can flip similarly to a dipole in the lattice[2–4].

We implemented both algorithms using Python and ran an appropriate number of iterations (see Results) to simulate the asymptotic behavior of the ferromagnet.

Both algorithms described above may be easily generalized to the antiferromagnetic case by flipping the sign of J (or h) and considering the interactions between dipoles of opposite instead of similar spin[2], including the "ghost spin."

Results

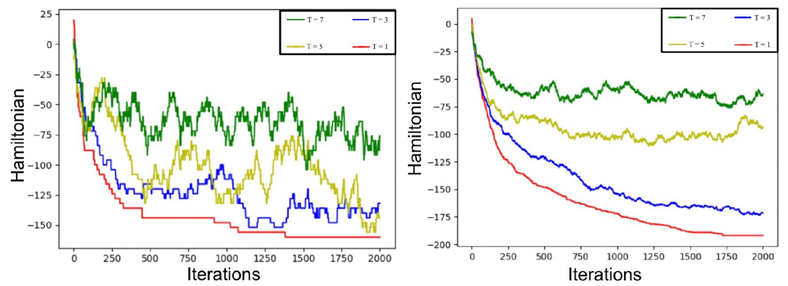

Figure 3. Both graphs simulate the time evolution of Hamiltonians modeled in an Ising Ferromagnet at varying temperatures. The graph on the left represents a single Hamiltonian, whereas the right represents an average of 10.

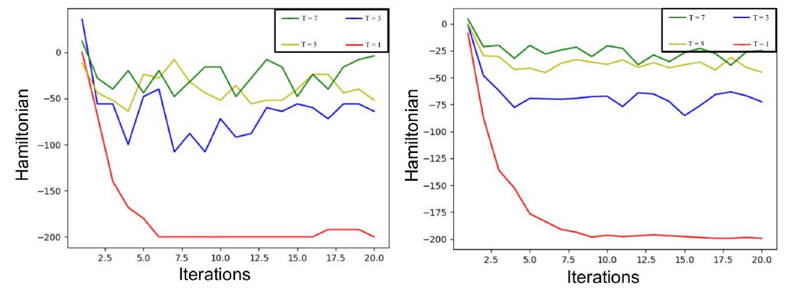

Figure 4. The above graphs simulate the time evolution our cluster model's Hamiltonian at varying temperatures. The graph on the left represents a single Hamiltonian, whereas the right represents an average of 10.

Conclusion

Based on our findings, we conclude that temperature significantly affects the time evolution of the Hamiltonian. Our data provides the conclusion that Hamiltonian variation is strongly correlated with temperature. This demonstrates the necessity for near absolute zero cooling to prevent unwanted fluctuations in spin.

The convergence rate for Metropolis-Hastings is on the order of requiring hundreds of iterations. Conversely, the convergence rate for the Swendsen-Wang algorithm is on the order of tens of iterations.

Further modelling can be done using the Quantum Heisenberg Model, which allows the simulation of rotations to have non-binary spins. This model allows more flexibility with spins and uses Quantum Mechanics rather than a semi-classical approach like the Ising Model.

Our findings and models provide an alternative to collecting data for large sample sizes or for expensive materials, allowing reasonable predictions for the behavior of (anti)ferromagnetic materials and their time evolution with or without an external magnetic field.

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[4] Suzuki, M. (2005). Topological and ghost interaction methods in equilibrium and non-equilibrium systems. *Progress of Theoretical Physics*, 113(6), 1391–1396. https://doi.org/10.1143/ptp.113.1391