Modeling Magnetic Phase Transitions

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1 Introduction

Any magnetic substance has charged atoms in its lattice, and the positive poles of these charged atoms must all point in the same direction. This alignment property is called ferromagnetism, and most magnetic substances we encounter on a daily basis are ferromagnetic. Above a certain temperature, called the Curie point, there is enough energy in the lattice to knock atoms out of alignment, so the substance loses its magnetism. We model this process using stochastic mechanics and attempt to recreate the phase transitions associated with the Curie temperature by observing simulated energy vs. temperature.

2 Model

2.1 Gibbs Distribution of Statistical Mechanics

In statistical mechanics, randomly arranged micro-components are used to determine the macro properties of mechanical systems. The balance between energy and entropy of a material is stochastically influenced by its thermodynamic temperature. Let Σ be a random variable over all possible states of a system and $\sigma^{\hat{\imath}}$ be some particular state of system. The Gibbs distribution [1] has

$$P\left(\Sigma = \sigma^{\hat{\imath}}\right) = \frac{e^{-E\left(\sigma^{\hat{\imath}}\right)/kT}}{\sum_i e^{-E\left(\sigma^i\right)/kT}},$$

where $E(\sigma^i)$ is the energy associated with the state σ^i, T is the thermodynamic temperature and k is a parameter that determines the temperature scale. We assume the probability space of Σ is finite, so we use a summation in the denominator as a partition function which sums over all possible values of σ^i.

Any system that follows the Gibbs distribution seeks to maximize entropy as time progresses. The entropy of a discrete probability distribution p is

$$-\sum_i p_i \ln(p_i),$$

where each $p_i > 0$ and $\sum_i p_i = e^T p = 1$.

The average energy of a system where each state σ^i occurs with probability p_i is

$$\langle E \rangle = \sum_i E\left(\sigma^i\right) p_i = E^T p,$$

where the components of E are $E\left(\sigma^i\right)$. We solve the following optimization problem to find the maximum entropy of the system given average energy $\langle E \rangle = \hat{E}$ as a parameter:

$$\begin{aligned} \max_p \quad & -\sum_i p_i \ln(p_i) \\ \text{such that} \quad & \\ & E^T p = \hat{E} \\ & e^T p = 1. \end{aligned}$$

We form a new optimization problem with objective function $\min \sum_i p_i \ln(p_i)$ and then negate the minimum. The Lagrangian of this new optimization problem is

$$\mathcal{L}(p, \lambda, \omega) = \sum_i p_i \ln(p_i) - \lambda\left(E^T p - \hat{E}\right) - \omega\left(e^T p - 1\right).$$

The problem is convex, so the first order optimality conditions,

$$\nabla \mathcal{L}(p, \lambda, \omega) = 0,$$

are sufficient to find a global minimum. We find that

$$p_i = \frac{e^{-\lambda E(\sigma_i)}}{\sum_i e^{-\lambda E(\sigma_i)}},$$

where λ satisfies

$$\hat{E} = \sum_i E(\sigma_i) \left(\frac{e^{-\lambda E(\sigma_i)}}{\sum_i e^{-\lambda E(\sigma_i)}} \right)$$

The Gibbs distribution is used to assess the probability for each microscopic state, i, to maximize entropy for low energy configurations. The thermodynamic temperature T is the cost of balancing between minimum and maximum entropy. The interactions between these microscopic states is used to understand larger systems developed using an Ising model.

2.2 The Ising Model

The Ising Model uses a finite lattice of particles with a fixed set of possible interactions between those particles, such as in figure 1, to model the Gibbs distribution.

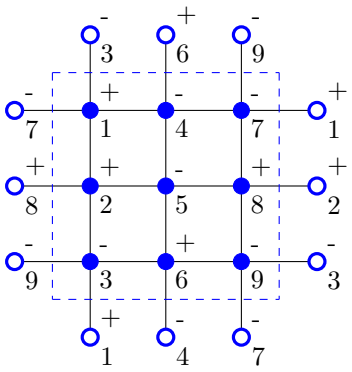


Figure 1: Square Lattice

Each point in the lattice model is assigned a spin of either a positive or negative 1, representing the magnetic orientation of each atom in a lattice. A periodic boundary condition is assumed, where the atoms above the top row are assumed to be those on the bottom row, and the ones to the left of the first row are assumed to be those in the final row. This boundary condition enforces that the topology of the lattice is in fact a torus.

The lattice state is represented by either an array or a vector of positive and negative ones. The example in figure 1 is represented both as

$$\begin{bmatrix} 1 & -1 & -1 \\ 1 & -1 & 1 \\ -1 & 1 & -1 \end{bmatrix}$$

or

$$\sigma = (1, 1, -1, -1, -1, 1, -1, 1, -1).$$

We always use column-major order to convert from matrix to vector form, so an $n \times n$ matrix A has vector form $\sigma_i = A_{(q+1)(r+1)}$, where q and r are given by the Euclidean division

$$(i-1) = qn + r.$$

Given a set of spins σ, the energy is modeled as the Hamiltonian

$$E(\sigma) = -J \sum_{(i,j)\in\mathcal{A}} \sigma_i \sigma_j - H \sum_i \sigma_i,$$

where $\mathcal{A}$ is an array of nearest neighbors. The lattice in Figure 1 has

$$\mathcal{A} = \{(1,4),(2,5),(3,6),(4,7),(5,8),(6,9),(1,3),(2,8),(3,9),(7,1),(8,2),$$
$$(9,3),(1,3),(4,6),(5,9),(3,1),(6,4),(9,7)\}$$

The first of the two summations in the Hamiltonian models the inter-atomic interactions while the second models external contributions. Ising models are most often studied without external contributions, but our survey models systems with and without external contributions. The parameter J determines whether the material is ferromagnetic or or antiferromagnetic. Ferromagnetic materials have $J > 1$ while antiferromagnetic materials have $J < 0$.
The Ising model for ferromagnetic materials is generally studied under the assumption that $J = k = 1$, which sets a temperature scale. These parameters could be customized to agree with a specific material, but there is no current theory that explains how to calculate J for a specific material. For antiferromagnetic materials, the assumption that $J = -k = -1$ is used. With these assumptions, the Gibbs probabilities are

$$P(\hat{\sigma}) = \frac{e^{-E(\hat{\sigma})/T}}{\sum_{\sigma} e^{-E(\sigma)/T}} \text{ with } E(\sigma) = -\sum_{(i,j)\in\mathcal{A}} \sigma_i\sigma_j - H\sum_i \sigma_i$$

for ferromagnetic materials and

$$P(\hat{\sigma}) = \frac{e^{E(\hat{\sigma})/T}}{\sum_{\sigma} e^{E(\sigma)/T}} \text{ with } E(\sigma) = -\sum_{(i,j)\in\mathcal{A}} \sigma_i\sigma_j - H\sum_i \sigma_i$$

for antiferromagnetic materials.
Unfortunately, calculating the Gibbs probabilities is computationally unrealistic. Given a two dimensional lattice of size $n \times n = N$, there are 2^N possible states, a number that far exceeds computational abilities. Instead of restricting the model to tiny lattices, we approximate desired quantities by sampling the state space.
We transition from one state to another by simultaneously applying simulated annealing across a subset of the lattice to determine whether a subset of spins should reverse. Let σ^k be the current state and $\hat{\sigma}$ differ from σ_k by exactly one of the spins in the selected subset. A flip is applied according to the probability

$$P(\sigma^k, \hat{\sigma}T) = \begin{cases} 1, & E(\hat{\sigma}) < E(\sigma^k) \\ e^{(E(\sigma^k)-E(\hat{\sigma}))}, & E(\hat{\sigma}) \geq E(\sigma^k). \end{cases}$$

If $P(\sigma^k, \hat{\sigma}, T) \geq y$, with y being a sample from $Y \sim \mathcal{U}(0,1)$, then the sole reversal in $\hat{\sigma}$ is accepted. This is repeated for all of the lattice points selected for consideration. σ^{k+1} is then formed by flipping all of the accepted reversals at σ^k. Our definition of energy reduces the sample required to decide whether a flip occurs to just the nearest neighbors. The energy is written as

$$E(\sigma) = -\sum_{(i,j)\in\mathcal{A}} \sigma_i\sigma_j = -\sigma_{\hat{\imath}}(\sigma_{\hat{\imath}_1} + \sigma_{\hat{\imath}_2} + \sigma_{\hat{\imath}_3} + \sigma_{\hat{\imath}_4}) - \sum_{(i,j)\in\mathcal{A}'} \sigma_i\sigma_j,$$

where $\sigma_{\hat{\imath}_1}$, $\sigma_{\hat{\imath}_2}$, $\sigma_{\hat{\imath}_3}$ and $\sigma_{\hat{\imath}_4}$ are the nearest neighbors of $\sigma_{\hat{\imath}}$ and $\mathcal{A}'$ is the subset of $\mathcal{A}$ such that neither i nor j is $\hat{\imath}$. If σ^k and $\hat{\sigma}$ differ only by a spin at lattice

point $\hat{\imath}$, then

$$\begin{aligned} E(\sigma^k) - E(\hat{\sigma}) &= (-\sigma^k_{\hat{\imath}} + \hat{\sigma}_{\hat{\imath}})(\sigma^k_{\hat{\imath}_1} + \sigma^k_{\hat{\imath}_2} + \sigma^k_{\hat{\imath}_3} + \sigma^k_{\hat{\imath}_4}), \\ &= (-\sigma^k_{\hat{\imath}} - \sigma^k_{\hat{\imath}})(\sigma^k_{\hat{\imath}_1} + \sigma^k_{\hat{\imath}_2} + \sigma^k_{\hat{\imath}_3} + \sigma^k_{\hat{\imath}_4}), \\ &= -2\sigma^k_{\hat{\imath}}(\sigma^k_{\hat{\imath}_1} + \sigma^k_{\hat{\imath}_2} + \sigma^k_{\hat{\imath}_3} + \sigma^k_{\hat{\imath}_4}), \end{aligned}$$

which references only the nearest neighbors of lattice point $\hat{\imath}$
Given a system state, the average of the systems energy, $\bar{E_T}$, and the average of the systems magnetism, $\bar{M_T}$, at a given temperature T are

$$\bar{E_T} = \frac{1}{N}\sum_{i=1}^{N} E(\sigma_i) \approx \langle E_T \rangle \quad \text{and} \quad \bar{M_T} = \frac{\eta}{N}\sum_{i=1}^{N} \sigma_i \approx \langle M_T \rangle$$

where η is a scaling factor assumed to be one for our analysis. The heat capacity, C_T, and susceptibility, $\mathcal{X}_T$, of the system are then given by

$$C_T = \frac{\langle E_T^2 \rangle - \langle E_T \rangle^2}{kT^2} \quad \text{and} \quad \mathcal{X}_T = \frac{\langle M_T^2 \rangle - \langle M_T \rangle^2}{kT},$$

where $\langle M_T^2 \rangle$, $\langle M_T \rangle^2$, $\langle E_T^2 \rangle$, and $\langle E_T \rangle^2$ are approximated by the sample averages in our calculations.

3 Results

First, we confirm that the energy of the lattice decreases to a minimum as the simulation progresses. Figure 3 illustrates the results of running 500 iterations of a simulation for temperatures of $T = 1.5$ and $T = 3.5$ on a 30 by 30 lattice of points. At each step, 60% of the points are candidates for reversal. 1000 iteration equilibration videos for $T = 1.5$ and $T = 3.5$ are available at [1] and [2] respectively.

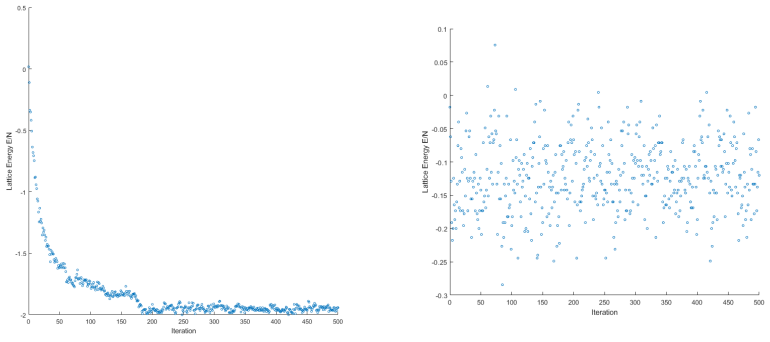


Figure 2: Energy per lattice point vs. iteration for simulations for a 30×30 lattice of points at temperatures of 1.5 and 3.5.

[1] https://youtube.com/shorts/Xxt0h8L3qtE?feature=share
[2] https://youtube.com/shorts/klTChmp7aW8?feature=share

At low temperatures, below the Curie point, the energy per lattice point decreases from a random state, and thus the magnetism increases with time. The temperatures appear to reach a minimum after about 200 iterations. At temperatures above the Curie point, the temperatures fluctuates randomly throughout the simulation.

The energy, magnetism, heat capacity, and susceptibility of a simulated 50×50 square lattice are shown below. We ignore the first 1000 states to allow the system to come to equilibrium.

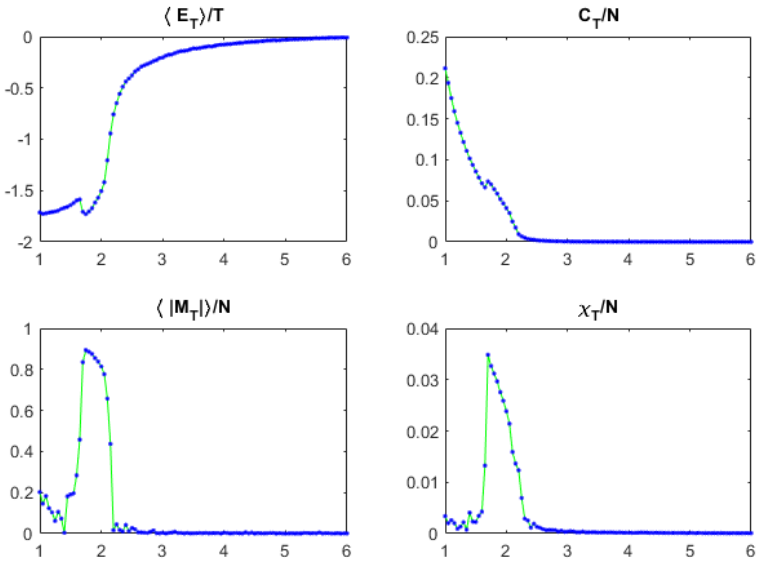


Figure 3: Square Lattice Observables

The model parameters are $k = 1, H = 1$, and $H = 0$. Temperatures were taken between $T = 1$ and $T = 6$ with uniform time steps of $\Delta T = 0.05$. The graphs display a phase transition, showing an increase in energy per lattice point and a decrease in magnetism at a temperature of about 2.15.

We also consider examples on hexagonal and triangular lattices like those shown in Figure 4.

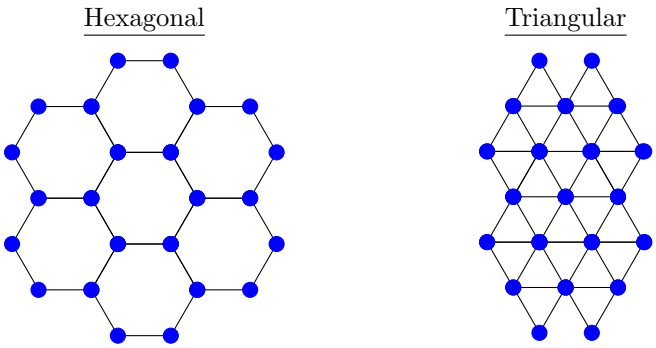
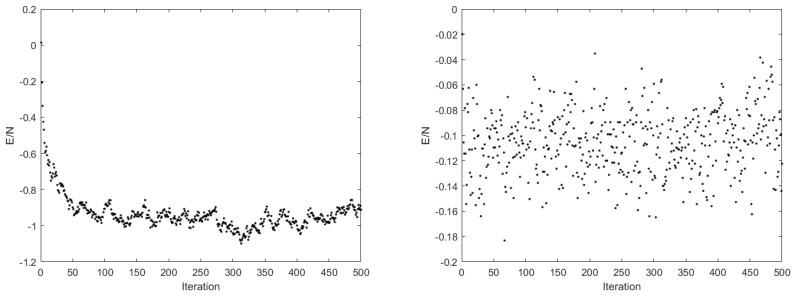


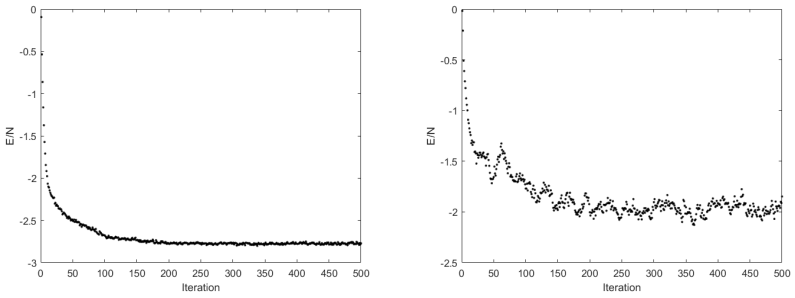
Figure 4: Alternative Lattices

Again, the energy of each lattice decreases to a minimum as the simulation progress. Figures 5a and 5b illustrate the results of running 500 iterations of a simulation for temperatures of $T = 1.5$ and $T - 3.5$ on a 50x50 hexagonal lattice of points. Figures 6a and serve the same purpose for a 50x50 triangular lattice of points. The hexagonal lattice demonstrates similar behaviour to the square lattice at $T = 3.5$, but takes far long to equilibrate when $T = 1.5$. The triangular lattice demonstrates the opposite. At $T = 1.5$ it equilibrates more quickly than the square lattice, but at $T = 3.5$ it produces an equilibration trend unique to itself. Unlike the square and hexagonal lattice, its energy decrease to approximately -2 rather than hovering around 0. At each step, 60% of the spins are candidates for a reversal in spin.



(a) $T = 1.5$ (b) $T = 3.5$

Figure 5: Equilibration of a Hexagonal Lattice



(a) $T = 1.5$ (b) $T = 3.5$

Figure 6: Equilibration of a Triangular Lattice

We generate the same sets of plots showing energy, specific heat, magnetism, and susceptibility as before. Figure 7 shows these figures for a 50x50 hexagonal lattice with $k = 1, = 1$, and $H = 0$ that was equilibrated for 1000 iterations before 750 samples were taken at temperatures between $T = 1$ and $T = 4$ with $\Delta T = 0.05$. It is evident that the trends in magnetism and specific heat have not converged to the trends expected, but time did not allow for larger grids to be simulated. While the trend in susceptibility appears to have incorrect magnitude, it does display a clear maximum at $T = 1.5$ which corresponds to what appears to be very close to the Curie Temperature based on the energy plot as shown by the vertical black lines.

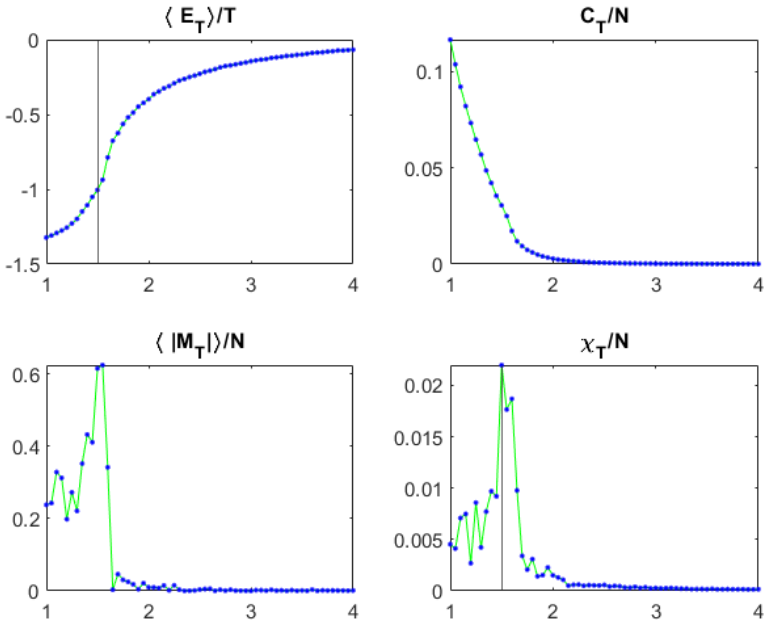


Figure 7: Hexagonal Lattice Observables

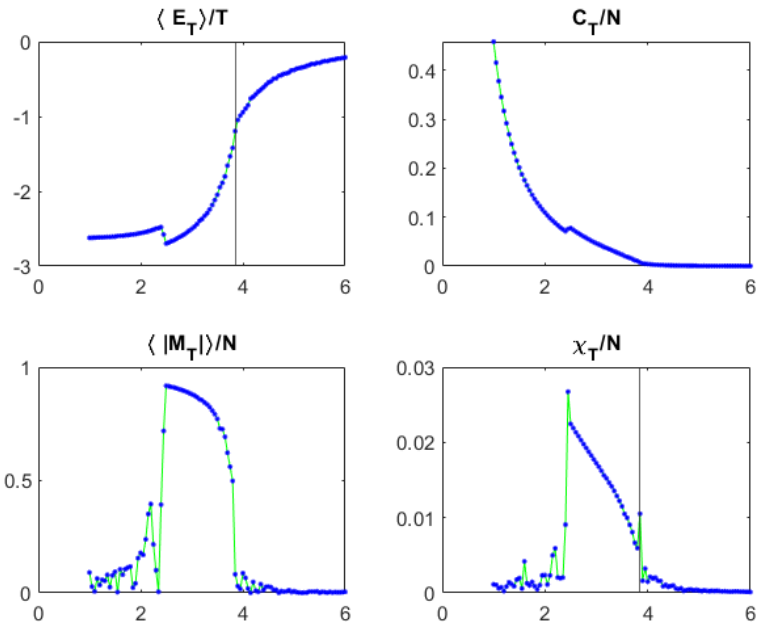


Figure 8: Triangular Lattice Observables

Figure 8 show the energy, specific heat, magnetism, and susceptibility for the triangular lattice. Again, a 50x50 lattice with $k = 1, H = 1$, and $H = 0$ was equilibrated for 1000 iterations before 750 samples were taken at temperatures between $T = 1$ and $T = 6$ with $\Delta T = 0.05$. It is evident that some of these plots are suspect, but the energy plot does seem reasonable. It is interesting to note that the Curie temperature for this arrangement is $T = 3.85$, much higher than that of the square or hexagonal lattice. Furthermore, despite the questionable trends in susceptibility, there remains a local maximum at this Curie temperature. If we reduce the grid size to 30x30, take 250 samples per temperature step, and set $H = 1$, we get the results shown in figure 9. Unfortuantley there is no clear local maximum in susceptibility to identify the Curie temperature, but the trend in energy suggests that it did not change.

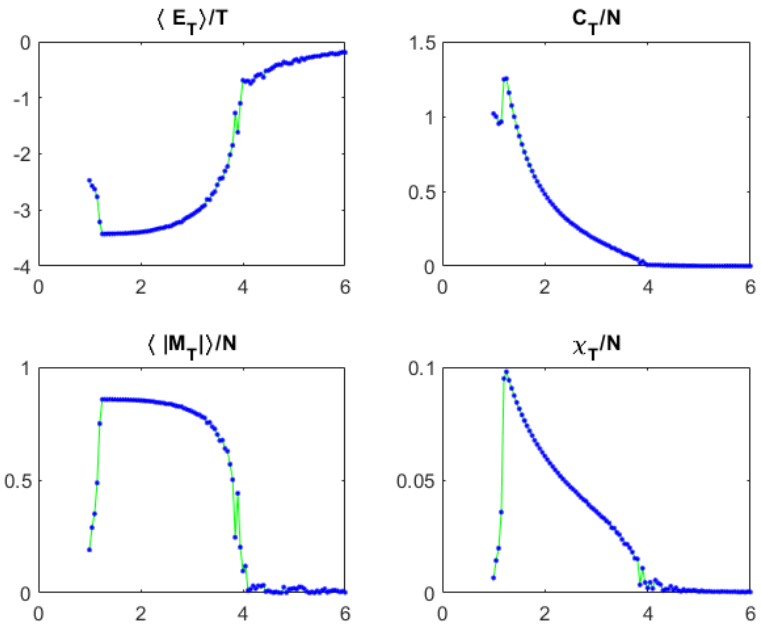


Figure 9: Triangular Lattice Observables with $H = 1$

4 Conclusion

Statistical mechanics of micro-interactions between atoms of a ferromagnetic material can be represented using an Ising model for square, hex, and triangular lattice structures. Applying Gibbs distribution to the lattice assess the probability for each atom to maximize entropy for low energy configurations. Slowly increasing the temperature of the atoms leads to a phenomenon known as the Curie point where the ferromagnetic material loses its magnetic properties. The Curie point for each lattice can be approximated with hex lattice at around 1.5, the square lattice around 2.15, and the triangle lattice near 3.85. These numbers show that there is a positive correlation between number of micro-interactions and the Curie point such that the 8 interactions per atom in a triangular lattice results in its high Curie point.

References

[1] Allen Holder and Joseph Eichholz. *An Introduction To Computational Science*. International Series in Operations Research & Management Science. Cham, Switzerland: Springer, 2019.

A Summary

Our paper used the 2-dimensional Ising model to simulate magnetic phase transitions in materials that occur as a function of temperature. Above a certain temperature known as the Curie temperature or Curie point, magnetic substances lose their magnetic properties. The Ising model is a statistical mechanics model that simulates atoms as a lattice of points and stochastically flips the spins of such particles according to a fixed temperature T to model time advancing.

We compared square, triangular, and hexagonal lattice structures with periodic boundary conditions to model the energy and magnetism stored in a material as time progresses. First, we ran the simulation at a constant, low temperature to establish an equilibrium state, then gradually increased the temperature and plotted how the energy and magnetism of the material changed with respect to temperature.

In all cases, we were successfully able to model the phase shifts associated with the material's Curie point. There was a sudden decrease in magnetism and sudden increase in energy at a certain temperature. Furthermore, different lattices had different behaviors. The approximate Curie temperature of the hexagonal lattice was the lowest at about 1.5, the square lattice had a a middling Curie temperature of about 2.15, while the triangle lattice had the highest Curie temperature at about 3.85.