Magnetic Phase Transitions

Owen Land, Zach Eme, Zibo Wang

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1 Introduction

Magnetism is a phenomenon that has been studied ever since lodestones-naturally magnetized pieces of magnetite were discovered. Since then, magnetism has become a commonly studied physical property, appearing in everything from elementary school science fair projects to special relativity. One specific property of magnetism, the Curie point, will be discussed in this report.

The Curie point is the temperature where a phase transition occurs in a magnet, causing it to lose magnetic attraction. This is possible to predict using an Ising model, and helps show the behaviour of physical models.

2 Method

The Ising model is a model developed to characterize ferromagnetism in metals. We use this model in its two-dimensional form to describe the interactions between neighboring atoms. The simplest form of the 2-D model creates a square lattice of atoms and defines spins as only having two states, positive or negative. The energy of the system can be described by

$$E(\sigma) = -H \sum_i \sigma_i - J \sum_{(i,j)\in A} \sigma_i \sigma_j, \tag{2.1}$$

where A is the collection of nearest neighbors. H is assumed to be 0 because the analysis is done with no external field. J is a material property constant that is positive for ferromagnetic materials and negative for anti-ferromagnetic materials. J is set equal to one in our model to study ferromagnetic behavior. This simplifies the energy model to

$$E(\sigma) = - \sum_{(i,j)\in A} \sigma_i \sigma_j. \tag{2.2}$$

The σ matrix has a periodic boundary condition which adds a level of complexity to the way the collection matrix is formed. To counteract this, extra rows and columns are added to all sides that mirror the boundary conditions

so that finding the collection points near the edges of the original σ matrix is trivial.

After the energy is found from the collection matrix using equation 2.2, the value is halved due to the collection matrix double counting points.

Atom's states are flipped to simulate lattice structure's tendency to approach a lower energy state Suppose σ_k is the current state, and $\hat{\sigma}$ is the state after the flip. The new state is accepted according the probability

$$P(\sigma_k, \hat{\sigma}, T) = \begin{cases} 1, & \text{if } E(\hat{\sigma}) < E(\sigma_k) \\ \mathrm{e}^{\frac{E(\sigma_k)-E(\hat{\sigma})}{T}}, & \text{if } E(\hat{\sigma}) \geq E(\sigma_k). \end{cases} \tag{2.3}$$

If $P(\sigma_k, \hat{\sigma}, T) \geq y$, where y is a sample of $Y \sim U(0,1)$, then the new state $\hat{\sigma}$ is accepted. To compare σ_k and $\hat{\sigma}$, we do not need to recalculate the energy of the whole lattice, but instead only have to focus on the changed atom σ_i^k and its nearest neighbors σ_{i1}^k, σ_{i2}^k, σ_{i3}^k, and σ_{i4}^k,

$$\begin{aligned} E(\sigma_k) - E(\hat{\sigma}) =& (-\sigma_i^k + \hat{\sigma})(\sigma_{i1}^k + \sigma_{i2}^k + \sigma_{i3}^k + \sigma_{i4}^k) \\ =& -2\sigma_i^k(\sigma_{i1}^k + \sigma_{i2}^k + \sigma_{i3}^k + \sigma_{i4}^k). \end{aligned} \tag{2.4}$$

The state σ can be used to find other physical quantities than the energy state.

$$\text{Magnetization} \qquad M(\sigma) = \eta \sum_i \sigma_i, \text{ where } \eta \text{ is a scalar,} \tag{2.5}$$

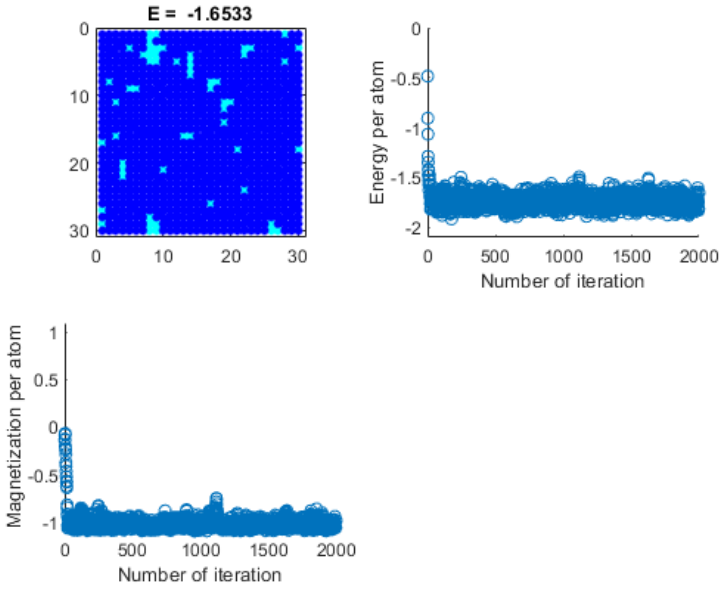
$$\text{Heat Capacity} \qquad C_T = \frac{\langle E_T^2 \rangle - \langle E_T \rangle^2}{kT^2}, \tag{2.6}$$

$$\text{Susceptibility} \qquad \chi = \frac{\langle M_T^2 \rangle - \langle M_T \rangle^2}{kT}. \tag{2.7}$$

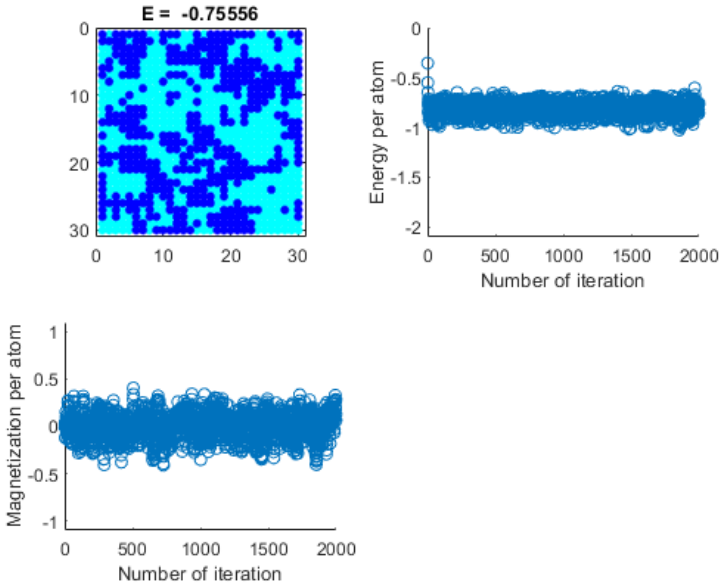
$\langle E_T \rangle$ or $\langle M_T \rangle$ are sample average of E or M at a specific temperature. $(\langle E_T^2 \rangle - \langle E_T \rangle^2)$ or $(\langle M_T^2 \rangle - \langle M_T \rangle^2)$ are essentially the variance of E or M.

3 Results

Figures 1a and 1b show the configuration of spins, σ, changes over iterations at different temperature. In order to obtain a better sample of the data, early iterations are thrown out to ensure that the data is taken closer to equilibrium. This gives time for the random flipping to more closely approach its smallest energy value and its highest entropy value.



(a) $T = 2$.



(b) $T = 4$.

Figure 1: Simulation of a 30 by 30 lattice at different temperatures.

Figure 2 shows the results of a simulation with a 30 by 30 lattice. The temperature ranges from $T = 1$ to $T = 4$ with step size 0.03. From this simulation, the Curie temperature is somewhere between $T = 2.2$ to $T = 2.3$. At about $T = 2.2$, the energy per atom increases at its maximum rate. The peak value of heat capacity per atom and susceptibility per atom also occurs near $T = 2.2$. After $T = 2.3$ there is no net magnetization. This is proof of a Curie point, and shows the behaviour of different physical properties of the model around this temperature.

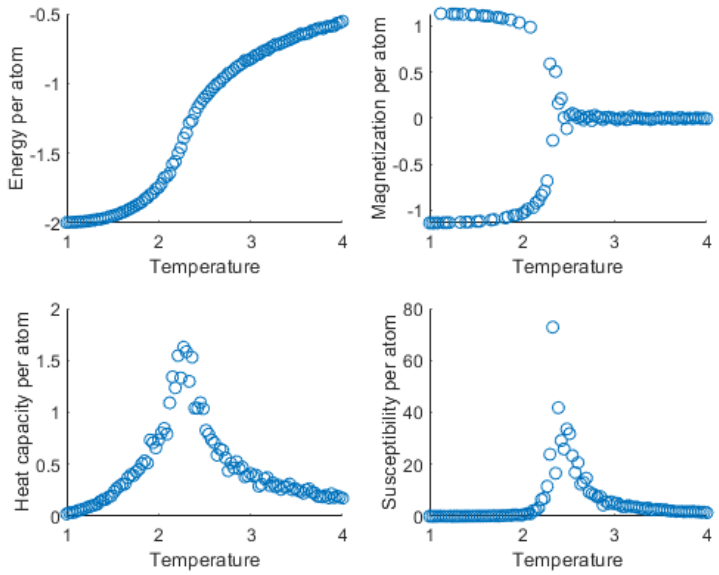


Figure 2: Simulated result for a 30 by 30 lattice.

4 Conclusion

While the Ising model is good at showing the behaviour of 2-Dimensional and 1-Dimensional magnetism properties as a function of temperature, a 3D model is intractable. This means that while our data shows how a magnet should theoretically interact with its surroundings through its energy storage and its magnetism, these can not be used to predict the real behaviour of magnets. Because of this, our model only exists of a proof of concept for a Curie point.

5 Future Work

The model currently only evaluates all properties in two dimensions and with a square geometry. Real world materials are not perfectly square nor do

they exist in only two dimensions. In order for the model to be more realistic it should be able to evaluate for different geometries as well as in three dimensions.

Bibliography

[1] Holder, Allen. "Chapter 12. Magnetic Phase Transitions." *Modeling with Optimization and Simulation.* 432-442