Mary Ann Odete & Juliana Lumer

Computational Physics

2-D Ising Models

Abstract

By modeling magnetic material as a 2D lattice of atoms, we are going to find the magnetization of the system as a function of temperature. We will use a Python program that implements the Metropolis algorithm, a Markov chain Monte Carlo method (MCMC). Each atom on the lattice has a corresponding magnetic moment which is either up or down (± 1).

Introduction

A popular area of study in statistical mechanics is that of phase transitions. To understand these complex interacting systems is no small feat. In 1944, Lars Onsager lead a huge advancement in mathematical physics when he found the analytical solution for the two dimensional Ising model with no external magnetic field [1]. To date, there is no analytical solution for the generalized case. The 2D Ising model is one of the few models for statistical interactions that has actually been solved analytically. Appropriately named, the 2D Ising model is a higher dimensional generalization of the original one dimensional model proposed by Ising. The model describes a two-dimensional lattice of variables, spins, which take on two values defined as ± 1 or $\uparrow\downarrow$. These spins interact with their nearest neighbors and, if it is present, an external magnetic field. Our job is to simulate this process by tracking the interactions between neighboring atoms, i.e., the changes in the system's energy, to observe how the magnetization of the system evolves over time with respect to temperature.

Theory

Spin & Magnetization

In this model, we look at a property of the lattice atoms' electrons, spin. Spin is a characteristic property elementary particles that can occupy on of two states ("up" or "down"). The spin electron decides the electron's spin angular momentum. This, along with the electron's orbital angular momentum and charge, forms the electron's magnetic moment.

The magnetic moment , μ, is given by:

$$\mu = g\frac{eJ}{2m_e}$$

J being the total angular momentum. Thus, the electron's spin is proportional to its magnetic moment, so the nearest neighbor magnetic dipole-dipole interactions can be viewed more simply as spin-spin interactions.

In the lattice of atoms, there are unpaired electrons. Nearest neighbors spins will align as either parallel $\uparrow\uparrow$, $\downarrow\downarrow$ or anti-parallel $\uparrow\downarrow$. This interaction causes a difference in energy between states: working with a magnetic material spins are more likely to align in the same direction since aligned spins will decrease the magnitude of the repulsion between electrons, bringing the system into a lower energy, more stable state.

The magnetization of the system can be defined as: [3]

$$M = \sum_i s_i$$

Where s_i is the spin state. If all spin states are aligned, we can see that will produce the greatest magnetization. The magnetization will also show how the system reacts to an external field.

Temperature & Magnetization

The system we are studying is thermodynamic. The temperature of the system affects the thermal motion of the dipoles, thus it also affects how the spins align, i.e., the magnetization. On their own, or with an applied field, ferromagnets will tend to spontaneously magnetize. However, as temperature rises, thermal effects start to influence the magnetization of the system. There is a critical point, the Curie temperature, beyond which the magnetic material cannot spontaneously magnetize. This is the aforementioned phase transition (ferromagnet $\rightarrow$ paramagnet). At this point, the material can no longer be magnetized.

Energy due to spin states

The energy E of a spin configuration σ is:

$$E(\sigma) = -\sum_{ij} J\sigma_i\sigma_j - \mu \sum_i B_i\sigma_i$$

Where J is a constant (the exchange energy), which is positive if the spins of neighboring electrons are the same, negative if opposite, or zero if the material has reached its Curie temperature and is no longer ferromagnetic. We can see that for aligned spins, the energy is lower. μ again denotes the magnetic moment, B_i is the external magnetic field at a certain point on the lattice. When B_i is zero, there is no external influence on the system, when it is positive, energy is lowered (aligned spins) and vice versa when B_i is negative.

The energy in a canonical ensemble, such as our system, is probabilistic. The probability $P(E,T)$ at temperature T of the system being in a certain state is given by the Boltzmann distribution: [2]

$$P(E,T) = \frac{e^{-E(\sigma)/k_BT}}{Z(T)} \quad , \quad Z(T) = \sum_{\sigma} e^{-E(\sigma)/k_BT}$$

Methods

The Metropolis algorithm is a MCMC method specifically for computing random samples from a probability distribution that would be difficult to obtain otherwise.

Results & Data

The first test we ran was raising the temperature for both a fully magnetized lattice (all spins +1) and a randomly magnetized lattice.

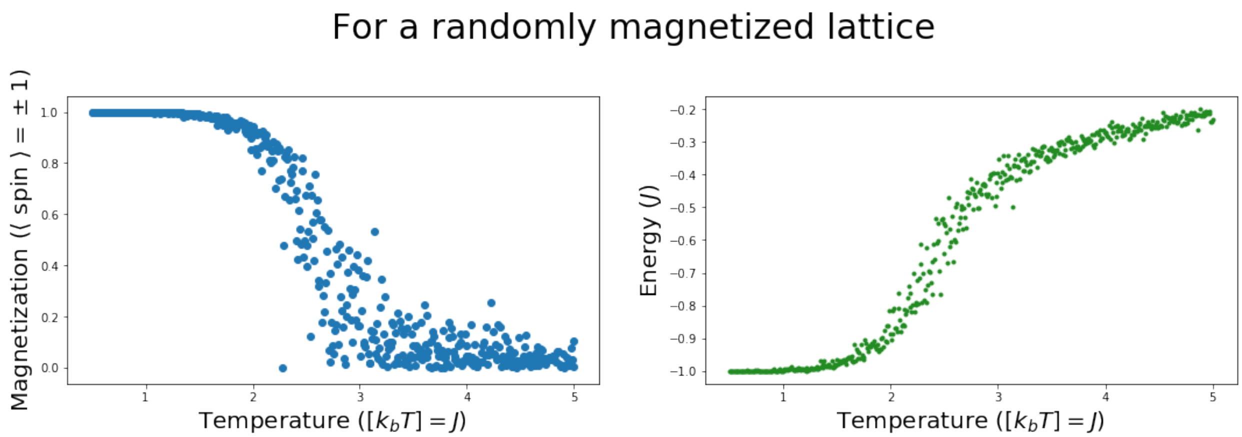

Figure 1: For both graphs, around $2k_bT$ (the Curie temperature), there is a steep change. For the magnetization, the lattice is quickly demagnetized, and the energy increases suddenly.

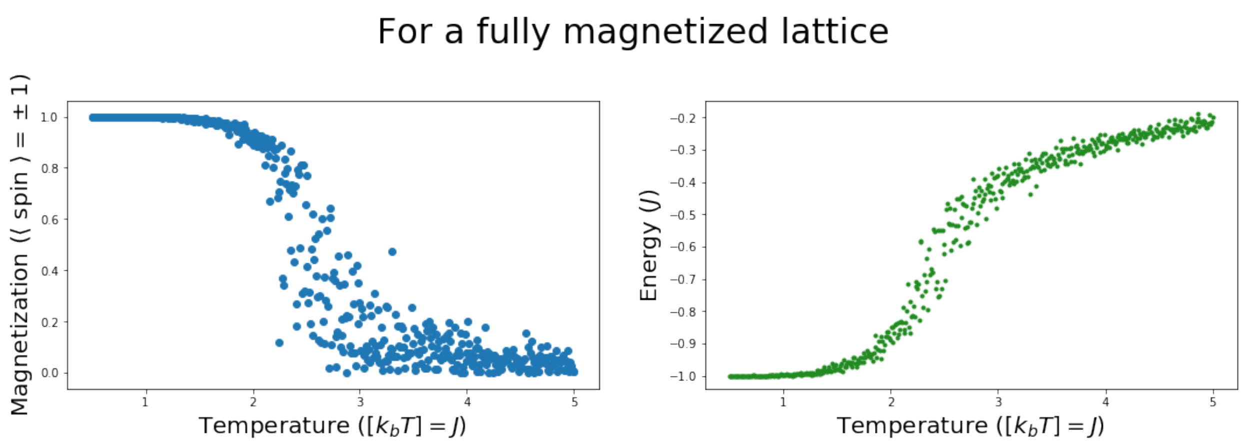

Figure 2: Again, both graphs experience a steep change close to $2k_bT$

These graphs show that the initial lattice arrangement does not matter, the end result is the same. At the Curie Temperature, the magnetization drops to zero and the energy will quickly increase. The slopes of these curves indicate a phase transition at T_c. Pushed past its Curie temperature, a ferromagnetic material will become paramagnetic. Cooling the now paramagnetic material past T_c will cause the material to become anti-ferromagnetic, i.e., spins will align ↑↓↑↓↑... etc. in each row.

The next test we ran was including an external magnetic field. The magnetization is now defined as [3]

$$M = H \sum_i s_i$$

We tested for both positive and negative H.

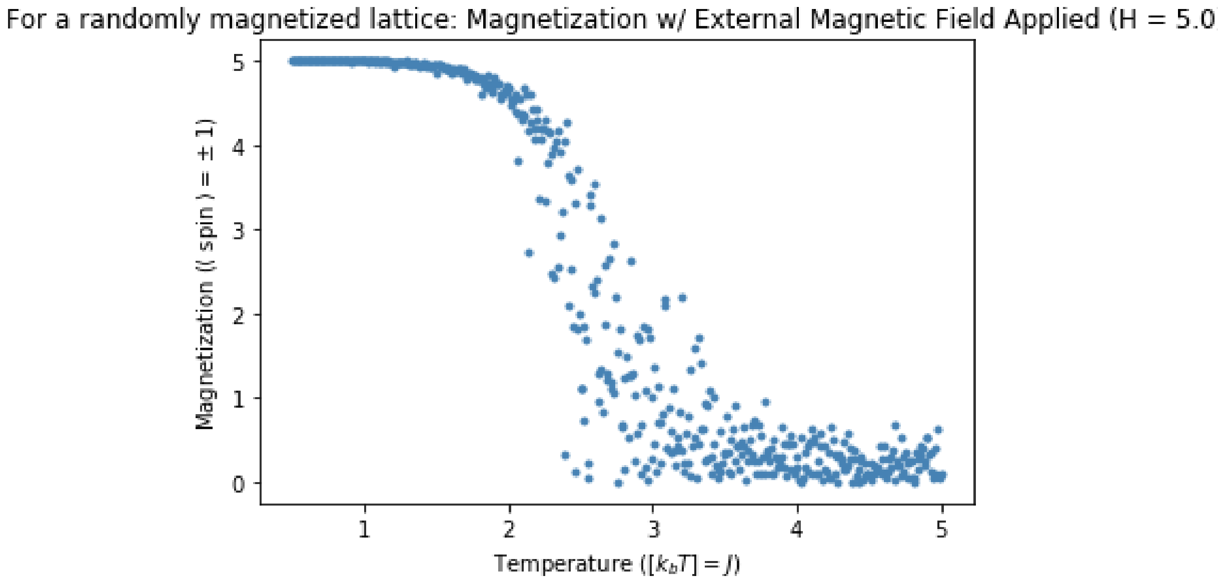

Figure 3: The effect on the magnetization when the external field applied is positive.

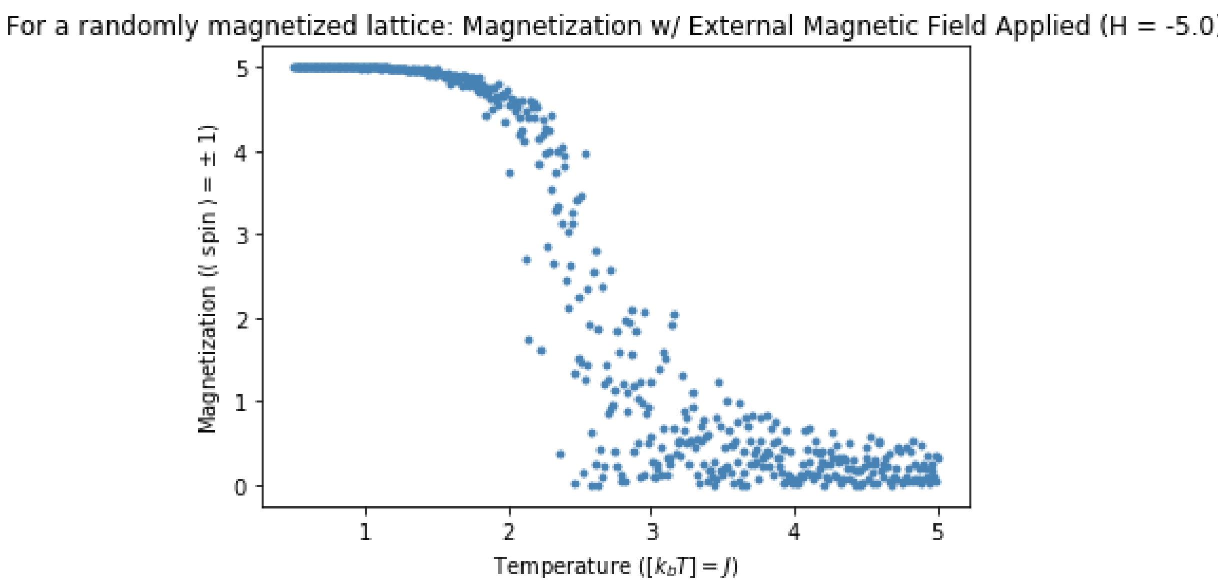

Figure 4: The effect on the magnetization when the external field applied is negative

While we cannot see it graphically, the application of an external magnetic field should cause the Curie Temperature to rise. More energy is need to demagnetize the lattice, so more heat has to be put into it for the ferromagnet to become a paramagnet.

And finally, we lowered the temperature.

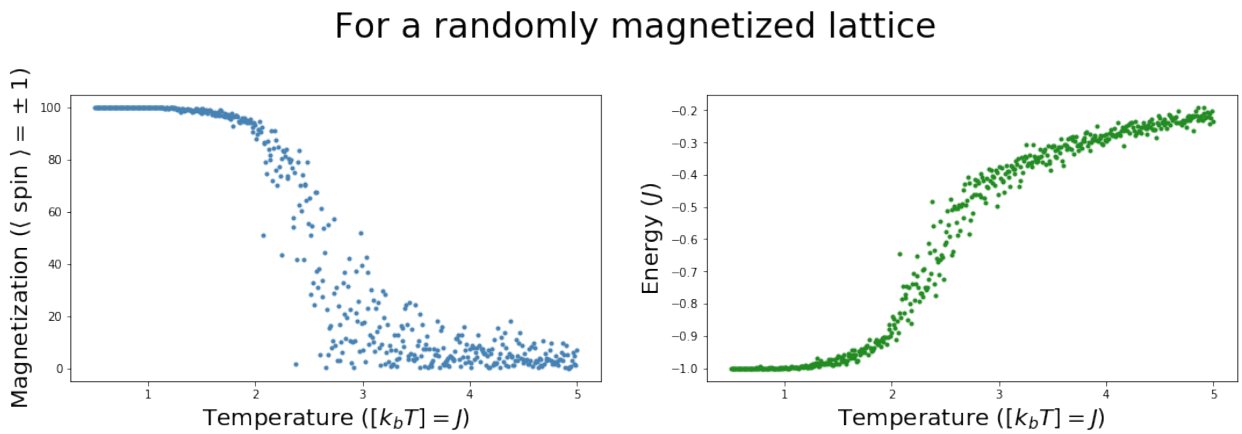

Figure 5: The effects on the lattice when the temperature is lowered

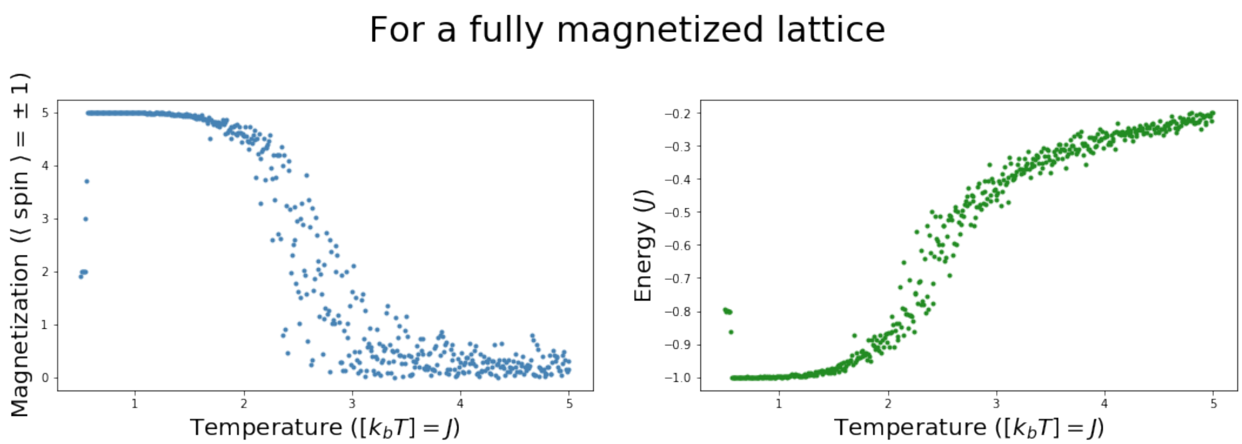

Figure 6: The effects on the lattice when the temperature is lowered

While the graphs in this section share the same general shape as the previous graphs, the scaling is vastly different in terms of the magnetization, especially for the randomly magnetized lattice. The energy does not seem to be too affected, though.

Then, we applied an external field while we cooled the lattice down.

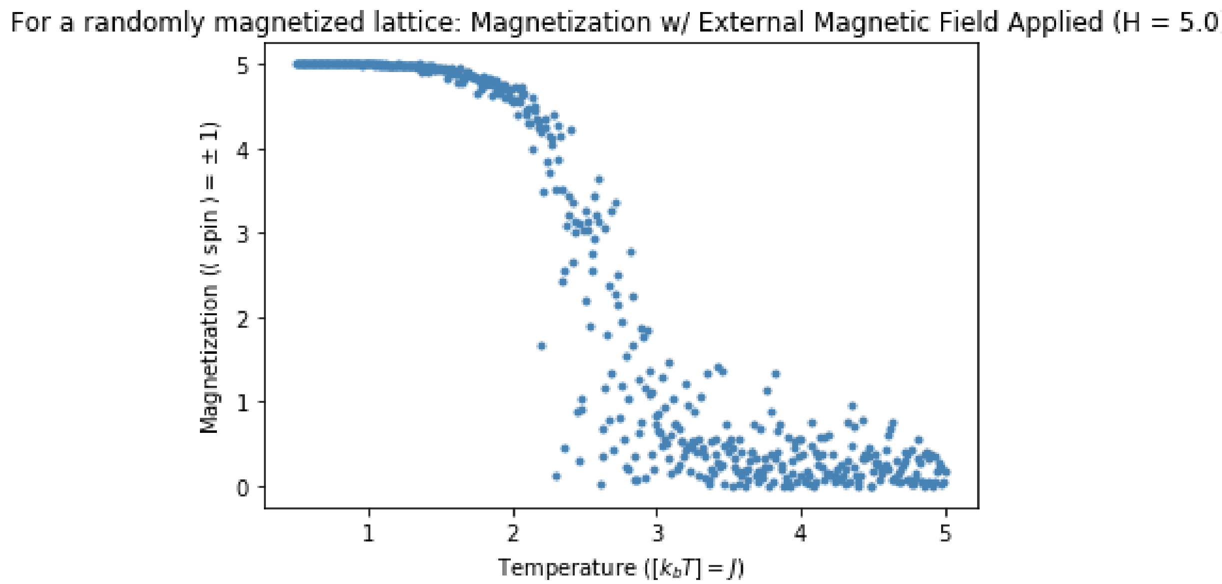

Figure 7: The effects on a lattice when the temperature is lowered and there is an external magnetic field applied. Similar to Figure 3.

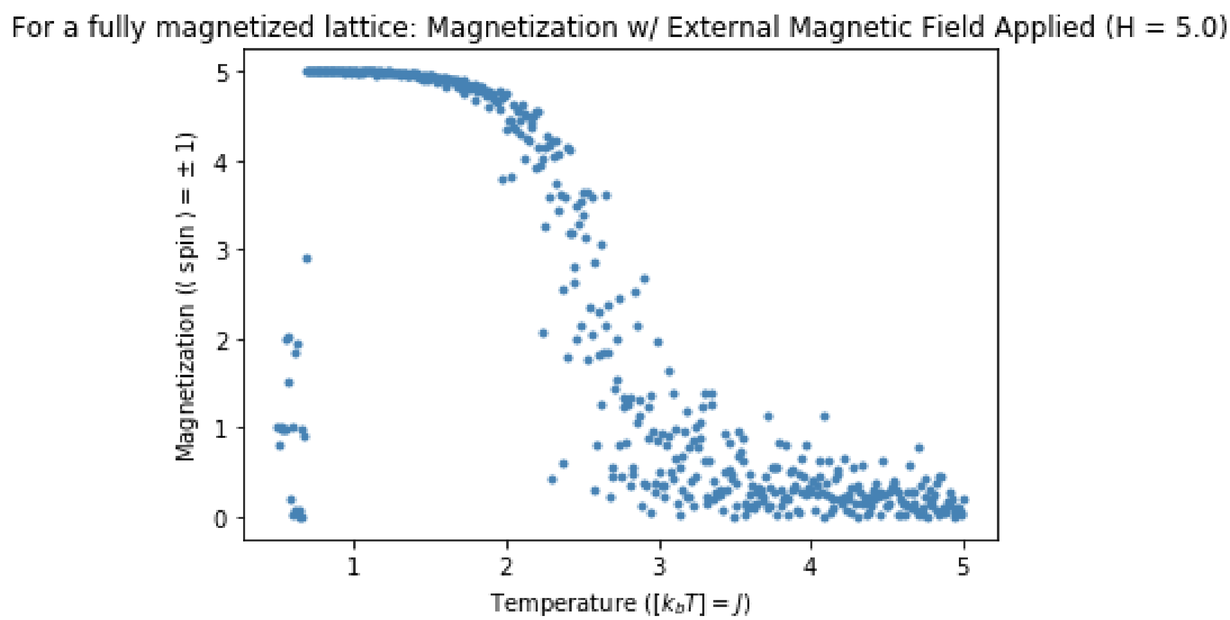

Figure 8: The effects on a lattice when the temperature is lowered and an external magnetic field is applied. Similar to Figure 4.

Conclusion

For the 2D lattice, all the graphs kept the same general shape, a $\pm \tanh$ curve. This agrees with the analytical solution and served as a preliminary measure of how accurate our results were. Under all the tested variations in initial conditions, the lattice behaves in a similar manner across the board. With regards to the energy, even the scaling remained the same under different situations. The main changes took place within the magnetization of the lattice. With an applied field, the Curie Temperature appears to increase so that the phase transition happens later than it does without the field.

The strength of the overall magnetization changed significantly under certain circumstances. The obvious case was the increase in strength when an external field is applied - the field increases the tendency for spins to align according to the direction of the field. Another difference in strength arises between raising the system temperature past T_c versus decreasing below T_c. The latter having the stronger overall magnetization. Moreover, this was the only instance in which the randomly magnetized lattice and the fully magnetized lattice started at different overall magnetizations. When the lattice is cooled down, instead of a ferromagnet, paramagnet swap there is a paramagnet, antiferromagnet swap. This is probably what led to such a big difference.

References

[1] "Lars Onsager — Array of Contemporary American Physicists". Aip.org.

[2] Landau, Rubin H. *Computational Physics , Third Edition*. Wiley-VCH, Verlag GmbH & Co. KGaA:Weinheim, Germany. Pg(409-443). 2015

[3] Blanton, Michael: "Computational Physics Project / 2D Ising Models"
`https://blanton144.github.io/computational/pdf/project-ising.pdf`