The energy of the lattice is calculated using the formula. We can represent this in code as below. The circshift function is used to find how the atoms align with the neighbouring points in the lattice. This sums out the total number of aligned and anti-aligned neighbours in the lattice.

Looking at the case of a lattice with random spins you can see a high energy (well relatively) and in the case of a lattice where all spins are aligned we can see a much lower energy

Numerically it is impractical to solve for all possible evolutions in the Ising model as there are simply too many possible evolutions. The partition function for the Ising model which can be used to calculate the macroscopic properties is given by the formula

$$Z = \sum\_{s\_i} e^{-\beta U}$$

As an example, for a tiny matrix of 10 by 10 lattice this partition function contains 2^100 terms, a number impossibly big for a computer to calculate in any reasonable timeframe [3].

While it is impossible to compute the probabilities of all the possible states, using the Metropolis algorithm we can evolve the system using the Boltzmann factors as probability of a particular evolution of the system. This algorithm, as described in the 341 Thermal textbook by Schroeder [3], chooses a random molecule

If the molecule has a high energy

A picture containing crossword puzzle

Description automatically generated

such as its spin is opposite to its neighbors, flipping the spin of the molecule would reduce the energy of the system. If this is the case the spin is flipped.

On the other hand, if the molecule has low energy

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Such as its spin is aligned with its neighbors, flipping the molecule would reduce the energy of the system. In this case it would make sense to not flip the molecule as energy is required to do so. However, In the Ising model the molecule is flipped with probability given by the formula $P = e^{-\beta \Delta E}$. Meaning When Temperature increases, probability of flipping increases. This occur even though energy increases, as with higher temperatures, the energy to flip the spin is available.

Representing this in code we can make a function that can return the probability of flipping a particular node at each step.

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We can see that in the case that Flipping the spin decreases the energy we flip the spin.

While in the case that flipping the spin increases the energy we flip with the probability based on the temperature as per the formula above where increasing the temperature means increasing likelihood of flipping the spin.

This process is then repeated to simulate the evolution of the system.

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To find the critical temperature at which phase transition occurs, computationally, we would run the Metropolis algorithm for sufficient number of evolutions at different temperatures and compare the energy to the temperature.

**Results**

To accurately compare our model to the Onsager’s analytical solution we use the Monte-Carlo method and average out over the last 1000 evolutions after evolving the system for 10000 steps. Doing this we get a smooth line for our high temperature runs but we notice at low temperatures there is some jitteriness. With further investigation we find that this is caused by at low temperatures the system evolves to a meta-stable solution that form due to the limited matrix size.

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Here we have an example a low temperature evolution which finishes with a line straight through the middle, increasing energy. This a meta stable solution that is very unlikely to evolve to a lower energy state over a reasonable timeframe.

A picture containing shape

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In contrast here we have a evolution of the same temperature which finishes with all atoms with the same spin with the minimum possible energy.

Chart, line chart

Description automatically generated

To get a smoother line at these points we ran the same simulation 50 times. This is the evolution of 70 different temperatures in a 60 by 60 lattice with 10000 steps of evolution each after which we average out the energy over the last 1000 steps. All this is then repeated 50 times making us have to deal with a run time of around 2500 seconds.

With this we can find the steepest point on the temperature vs energy graph as the critical point of our model where it changes from zones with aligned spins like that in a ferromagnet to chaos no obvious zone with aligned spins.

Comparing the Onsager’s analytical solution which gives a value of 2.269 we can see that our computational model gave a value that agrees highly with the analytical solution.