# Computational Array of Ferromagnetic Effect "Ising Model"

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## Overview

Electron's spin has two possibilities of order: order and disorder or stable and unstable. Order helps to sustain a process while disorder adapts to new changes. Moreover, atoms are perceptible to have same orders because they are very similar to each other. During interactions, their environment eventually becomes similar. On the other hand, increasing temperature can weaken those bonds and misalign atoms from each other.

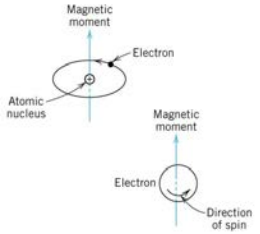
These effects are very difficult to calculate or measure because atoms are very small and many. Although using simple probabilistic statistics similar to "throwing a dice" by taking random numbers, we can find reliable solution with more efficient calculation. In this method we will look at a system and take average over many trials in order to get a result.

## Ising Model Derivation

Particles tend to favor lower energy state, because it is more stable for them. At zero temperature, particles tend to go to minimum energy. Moreover, atoms go to minimum energy by making bonds with other atoms.

Due to precession of electrons called "spin" atoms have magnetic moments and magnetic moment have lower energy when they align with magnetic field.

$$u = -\mu \cdot B$$




Therefore, two atoms' interaction has an effect of two magnet interacting with each other. Although, with Ising Model we simplify magnetic moment in to two terms: upstate and down state or spin up and spin down. S1 represents the spin of particle 1 and S2 represents the spin of particle 2.

Additionally, the interaction energy between two particle is simplified as constant J. Therefore J is negative when both particles are aligned. (Fig.4) And J is positive when two particles have opposite spin state. (Fig.3) Since -J is a lower energy value, we can derive that particles want to be aligned.

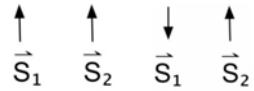



Fig. 4 Fig. 5

Ferromagnetic interaction occurs when J is positive and when J is negative antiferromagnetic interactions occur, where all the neighboring atoms want to have opposite spin from each other.

$$u = -J\,\vec{S}_1 \cdot \vec{S}_2$$

## Curie Temperature

The magnetic dipole moment created by spin can be viewed as a "small magnet." When the temperature is increased, these tiny magnets fluctuate as seen on figure 3. These small magnets lose magnetization as they reach the curie temperature.

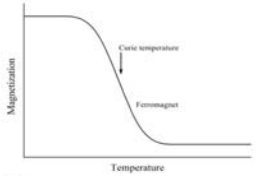



Fig. 7

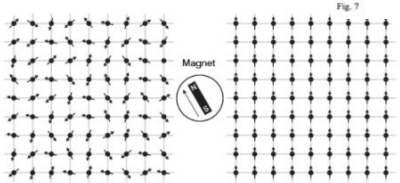



Fig. 3

Ferromagnetic material has a phase transition before and after meeting the curie temperature as seen on Fig. 7. This phenomena is caused by the alignment of spins at 0 temperature and misalignment of the spins after the curie temperature. The misalignment causes an object to lose its magnetic properties due to spin pair coupling.

## Monte Carlo Method

The probability of spin energy equals to Boltzmann's Statistical equation.

$$Boltzmann\ Probability = e^{-J/k_B T}$$

Conventional methodology is to account for all possibility at a certain energy and calculating the probabilities at that energy. Therefore, integration over all possible state, which is the probability of being at certain energy multiplied by the magnetization at that energy equals to the expectation of magnetization.

$$\int_i P(E_i) \cdot M(E_i)\, dE_i = \langle M \rangle$$

Contrast to sampling the whole system to take the possibility, Metropolis Algorithm or Monte Carlo Method, samples a system with relevant probability and averages it out. Therefore, instead of finding all possible state and averaging them according to probability, we take the states according to their probabilities and average them out.

Energy of a component:

$$E = -S_{i,j} \cdot (S_{i+1,j} + S_{i-1,j} + S_{i,j+1} + S_{i,j-1})$$

To be specific, a change in energy system ΔE(caused by the move of a spin) is calculated; If ΔE is smaller than zero, the change would bring the system to a lower state energy. We allow the move and put the particle into new position. If ΔE is bigger than zero, we allow the move with the probability according to Boltzmann's equation.

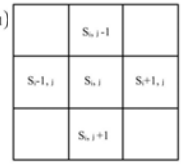
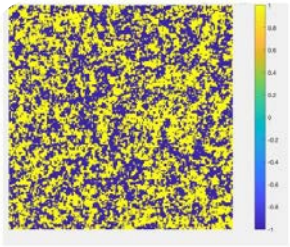



Fig. 6



Boltzmann's constant k=3

Fig. 1

Blue - spin down
Yellow - spin up

Boltzmann's constant k=0.001

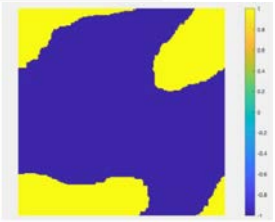


Fig. 2

## Results

We used Matlab program to simulate Monte Carlo Method and ran the system for 10,000 cycles; each cycle a random cell in 200 x 200 matrix was chosen to be flipped or not with a 50% chance. J =1 was used for the strength of interaction and temperature was manipulated with Boltzmann's constant k. Figure 1 had k = 3 which was a maximum temperature and figure 2 at k = 0.001, which is close to the minimum temperature. The phase transition can be clearly seen between two samples.
At lower temperature, the system strongly favors the two ground states, which can be speculated by observing the formation of their domains. Also, one of the domain dominated and flipped surrounding spins. Moreover, we could not observe those domains at high temperature as expected, while we observe random distribution of spin up and down at about 50% rate.

## References

Nicolas Metropolis.The Beginning of the Monte Carlo Method. *Los Alamos Science*, No. 15, Page 125.

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