Ising model

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December 6, 2024

1 2D Ising Model

1.1 Preparation

First off, we need to create a square grid in which each element contains spin of the particle inside that cell. This number is either 1 (up) or -1 (down).

1.2 Flip or Not Flip That Is The Question!

Starting from the initial condition of our system, we have to start sweeping the entire grid and decide if the spin of a cell needs to be flipped or not. In order to do this, first, we need to compare the energy of a cell in interaction with its four neighbors with its energy in a hypothetical configuration where its spin is flipped. Next, a decision needs to be made, ”Is the spin of this cell to be flipped ?”. There are two different possibilities,
(1) E_{flipped} is less than E_{current}, in this case the spin needs to be flipped so that energy goes to the lower state.
(2) E_{flipped} is greater than E_{current}, in this case we turn to Boltzmann factor to decide if our system is going to jump to a more energetic configuration or not. Let me walk you through this process:

Jumping decision Let us define a probability which will save the day! Using Boltzmann factor, we define $P_{\Delta E} = \exp(-\beta \Delta E)$, where $\Delta E = E_{\text{current}} - E_{\text{flipped}}$. Then let us call a random number generator from a uniform distribution to give us a random number between zero and one. If $P_{\Delta E}$ is greater than that random number, the spin is flipped. Otherwise, the spin is left untouched.

1.3 Energy

So far we discussed the idea behind spin flip, now let us shed some light the the format of energy in this system. It is given by the following equation

$$E = -J_1 \sum_{<ij>} s_i s_j - J_2 \sum_{<<ij>>} s_i s_j - J_3 \sum_{<<<ij>>>} s_i s_j \tag{1}$$

where <ij> indicates summation over the closest neighbors, i.e. (i+1, j), (i, j+1), (i+1, j+1), and (i+1, j+1), $<< ij >>$ indications summation over next set of neighbors, and finally $<<< ij >>>$ is summation over those even further from our particle.

1.4 Sweeping The Entire System

The only process left to do is to simply do the 1.2 algorithm for all of the cells in our system. Then doing it over, again and again. Consequently, the system is to reach the lowest energy configuration at that temperature.

2 Testing the program

In this section, we are going to test our code using the physics of the problem. In other words, we want to see if the program can predict behavior of the system correctly or not. (It should be noted that the numbers are considered to be dimension less)

2.1 Low Temperature

In low temperature the system should move to either Magnetization of 1 or -1. First off, let us take $J_1 = -1, J_2 = J_3 = 0$ and see what happens for a 10 by 10 grid.

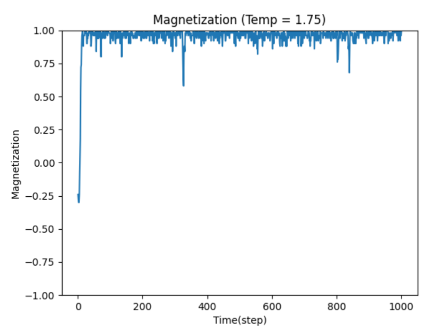


Figure 1: Temperature 1.75, # Particles 100, # Monte Carlo 1

Now, let us see what happens as the number of Monte Carlo increases.

The only considerable change is that the jumping point from around zero to 1 is omitted as doing 10 Monte Carlo in the first step moves the system towards 1 in the same step.

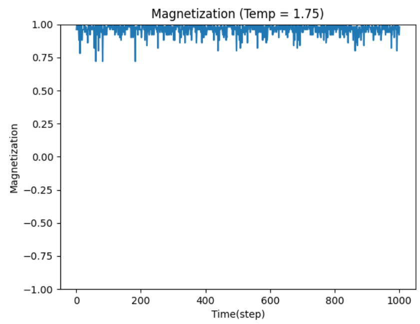


Figure 2: Temperature 1.75, # Particles 100, # Monte Carlo 10

2.1.1 Size of the grid

Increasing the size of grid from 10 to 15 and 20. Other than the size keeping conditions the same as in 2.1, yields

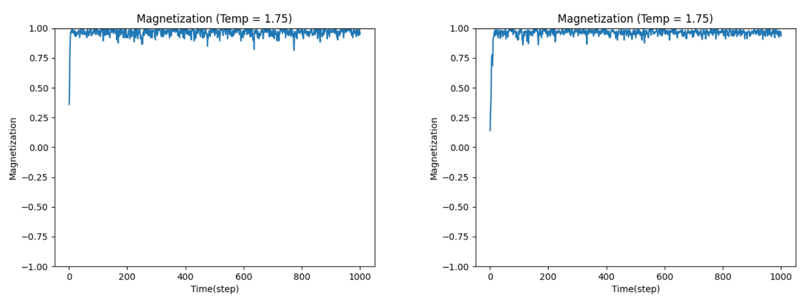


Figure 3: Temperature 1.75, Left: # Particles 225, Right: # Particles 400, # Monte Carlo 1

As it can be seen in the figures, more the number of particles in the system, less the fluctuation of system's magnetization.

Let us compare these three conditions again, this time on the same graph.

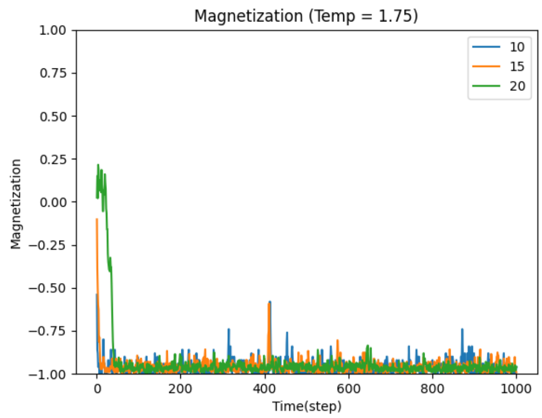


Figure 4: Temperature 1.75, # Particles 100, 225, and 400, # Monte Carlo 1

2.2 High Temperature

On the contrary to low temperature, in case of warmer conditions the system experiences a random behavior, fluctuating around Magnetization of 0.

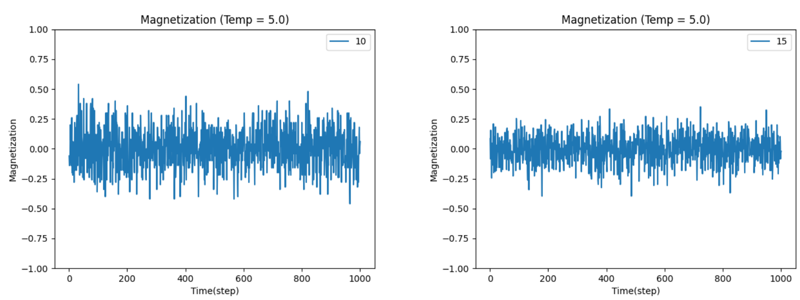
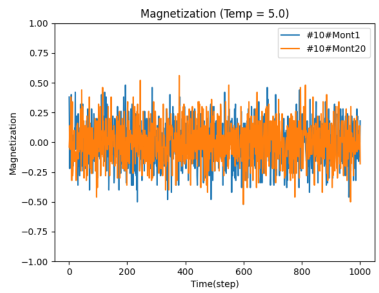


Figure 5: Temperature 5, # Particles Left: 100, Right: 225, # Monte Carlo 1

As expected, magnetization of the system fluctuates around 0. Moreover, increasing size of the grid decreases fluctuation amplitude.

Let us take a look at how increasing the number of Monte Carlos can effect the system.



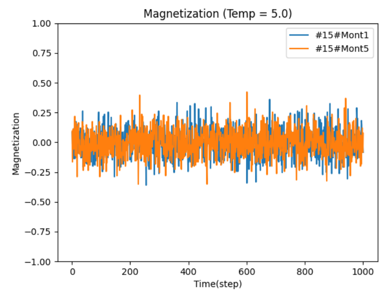


Figure 6: Temperature 5, # Particles Left: 100, Right: 225

It seems not much changes in these cases !

3 Curie Temperature

The Curie temperature (T_C), or Curie point, is the temperature above which certain materials lose their permanent magnetic properties, which can (in most cases) be replaced by induced magnetism. The Curie temperature is named after Pierre Curie, who showed that magnetism is lost at a critical temperature.

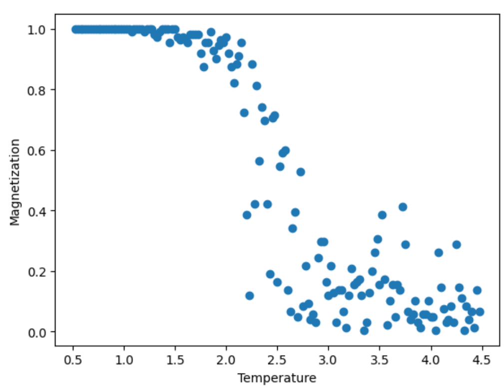


Figure 7: Magnetization Vs Temperature graph for a system with 225 particles. 1000 Monte Carlo was done for each temperature.

Using the data graphed in 3, Curie temperature for this system was

$$T_C \approx 2.225$$

Comparing this number with the exact value from the analytic solution (2.27), it can be deduced that our system works properly. I would argue that the error of the system is due to the number of Monte Carlo done on the system. Probably increasing the number of Monte Carlos will reduce error of the system.

4 Energy

For the sake of visualization, all energies presented in this file are divided by 100.

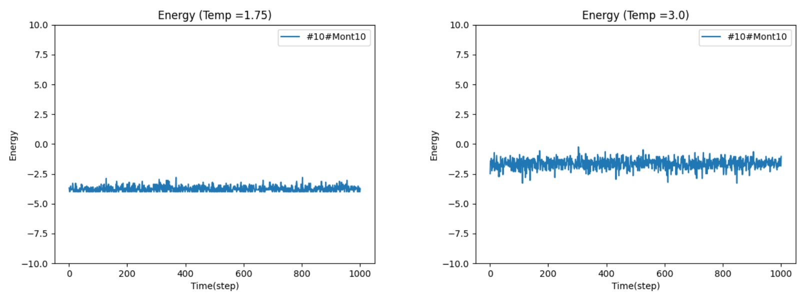


Figure 8: Temperature Left: 1.75, Right: 3.0, # Particles 100

Unlike magnetization fluctuation amplitude in energy increases by increasing the number of particles in the system.

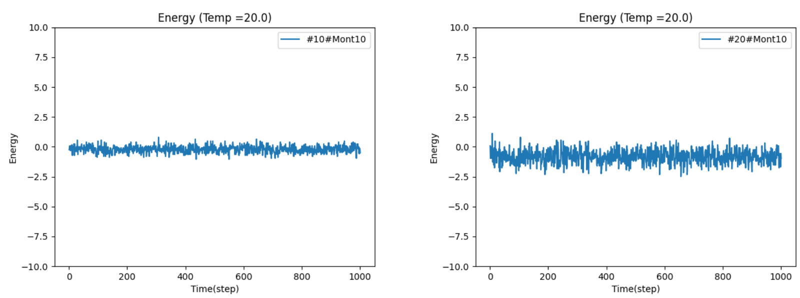


Figure 9: Temperature 20, # Particles Left: 100, Right: 400, # Monte Carlo 10

5 Non zero J_2 and J_3!

So far in our simulations, we took $J_2 = J_3 = 0$. From now on, however, we take J

5.1 Effect of Size of the grid on Magnetization

As before, by increasing the number of particles in the grid, fluctuation amplitude around magnetization of the system decreases.

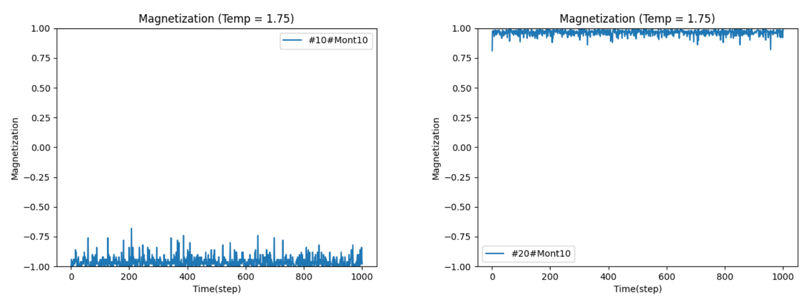


Figure 10: Temperature 1.75, Left: # Particles 100, Right: # Particles 400, # Monte Carlo 10

5.2 Magnetization

As it can be seen in figure 5.2, behavior of system is pretty much similar to the previous configuration. It is interesting to note that for $T = 2.22$, the system jumps between magnetization of 1 and -1.

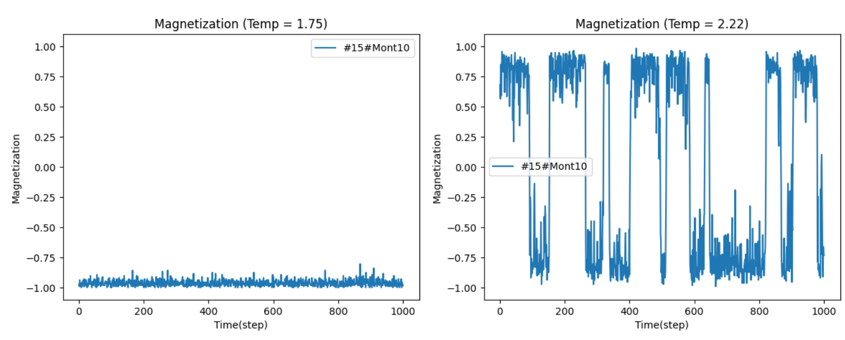


Figure 11: Magnetization graph for a system with 225 particles.

5.3 Curie Temperature

The only substantial change in this graph is that Curie temperature has shifted to right a little bit. Changing our estimated temperature to $T_C \approx 2.25$

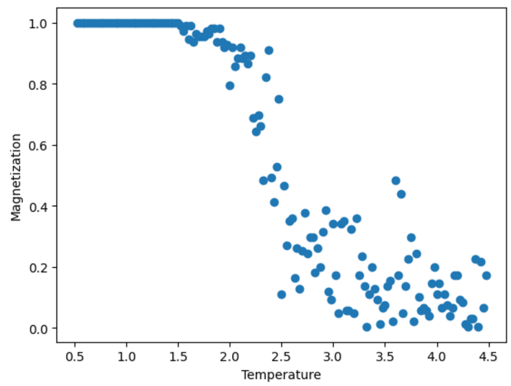


Figure 12: Magnetization Vs Temperature graph for a system with 225 particles. 1000 Monte Carlo was done for each temperature.