Computational Physics Homework Report

Fateme RamezanZade-99100693 Problem Set 8

Ising Model Simulation

1. **Functions Description**

E(arr,J):

This function calculates the total energy of the system (arr) using the formula:

$$E = -J \sum_{<i,j>} s_i s_j$$

It is worth mentioning that we use periodic boundary conditions in this model.

dE(x,a,b,c,d):

This function calculates the change of energy for flipping the spin of x, where a, b, c and d are its neighbor spins. Then returns the value (E+8)/4. This value would later be used as index to determine the Boltzmann factor from its array.

metro_steps(arr,T,N):

This function performs N Monte Carlo steps on a system in temperature T which is represented by the array arr and returns the result. Firstly, the b_factor array is defined which contains five elements, each corresponding to the Boltzmann factor for a specific change in energy. Since there are only five different values of energy change, calculating them once and for all would reduce runtime. Then a loop of N turns starts, each corresponding to a Monte Carlo step, where metropolis algorithm is performed for len(arr)^2 times. This is because we require that each spin gets the chance of flipping in each Monte Carlo step. In the metropolis algorithm, a spin is chosen randomly, and energy change duo to its flip is calculated. If the change is accepted, the spin would be flipped.

2. **Main Code**

2.1

The initial conditions and parameters are assigned and a random 2-D array of 1 or -1 is created with desired size. Then Monte Carlo steps are performed with different temperatures and the resulted array is shown using a colormap for each one.

2.2

Firstly, the parameters of the simulation are assigned. Then an array of different temperatures is created, and a loop begins to run the simulation for each temperature. Now a random 2-D array of 1 or -1 is created with desired size. Then another loop starts to repeat simulation 20 times. In each time, N Monte Carlo steps is performed using metro_steps function and for the resulted array, the energy is calculated using the E function and magnetization is calculated by summing over all the spins (elements of the array). Then the averages of these quantities are stored in the corresponding array with index which relates to the temperature, and the variance of them is used to calculate the heat capacity and magnetic susceptibility using the following formulas:

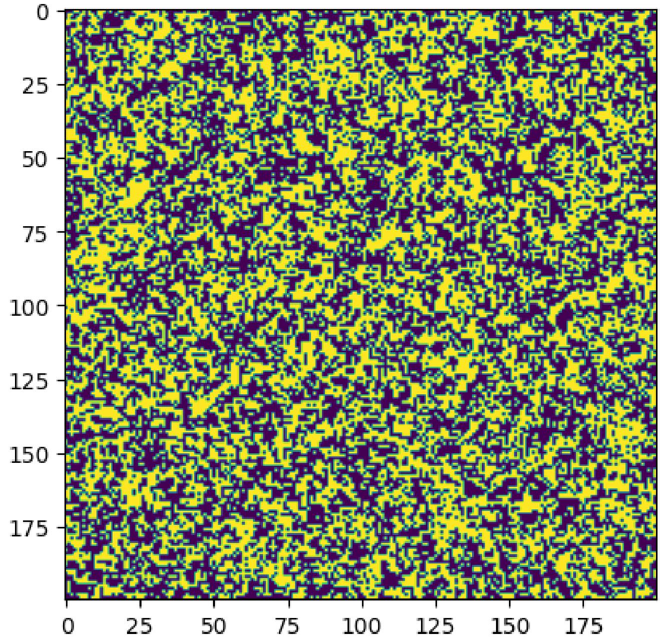
$$C_v = \frac{\sigma_E^2}{T^2} \quad , \quad \chi = \frac{\sigma_m^2}{T}$$

Lastly, each of the previous quantities are plotted vs the inverse of temperature.

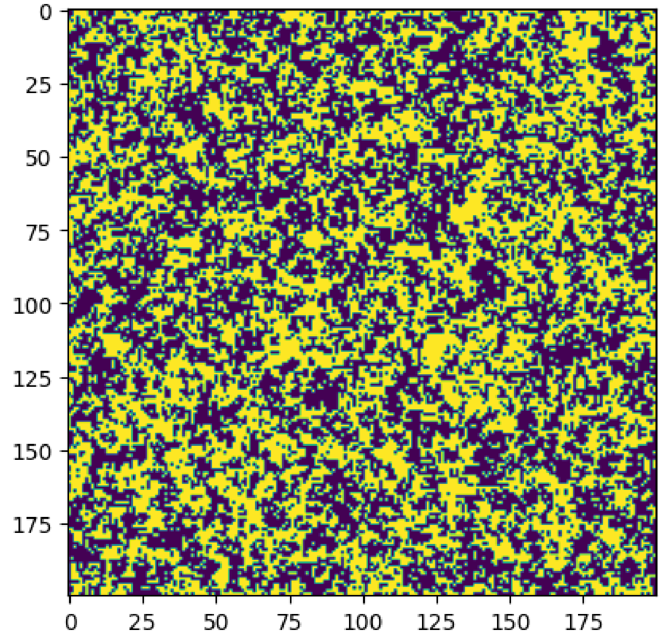
3. Results

3.1:

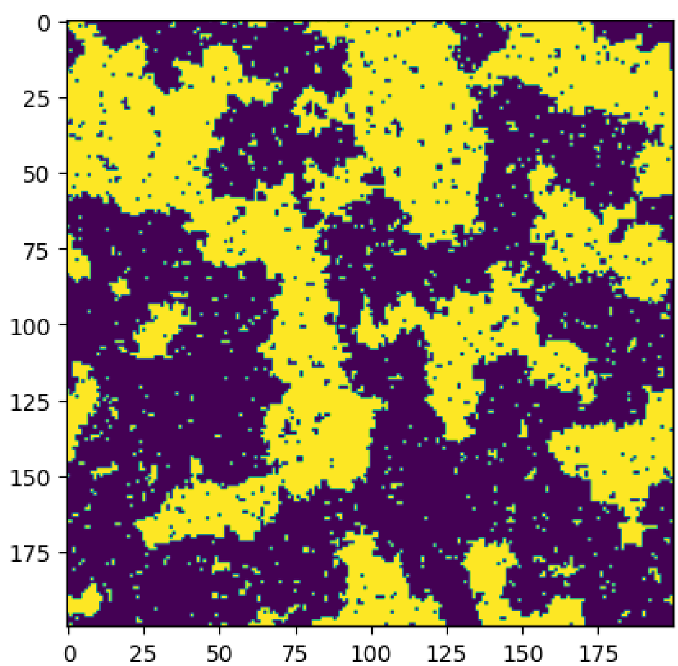
Lattice size(L)=200, Monte Carlo steps number N=50



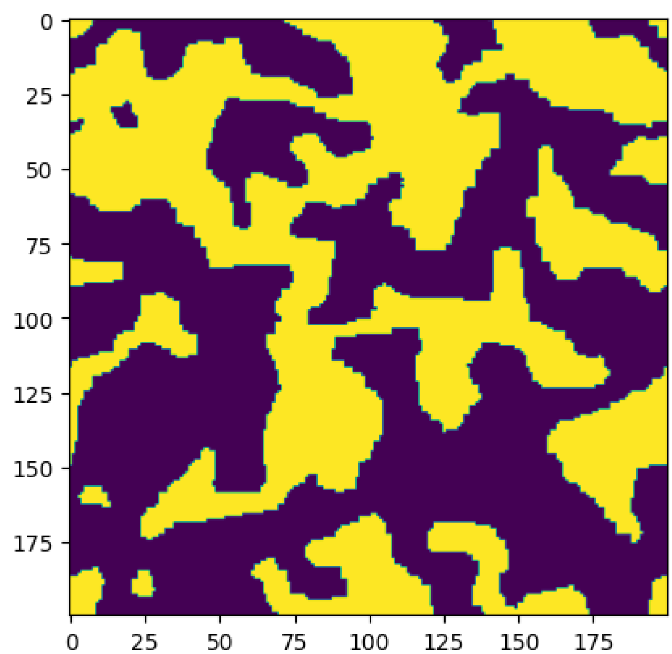
Temperature = 5



Temperature = 3.5



Temperature = 2.5

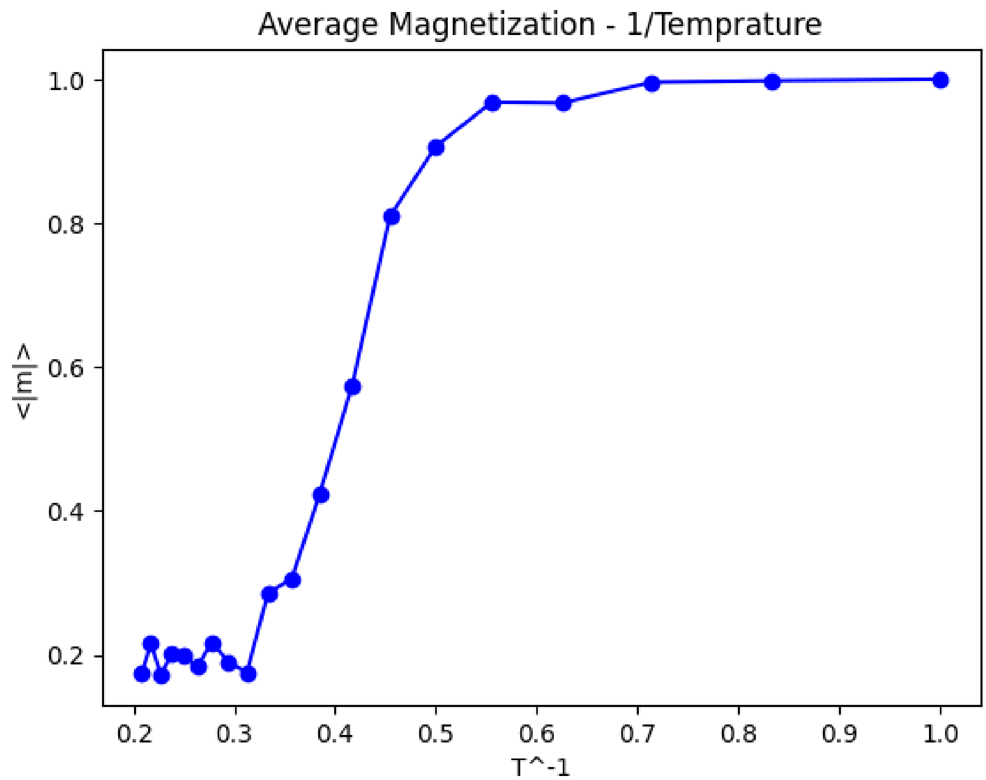


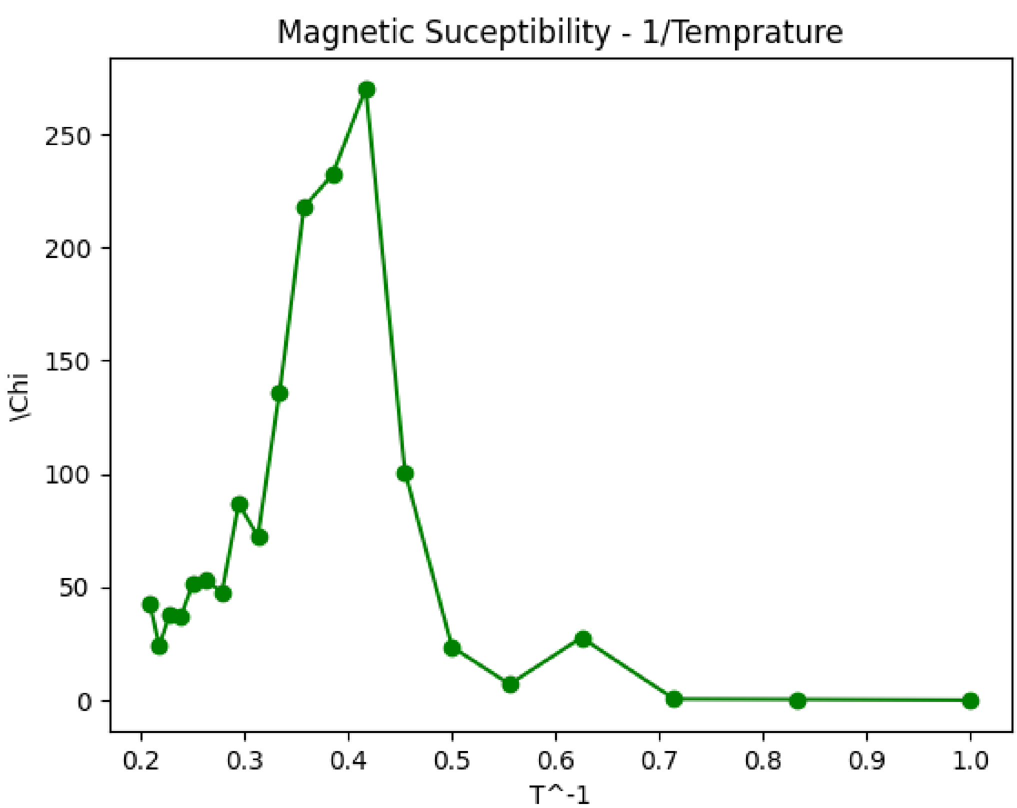
Temperature = 0.5

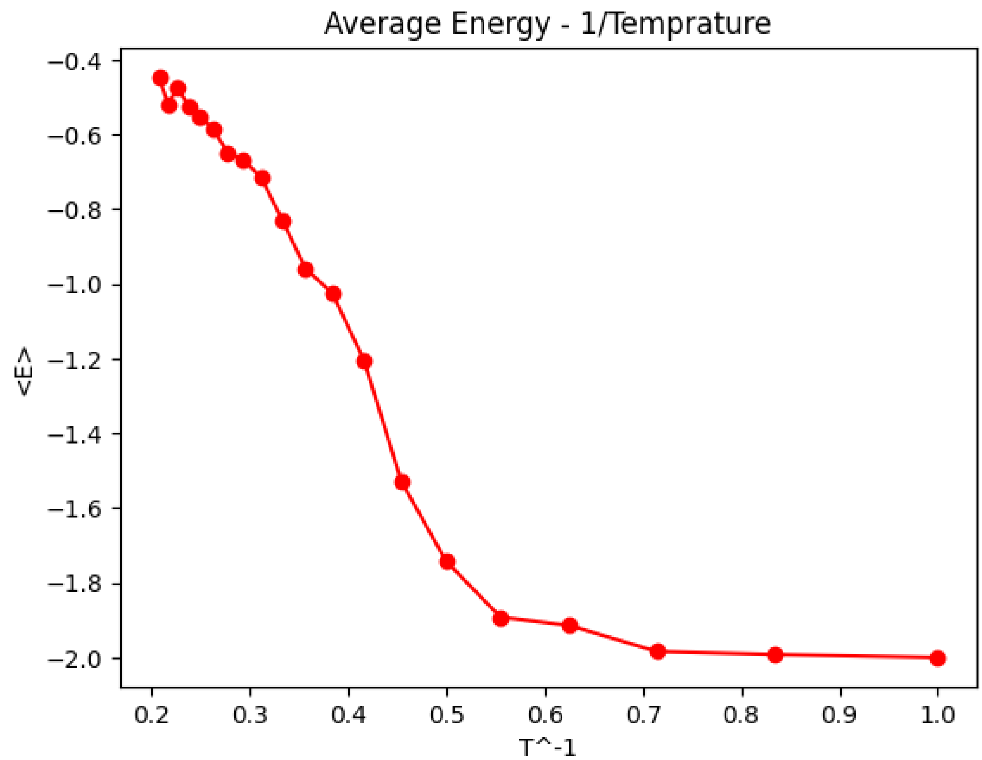
As expected, we can see that in lower temperatures, a phase transition from paramagnetic phase to ferromagnetic phase and more spins tend to have the same direction.

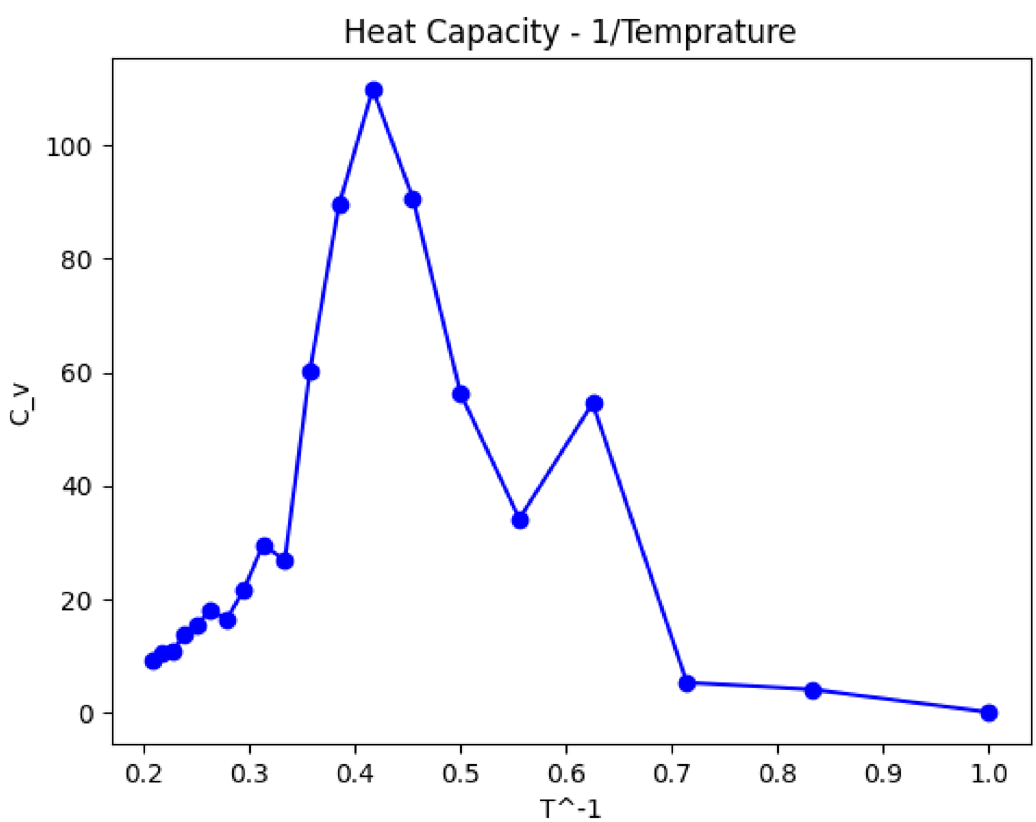
3.2

Lattice size(L)=10, Monte Carlo steps number N=100









Using the graphs, we can conclude that $\frac{1}{T_c} \approx 0.4 \Rightarrow T_c \approx 2.5$

In my calculations I have used units where $\frac{J}{k_b} = 1$. In order to find the physical temperature, we need to convert the units to standard ones.