Computational Physics
Set 5

Ali Ashtari
400100038

April 27, 2024

Introduction

In this report, we are dealing with Ising model. I will solve the 1D and semi-2D Ising model with transfer matrix method. Then I will solve 1D, semi-2D and 2D Ising model using Monte-Carlo simulation.

The general hamiltonian for Ising model is:

$$H = -\sum_{\langle i,j\rangle} J_{ij} S_i S_j - \sum_i h_i S_i \tag{1}$$

In which $\langle i, j\rangle$ denotes nearest neighbours.

Problem 1 : 1D Ising model with transfer matrix method

In this problem, I solve 1D Ising model using transfer matrix method. We assume that J and h are constant and equation (1) will get this form:

$$H = -J\sum_i S_i S_{i+1} - h\sum_i S_i \tag{2}$$

Note that $\sum_i S_i = \frac{1}{2}\sum_i (S_i + S_i + 1)$:

$$H = -J\sum_i S_i S_{i+1} - \frac{1}{2}h\sum_i (S_i + S_i + 1) \tag{3}$$

We first find the partition function by this relation:

$$Z = \sum_{\{S\}} e^{-\beta H(\{S\})} \tag{4}$$

Combining equations (3) and (4), we will get:

$$Z = \sum_{\{S\}}\prod_i e^{\beta J S_i S_{i+1} + \frac{1}{2}\beta h(S_i + S_{i+1})} \tag{5}$$

It is reminder of matrix multiplication, so I define:

$$\langle S_i|T|S_{i+1}\rangle = e^{\beta J S_i S_{i+1} + \frac{1}{2}\beta h(S_i + S_{i+1})} \tag{6}$$

T is denoted as the "transfer matrix". Now by assuming periodic boundary condition, $S_{N+1} = S_1$, the partition functions can be written as:

$$Z = \sum_{\{S\}}\langle S_1|T|S_2\rangle\langle S_2|T|S_3\rangle ... \langle S_N|T|S_1\rangle \tag{7}$$

All of $S_2, S_3, ...$ will become resolution of identity by transferring summation on them inside, and the summation on S_1 will become the trace, so the expression for Z will become:

$$Z = tr(T^N) \tag{8}$$

By diagonalizing T, this simplifies to:

$$Z = \lambda_+^N + \lambda_-^N \tag{9}$$

In which λ_+, λ_- are larger and smaller eigenvalues of T respectively.

For numerical computation, I assume a chain of 60 spins, and periodic boundary condition, and also $\frac{J}{k_B T} = 0.3$ and $\frac{h}{k_B T} = 0.1$. By running the code, we will obtain $Z = 2.83707 \times 10^{19}$ for the partition function.

We have for average spin in i-th site:

$$\langle S_i \rangle = \frac{1}{Z} \sum_{\{S\}} S_i e^{-\beta H(\{S\})} = \frac{1}{Z} tr(T^{i-1} \sigma_z T^{N-i+1}) \tag{10}$$

In which σ_z is Pauli spin matrix of z-direction. Again by diagonalizing T and writing equation (10) in that basis, we will obtain:

$$\langle S_i \rangle = \frac{1}{Z} (\lambda_+^N \langle + | \sigma_z | + \rangle + \lambda_-^N \langle - | \sigma_z | - \rangle) \tag{11}$$

In which $|+\rangle, |-\rangle$ are eigenstates of T.

Average magnetization density is exactly this quantity, and its numerical value I obtain is $m = 0.17955$.

Now for the spin-spin correlation function, we can write:

$$\langle S_i S_j \rangle = \frac{1}{Z} tr(T^{i-1} \sigma_z T^{j-i} \sigma_z T^{N-j+1}) \tag{12}$$

Again writing the correlation function in the basis that diagonalizes the transfer matrix T, we will obtain:

$$\langle S_i S_j \rangle = \frac{1}{Z} (\lambda_+^N \langle + | \sigma_z T^{j-i} \sigma_z | + \rangle + \lambda_-^N \langle - | \sigma_z T^{j-i} \sigma_z | - \rangle) \tag{13}$$

As is observed from equation (13), the spin-spin correlation function is a function of distance j-i. The spin-spin correlation function is plotted in Figure 1. Its symmetry about j-i=30 is a consequence of periodic boundary condition; the chain is repeated before and after itself.

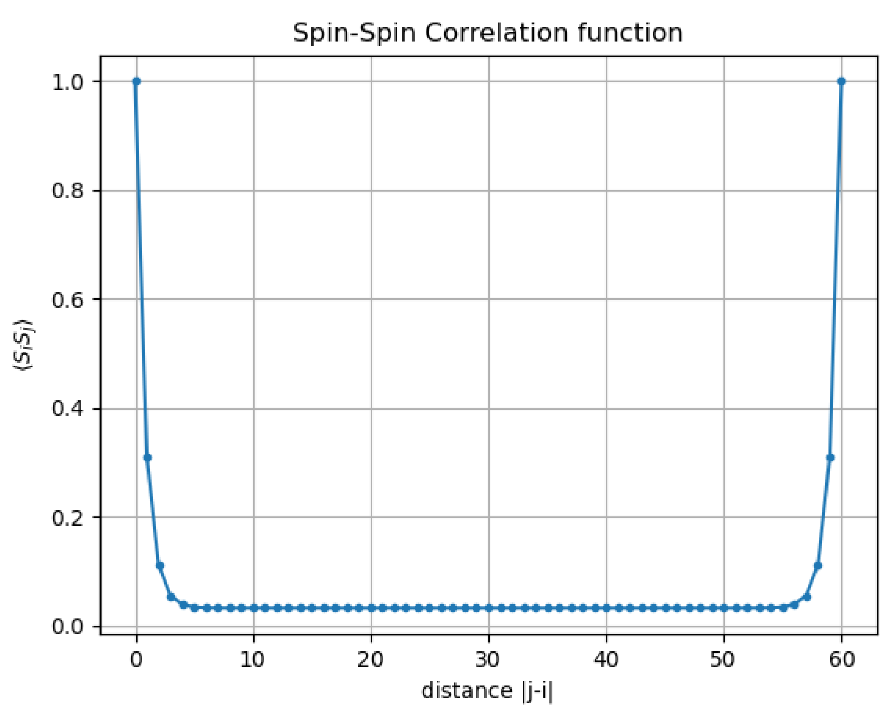

Figure 1: Spin-Spin correlation function for 1D Ising model using transfer matrix method

Problem 2 : 1D Ising model with Monte-Carlo method

In this problem, we are dealing with the same problem as problem one, except that now I use Monte-Carlo simulation and Metropolis algorithm to do obtain magnetization and spin-spin correlation function.

The Metropolis algorithm is simple; we will perform several Markov chains, each time with a random initial point. Then performing the chain and in each step, calculating ΔE; if the value $\exp(-\frac{\Delta E}{k_B T})$ was greater than rand(0, 1), then the spin in that site will be flipped; else, it won't be flipped.

Magnetization density can be evaluated by $\langle S_i \rangle_i$ (subscript i indicates averaging with respect to i) . By using Metropolis algorithm, the value obtained for magnetization is $m = 0.17456$. Relative error with respect to the value obtained by transfer matrix (exact answer) is about 2.8%, quite close!

The spin-spin correlation function can be evaluated by $\langle S_i S_{i+j} \rangle_i$, because correlation function is just function of distance. The obtained spin-spin correlation function by Monte-Carlo simulation is shown in Figure 2.

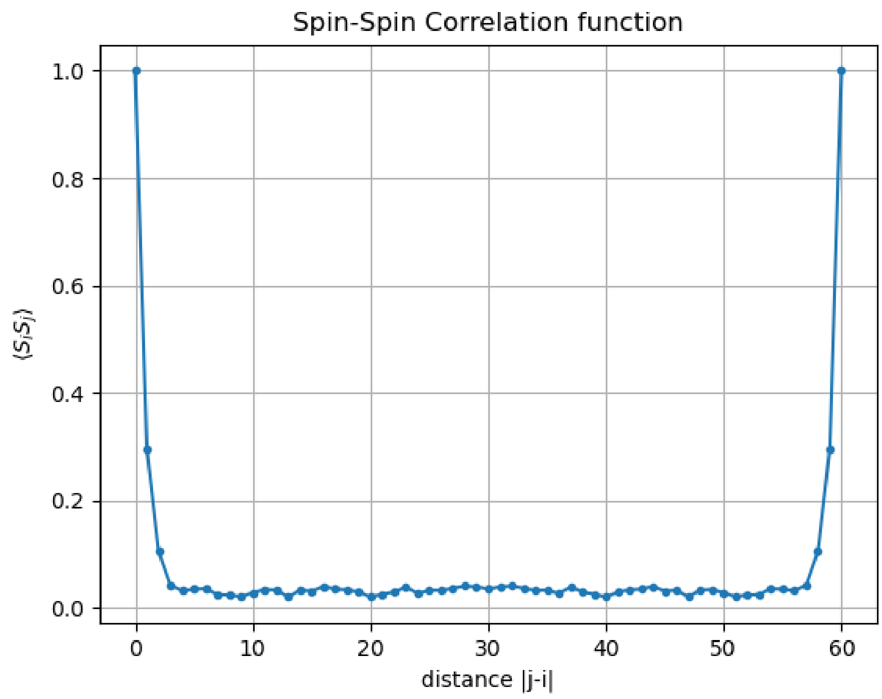

Figure 2: Spin-Spin correlation function for 1D Ising model using Monte-Carlo method

Problem 3 : semi-2D Ising model transfer matrix method

This problem is generalization of the problem 1, but with 4 chains coupled with each other. Numerical values are $\frac{J}{k_B T} = 0.3$ and $\frac{h}{k_B T} = 0.1$. Note that the hamiltonian is:

$$-\beta H = \sum_{i=1}^{N} f_{i,i+1} \tag{14}$$

$$f_{i,i+1} = \beta J \sum_{j=1}^{M} \left[S_{j,i} S_{j,i+1} + \frac{1}{2}(S_{j,i} S_{j+1,i} + S_{j,i+1} S_{j+1,i+1}) \right] + \frac{\beta h}{2} \sum_{j=1}^{M} [S_{j,i} + S_{j,i+1}] \tag{15}$$

So the partition function can be written as:

$$Z = \sum_{\{\mu\}} \langle \mu_1 | T | \mu_2 \rangle \langle \mu_2 | T | \mu_3 \rangle ... \langle \mu_N | T | \mu_1 \rangle \tag{16}$$

In which $|\mu_i\rangle = |S_{1,i}, S_{2,i}, S_{3,i}, S_{4,i}\rangle$. So the transfer matrix is $2^4 \times 2^4$. Now we can use equations (8) to (13), but we should note that we have to sum over all eigenvalues in equations (9), (11), (13). Also note that for correlation function and magnetization, instead of inserting σ_z, we have to insert each of this:

$$S_z^{(1)} = diag([1,1,1,1,1,1,1,1,-1,-1,-1,-1,-1,-1,-1,-1])$$

$$S_z^{(2)} = diag([1,1,1,1,-1,-1,-1,-1,1,1,1,1,-1,-1,-1,-1])$$

$$S_z^{(3)} = diag([1,1,-1,-1,1,1,-1,-1,1,1,-1,-1,1,1,-1,-1])$$

$$S_z^{(4)} = diag([1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1,1,-1])$$

By running the code, the resulting partition function would be $Z = 6.11029 \times 10^{85}$. (It is a very large number, but this is the partition function for a 4×60 spin system!)

The average magnetization density by using modified version of equation (10) would be $m = 0.51459$. But also we could use:

$$m = \frac{1}{MN} \frac{\partial \ln(Z)}{\partial \beta h} \tag{17}$$

By using equation (17), the answer would be $m = 0.51476$. Very close to the answer be taking the trace!

The spin-spin correlation function for this system is shown in two ways, first by a heat-map in Figure 3, and then by a 3D plot in Figure 4. Note the exponential decrease of correlation function and also its symmetry about its center because of periodic boundary condition; just like its 1D counterpart.

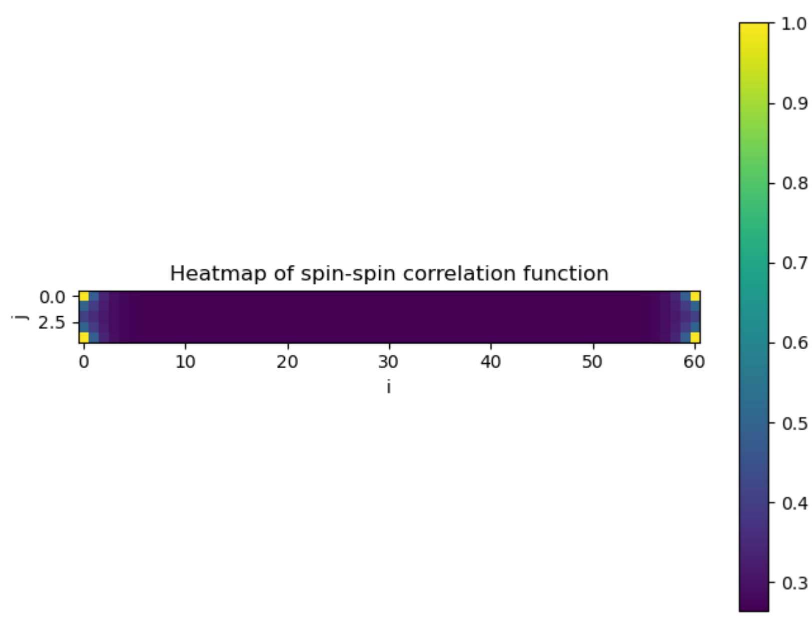

Figure 3: Heat-map of Spin-Spin correlation function for semi-2D Ising model using transfer matrix method

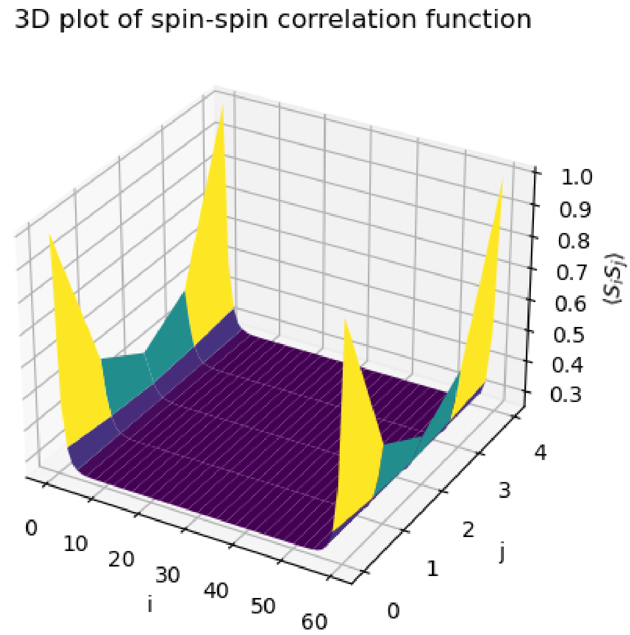

Figure 4: 3D plot of Spin-Spin correlation function for semi-2D Ising model using transfer matrix method

Problem 4 : semi-2D Ising model with Monte-Carlo method

In this problem we are dealing with the same spin system as problem 3, but with Monte-Carlo algorithm. I use Metropolis algorithm I've explained in problem 2, and also instead of using different Markov chains, I use one chain with random points in each step, but averaging the system when it reaches equilibrium. In Figures 5 and 6, energy and magnetization are plotted against time steps.

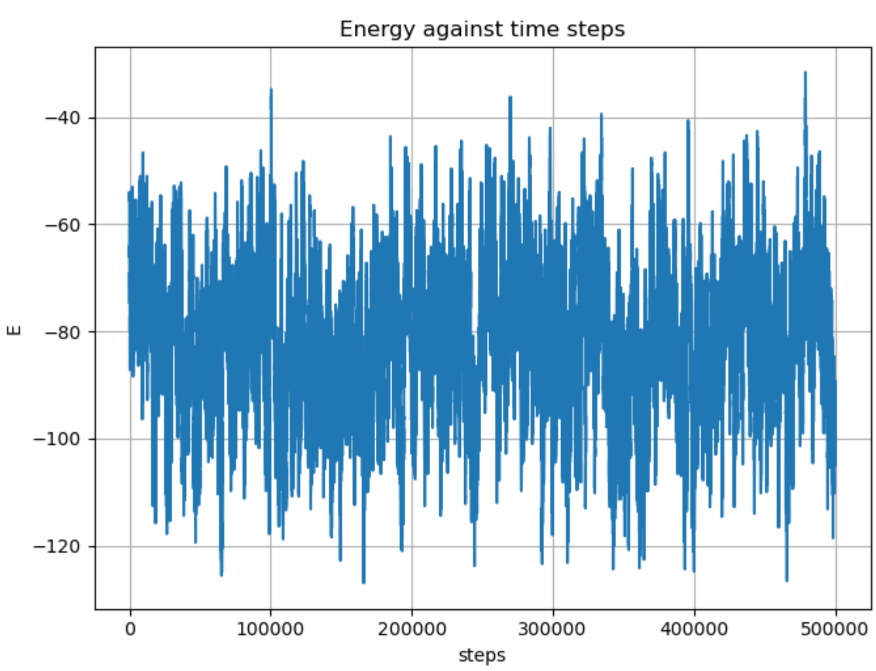

Figure 5: Energy against time steps for semi-2D Ising model by Monte-Carlo algorithm

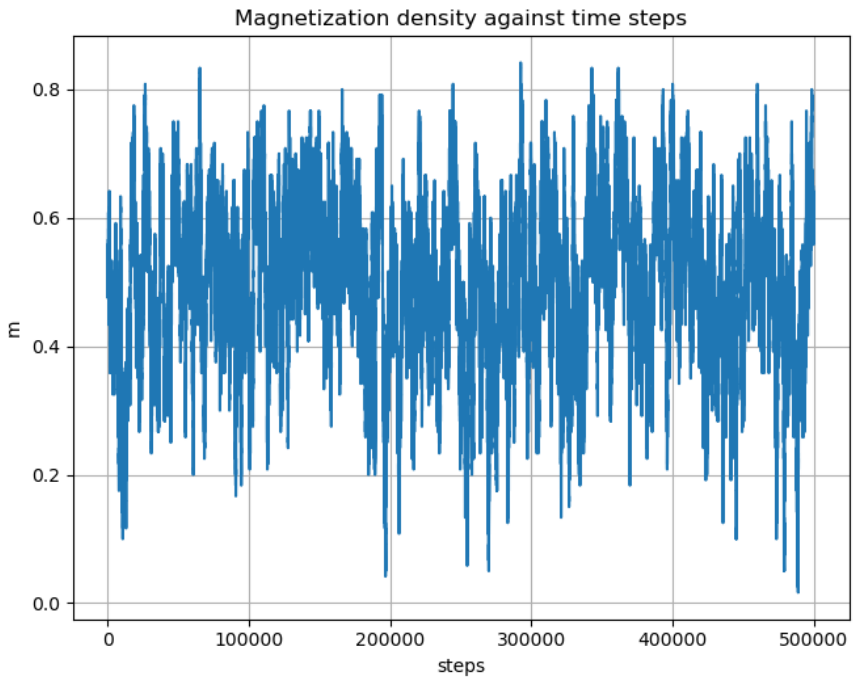

Figure 6: Magnetization density against time steps for semi-2D Ising model by Monte-Carlo algorithm

I've taken the averages in the tails of the plots, I mean, the last $\frac{1}{10}$ iterations, and considered the system had reached the equilibrium by then. The magnetization I've obtained by Monte-Carlo simulation is $m = 0.49778$. The relative error to transfer matrix method (the exact answer) is 3.3%, it's really close!

The spin-spin correlation function is can be evaluated by $\langle S_{k,l} S_{k+i,l+j} \rangle_{k,l}$; in which subscript "k, l" means averaging with respect to these indices and the final answer is only function of i and j. In Figure 7, the heat-map of spin-spin correlation function is shown, and in Figure 8 th 3D plot of it is shown. They are similar to their counterparts in problem 3.

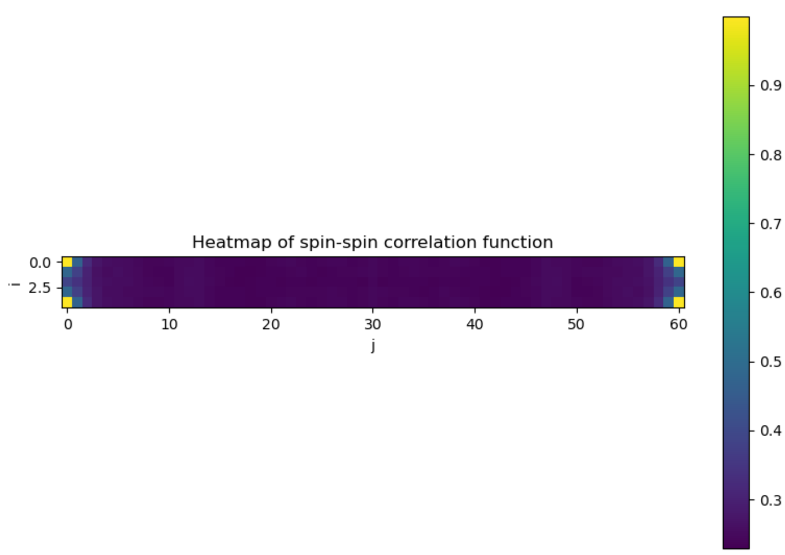

Figure 7: Heat-map of Spin-Spin correlation function for semi-2D Ising model using Monte-Carlo method

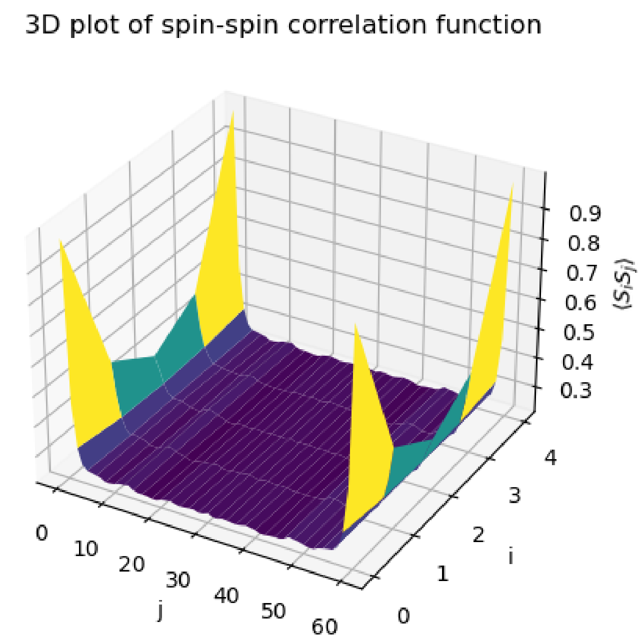

Figure 8: 3D plot of Spin-Spin correlation function for semi-2D Ising model using Monte-Carlo method

Problem 5 : 2D Ising model with Monte-Carlo method

In this problem, we are dealing with 20×20 lattice of spins and I use Monte-Carlo simulation to deal with it. First by considering $\frac{J}{k_B T} = 0.3$ and $\frac{h}{k_B T} = 0.0$, I've plot the energy and magnetization density against time steps in Figures 9 and 10 respectively.

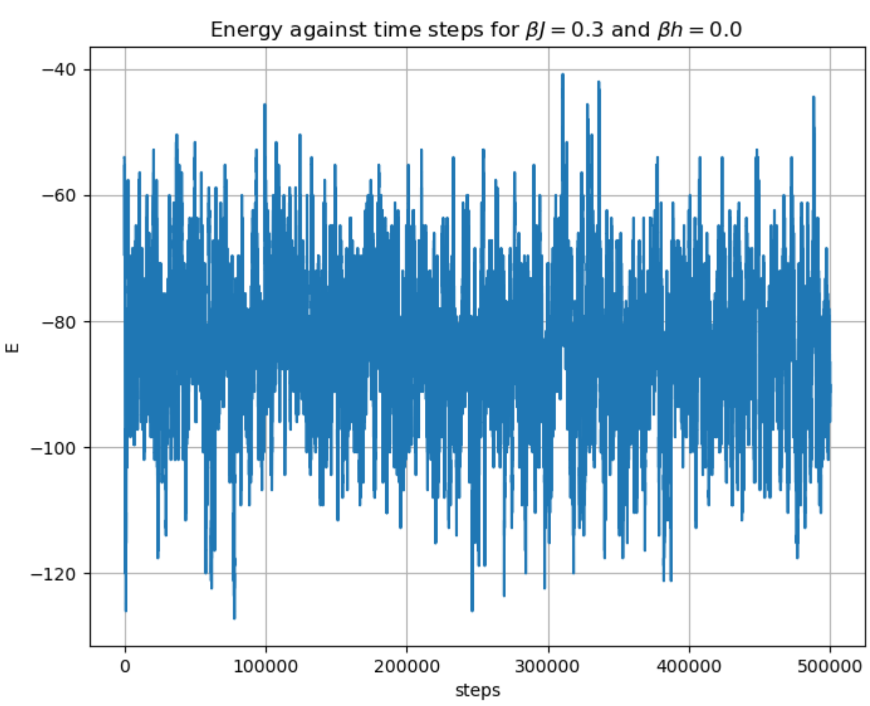

Figure 9: Energy against time steps for 2D Ising model by Monte-Carlo algorithm

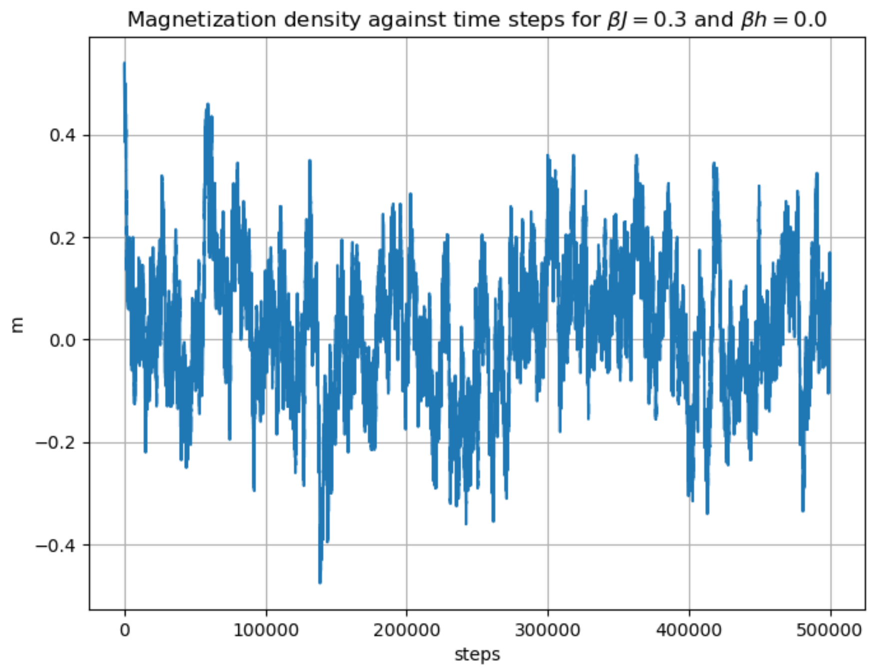

Figure 10: Magnetization density against time steps for 2D Ising model by Monte-Carlo algorithm

For this values of $\beta J, \beta h$, the spin-spin correlation function is shown in two ways, first by a heat-map in Figure 11, then by a 3D plot in Figure 12. Again, there is an exponential decrease in each $\frac{1}{4}$ of the plane, and also note the symmetry around the center; this is because of periodic boundary condition.

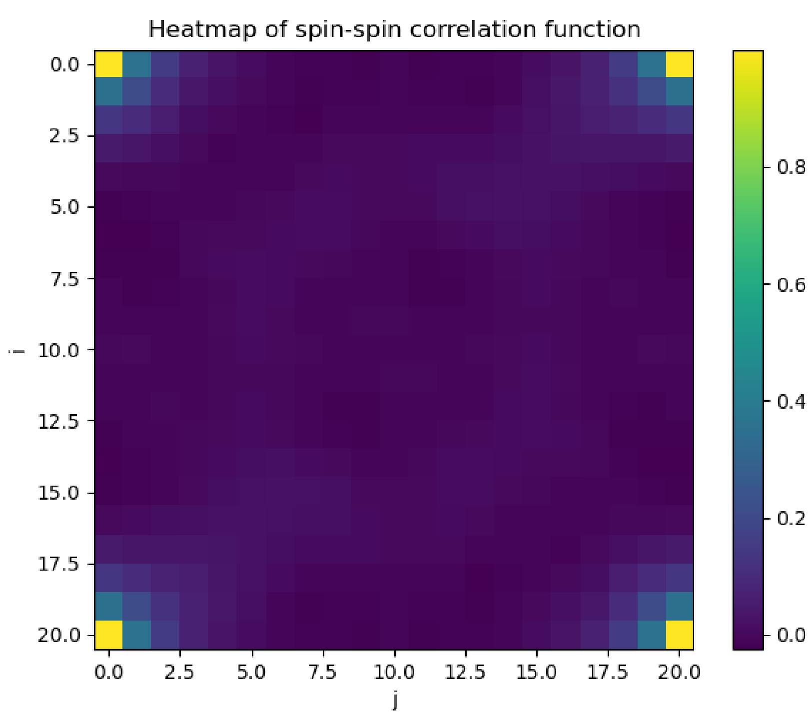

Figure 11: Heat-map of Spin-Spin correlation function for 2D Ising model using Monte-Carlo method

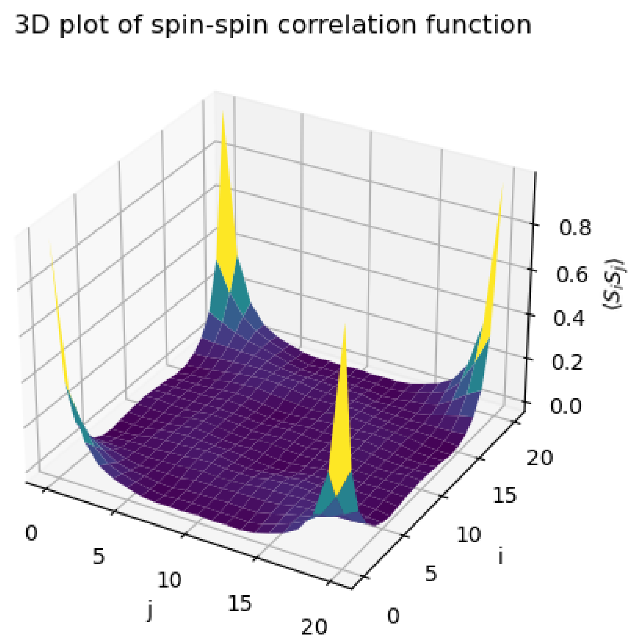

Figure 12: 3D plot of Spin-Spin correlation function for 2D Ising model using Monte-Carlo method

Now, we want to evaluate the transition temperature; we know that 2D Ising model exhibits the phase transition from ferro-magnet to para-magnet in T_c. Considering no external magnetic field (h=0), I've plot the magnetization density against inverse temperature J/k_BT in Figure 13. For high temperature ($J/k_BT \to 0$) magnetization would be zero due to thermal fluctuations. In low temperature ($J/k_BT \to \infty$), magnetization density would be 1 (all of spins align in the same direction). But there in between, the phase transition occurs. By using Monte-Carlo simulation, thereby Figure 13, the transition temperature would be obtained

$$\frac{J}{k_B T_c} = 0.42253$$

Onsager had solved 2D Ising model analytically and predicted that the transition temperature would be *:

$$\frac{J}{k_B T_c} = \frac{\ln(1+\sqrt{2})}{2} = 0.44069 \ \textit{(exact answer)}$$

The relative error is 4.1%, close enough!

Stephen J. Blundell, Katherine M. Blundell - Concepts in Thermal Physics-Oxford University Press (2009), Chapter 28, Figure 28.17

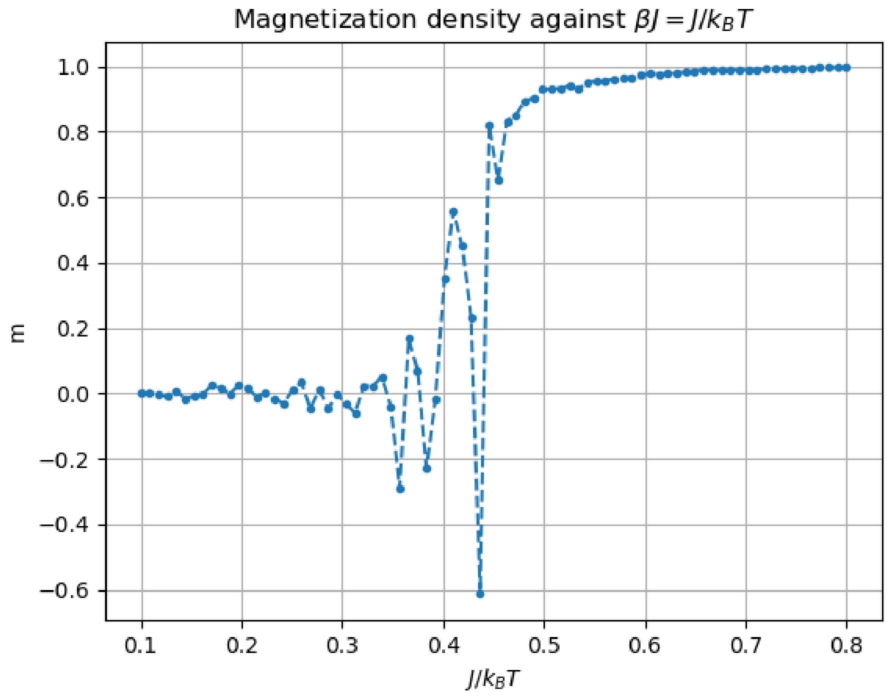

Figure 13: Magnetization density "m" against inverse temperature "$\frac{J}{k_B T}$" for 2D Ising model using Monte-Carlo method