Amirreza Vedadiyan Homework 5 April 27, 2024

Theory

Introduction

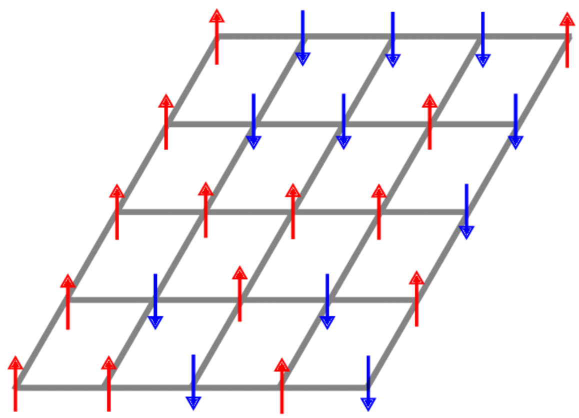
In this assignment, we embark on a journey into the realm of statistical mechanics, delving into the elegant and versatile Ising model. The Ising model stands as a cornerstone in the study of phase transitions and collective phenomena, offering profound insights into the behavior of magnetic systems, among other applications. Through this exploration, we aim to grasp not only the fundamental principles underlying the Ising model but also the methodologies employed in both exact analytical solutions and Monte Carlo simulations to elucidate its intricate dynamics.
Our exploration unfolds in two distinct but complementary dimensions: exact solutions and Monte Carlo simulations. We begin by unraveling the mathematical elegance of exact solutions, employing techniques such as transfer matrices and recursion relations to derive analytical expressions for thermodynamic observables. These exact methods provide invaluable insights into the behavior of the Ising model under various conditions, serving as a benchmark against which the efficacy of numerical approaches is measured.

In parallel, we delve into the realm of Monte Carlo simulations, harnessing the power of probabilistic algorithms to explore the phase space of the Ising model. Through techniques like the Metropolis algorithm, we navigate the vast configuration space of spins, sampling statistically significant ensembles to glean insights into thermodynamic properties and phase transitions. Monte Carlo simulations offer a versatile and computationally efficient tool for investigating complex systems, providing a bridge between theoretical predictions and experimental observations.

By embarking on this journey into the Ising model, we aim not only to deepen our understanding of statistical mechanics but also to cultivate essential skills in mathematical modeling, computational techniques, and critical analysis. Through a synthesis of theory and practice, we endeavor to unravel the mysteries of magnetic materials and pave the way for future explorations in condensed matter physics and beyond.

Ising Model

The Ising model , is a mathematical model of ferromagnetism in statistical mechanics. The model consists of discrete variables that represent magnetic dipole moments of atomic "spins" that can be in one of two states (+1 or -1). The spins are arranged in a graph, usually a lattice (where the local structure repeats periodically in all directions), allowing each spin to interact with its neighbors. Neighboring spins that agree have a lower energy than those that disagree; the system tends to the lowest energy but heat disturbs this tendency, thus creating the possibility of different structural phases. The model allows the identification of phase transitions as a simplified model of reality. The two-dimensional square-lattice Ising model is one of the simplest statistical models to show a phase transition.



In the Ising model, the Hamiltonian includes two types of interactions:
1-the external field term. As we remember from quantum mechanics, an external magnetic field h can split the energies of the spin-down and spin-up state, so that one is higher in energy and the other is lower.
2-the interaction term between neighboring spins – maybe they want to align with each other and point the same way, maybe they want to anti-align and point in different ways. Physically, we can imagine that this interaction arises because each spin in the magnet is its own mini magnetic dipole that sets up its own magnetic field, and its neighbors can feel that magnetic field.
So the Hamiltonian of the Ising Model can be written as :

$$H = -J \sum_{<i,j>} \sigma_i \sigma_j - H \sum_j \sigma_j$$

where the first term is the energy of each of the bonds between neighboring sites, and the second is the energy of each of the sites. Since we want to rewrite the Hamiltonian as a sum over bonds, we re-assign the energy of j'th site to its two neighboring bonds (bond j-1 to j, and j to j+1).(We also introduce a factor one-half to compensate for the fact that each site will now be counted twice). Now the Hamiltonian is sum over bonds :

$$H = \sum_j E(\sigma_j, \sigma_{j+1})$$

Where :

$$E(\sigma_j, \sigma_{j+1}) = -J\sigma_j\sigma_{j+1}\frac{H}{2}(\sigma_j + \sigma_{j+1})$$

is the energy of the bond between sites j and j+1.

Transfer Matrix

Now we know what is our Hamiltonian and our goal is find the partition function , magnetization and correlation function. We know the partition function is :

$$Z = \sum_{\{\sigma\}} e^{-\beta E_\sigma}$$

where the sum is over all possible states, but finding all possible state is too slow so because of that we use transfer matrix based on our problem and then use below formulas to find :

$$Z = Tr[T^n]$$

$$< \sigma_j >= Z^{-1}Tr[T^{j-1}S_zT^{N-j+1}]$$

$$< \sigma_i\sigma_j >= Z^{-1}Tr[T^{i-1}S_zT^{j-i}T^{N-j+1}]$$

Monte-carlo Simulation

We have learned about metropolis algorithm in the previous homework's so we can simply use it here and following the steps :

1. Start with a random configuration
2. Apply periodic boundary conditions to the system so that all the spins have the same environment. Periodic images are obtained by translating the system by assing multiples of n.

3. Start from first spin and change the spin of it.
4. Compute the change in the value of the Hamiltonian by using :

$$\Delta E = -2J \sum_{<i,j>} S_i S_j - 2HS_i$$

5. Determine wheter to accept or reject the move according to the following rules:
    - if $\Delta E \leq 0$ accept the move.
    - if $\Delta E > 0$ pick a random number r between 0 and 1
        - if $r \leq e^{-\beta \Delta E}$, accept the move.
        - else reject the move.
6. Calculate the magnetization and correlation function
7. Repeat all the steps.

Problem 1:

Determining Thermodynamic Properties for a 1D Lattice

In this problem, we undertake the task of elucidating key thermodynamic properties of a one-dimensional lattice consisting of 60 sites. The Ising model offers a powerful framework for understanding the collective behavior of magnetic moments in such systems, enabling us to compute essential quantities such as the partition function, magnetization, and correlation function.

The cornerstone of our approach lies in the utilization of the transfer matrix method, a powerful technique that allows us to systematically analyze the behavior of the Ising model. Specifically, we construct the transfer matrix for our 1D lattice, encapsulating the energetics of spin configurations and their interactions. The transfer matrix, denoted by T, takes the form of a 2×2 matrix, where each element represents the transition probability between two spin states. For a given pair of spins with values (σ_i, σ_{i+1}), the matrix elements are determined by the Boltzmann factor, incorporating the energy associated with the spin configuration. Thus, we express T as:

$$T = \begin{pmatrix} e^{-\beta E(+1,+1)} & e^{-\beta E(+1,-1)} \\ e^{-\beta E(-1,+1)} & e^{-\beta E(-1,-1)} \end{pmatrix} = \begin{pmatrix} e^{\frac{-J-H}{kT}} & e^{\frac{J}{kT}} \\ e^{\frac{J}{kT}} & e^{\frac{-J+H}{kT}} \end{pmatrix}$$

Here, $\beta = \frac{1}{kT}$ represents the inverse temperature, J denotes the coupling constant characterizing spin-spin interactions, H signifies the applied magnetic field, and k stands for the Boltzmann constant. The elements of the spin operator matrix S are defined to account for the possible orientations of individual spins within the lattice:

$$S = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

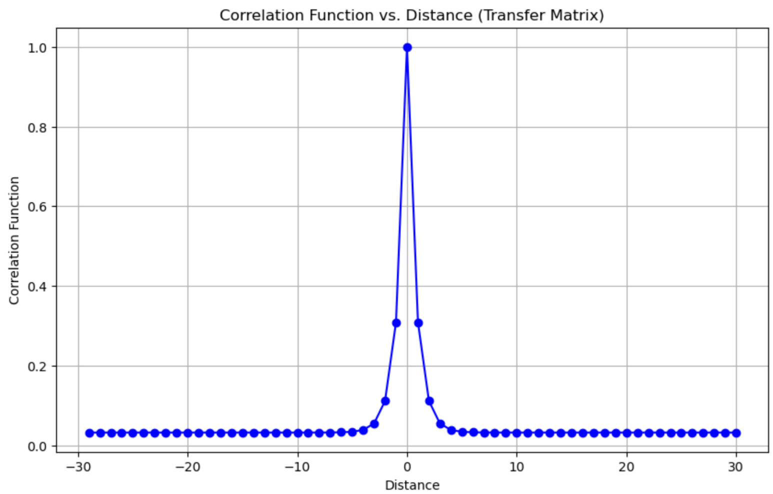
With these foundational components established, we are poised to embark on the journey of computing the partition function, magnetization, and correlation function for our 1D lattice. Through the application of rigorous mathematical techniques and physical insight, we aim to unravel the intricate thermodynamic properties inherent in the Ising model, shedding light on the behavior of magnetic systems at the microscopic level.

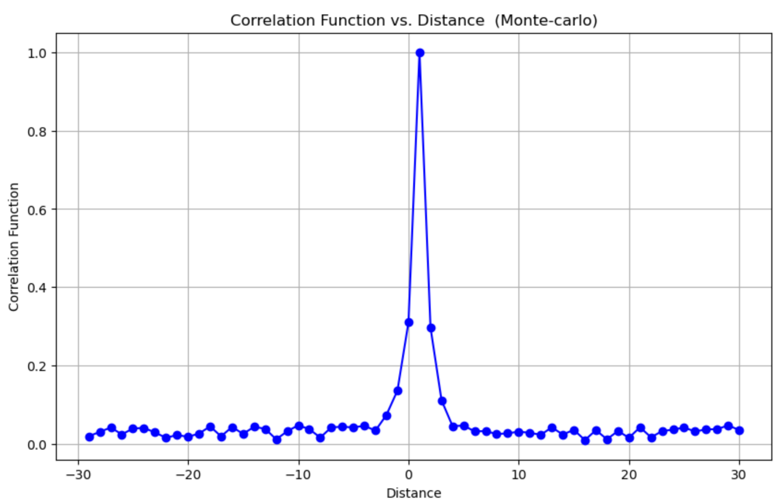
Result

The result with exact solution (Transfer Matrix Method) and monte-carlo simulation method is match and are given by :

Parameter	Value
Z	2.8×10^{19}
m	0.17955

The correlation function between middle spin (number 30) and all other spins are :





Problem 2 :

In this problem we want to solve a Ladder with four coupled Ising spin chains using Transfer matrix and monte-carlo simulation .
We consider now four coupled Ising spin chains (1,2,3 and 4). The intrachain interactions and the interchain (between the 1-st. and 2-nd chains and the 3-rd and 4-th chains) interactions are taken as in Theory section. The Hamiltonian is given by:

$$H = -J(S_{1,i}S_{1,i+1} + S_{2,i}S_{2,i+1} + S_{3,i}S_{3,i+1} + S_{4,i}S_{4,i+1}) -$$
$$\frac{J}{2}(S_{1,i}S_{2,i} + S_{2,i}S_{3,i} + S_{3,i}S_{4,i} + S_{1,i+1}S_{2,i+1} + S_{2,i+1}S_{3,i+1} + S_{3,i+1}S_{4,i+1}) -$$
$$\frac{H}{2}(S_{1,i} + S_{2,i} + S_{3,i} + S_{4,i} + S_{1,i+1} + S_{2,i+1} + S_{3,i+1} + S_{4,i+1})$$

The partition function can be written in a similar way :

$$Z = \sum_{S_{,i\pm1},S_{2,i\pm1},S_{3,i\pm1},S_{4,i\pm1}} exp(-\beta H) = Tr(T^N)$$

where T is now the $2^4 \times 2^4$- transfer matrix. To construct the transfer matrix we have to generate all possible states for $S_{i,j\mp1}$. To do that we generate numbers between 0 and $2^n - 1$ and go to the base 2 and consider 0's as up and 1's as down for $S_{1,i}, S_{1,i+1}, \ldots S_{4,i+1}$ so we will have :

$$0 = 00000000- > T(1,1)$$
$$1 = 00000001- > T(1,2)$$
$$2 = 00000010- > T(1,3)$$
$$3 = 00000011- > T(1,4)$$
$$\ldots$$

So we can have all possible states.
In this method we used here there is a difference between this problem and problem number 1 and It's the S operators because in the way we construct our transfer matrix we will have 4 S instead on 1 as:

$$S_1 = np.diag([1, 1, 1, 1, 1, 1, 1, 1, -1, -1, -1, -1, -1, -1, -1, -1])$$
$$S_2 = np.diag([1, 1, 1, 1, -1, -1, -1, -1, 1, 1, 1, 1, -1, -1, -1, -1])$$
$$S_3 = np.diag([1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1])$$
$$S_4 = np.diag([1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1])$$

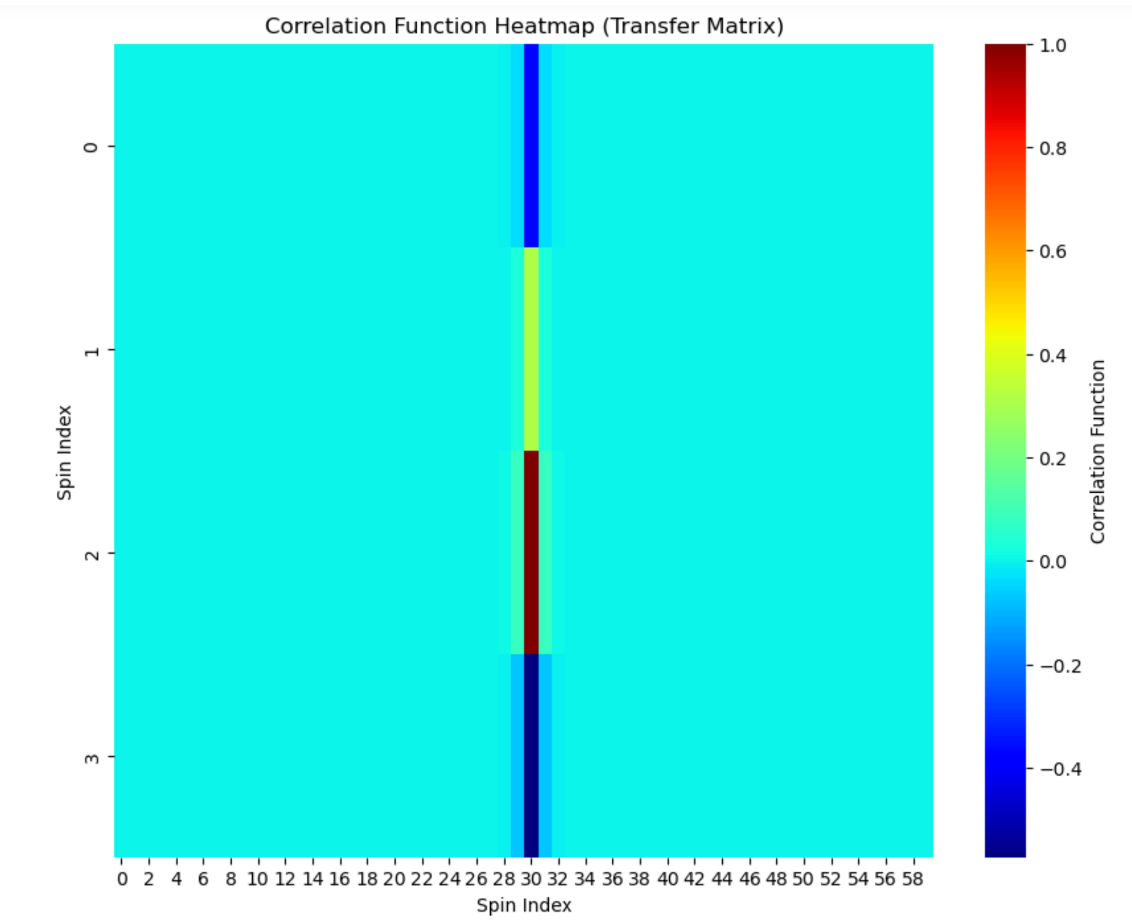
because in our method the sign of S_1 changes after 8 time, the sign of S_2 changes after 4 times S_3 after 2 times and S_4 every step.

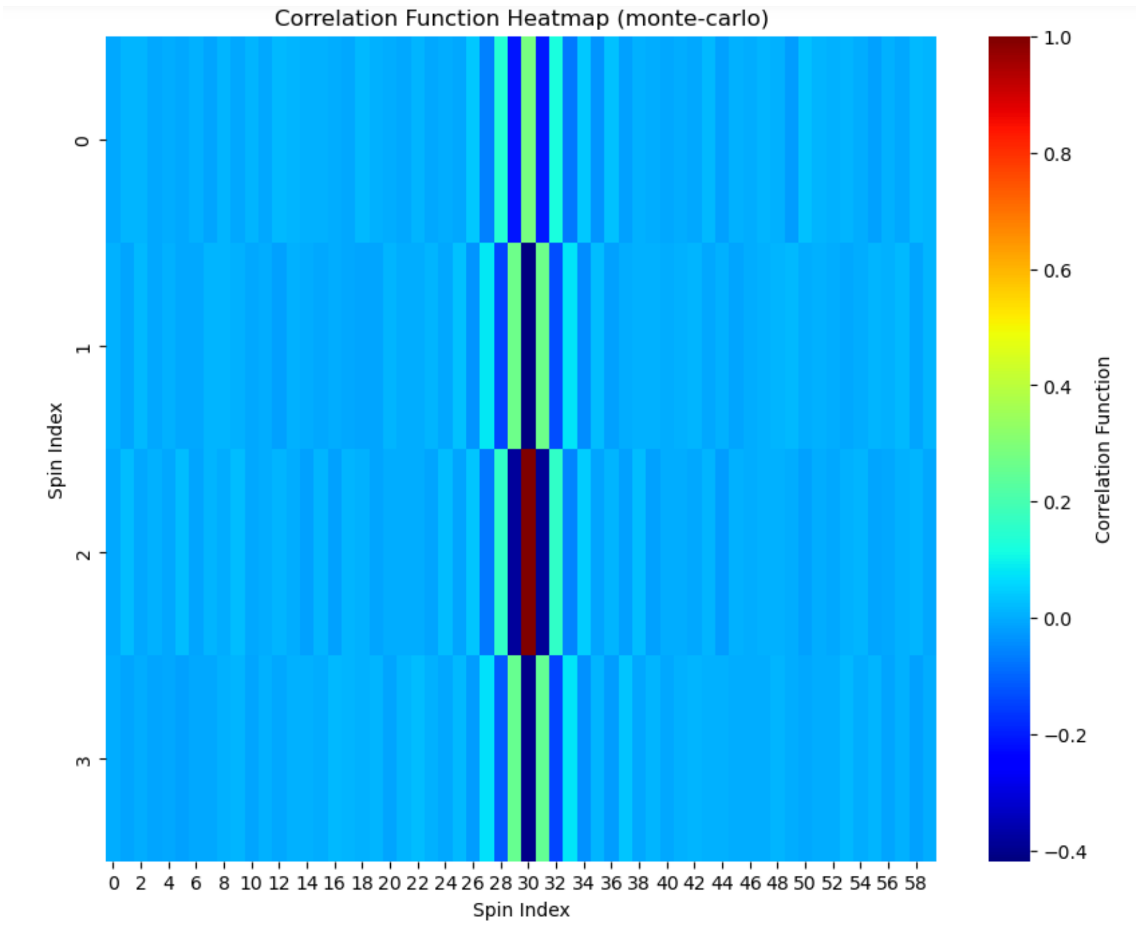
Result

The result with exact solution (Transfer Matrix Method) and monte-carlo simulation method is match and are given by :

Parameter	**Value**
Z	1.01×10^{85}
m	-0.03438

(Note that the Hamiltonian we saw in class doesn't have -1 so you can change the sign of J/KT and H/KT to get the result for that.)
The correlation function between middle spin (2,30) and all other spins are :

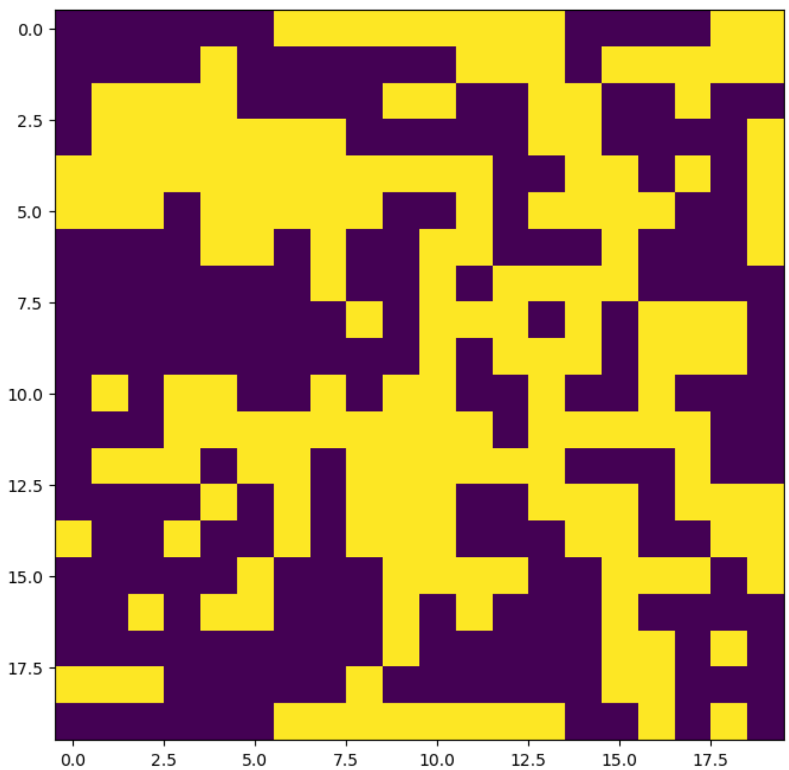




Correlation Function Heatmap (monte-carlo)
Spin Index
0
1
2
3
0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52 54 56 58
Spin Index
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
−0.4
Correlation Function

Problem 3 :

In this problem we want to simulate 2D Ising model using monte-carlo simulation and find the critical point of it. The method we use is metropolis algorithm as we mentioned in the Theory section. The initial config is like:

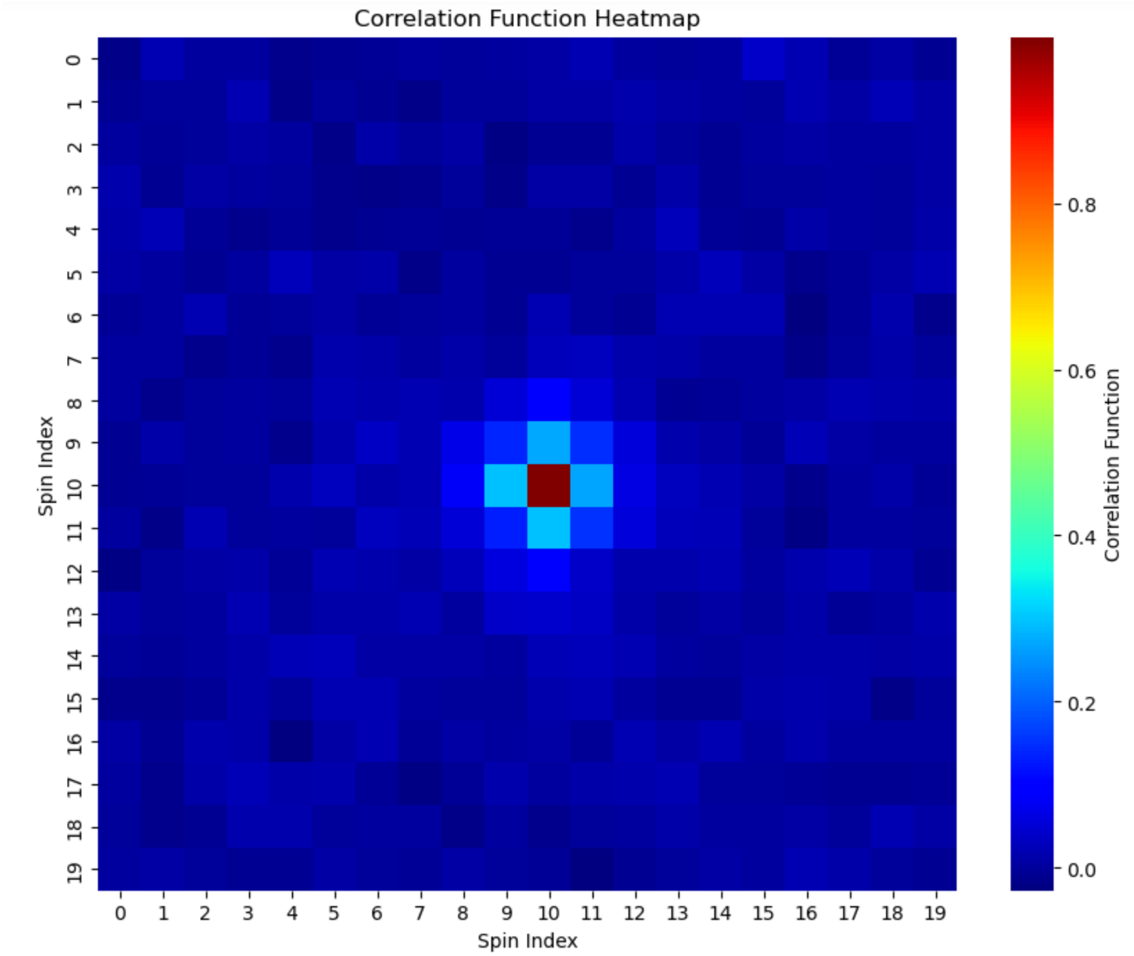


Result

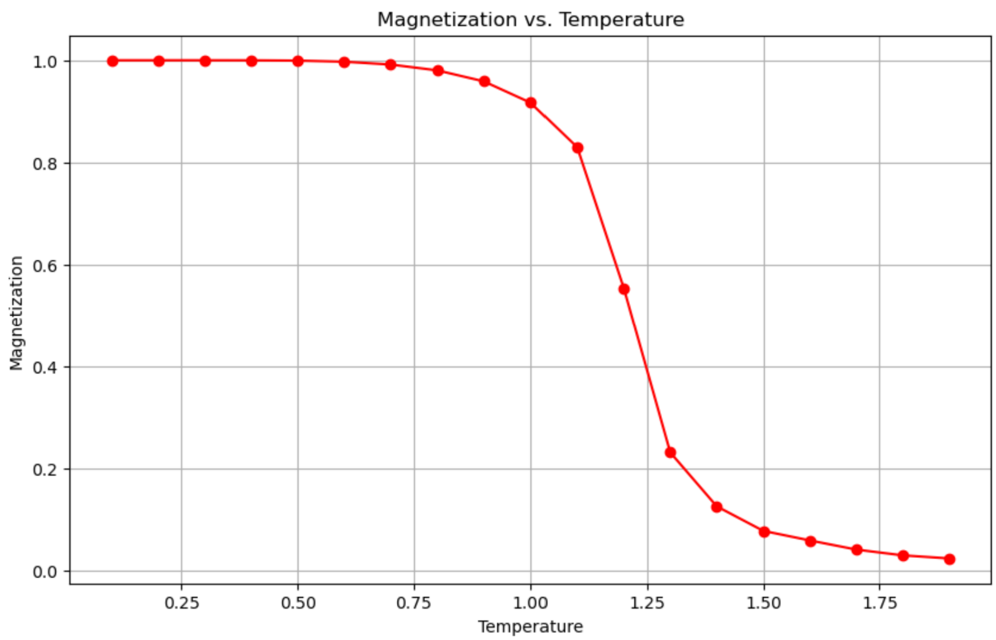
The result for an arbitrary J and H is :

Parameter	**Value**
J	-0.5
H	-0.01
T	2
m	0.0226

The correlation is :



To see the critical point for this model we plot the m by T and the result is :



(We can also first make and initial 2 configurations with almost up and almost down and see the transition.)

References

1 Okamoto, K. (1992). Ladders with two, three and four coupled Ising spin chains: Magnetic properties. *Physics Letters A*, 169(6), 433-438.

2 Jarzynski, J. (n.d.). Statistical Mechanics Lecture 4: The Ising Model. Retrieved from Stanford University website: `https://stanford.edu/~jeffjar/statmech/lec4.html`

3 Wikipedia contributors. (2024, April 27). Ising model. In Wikipedia, The Free Encyclopedia. Retrieved April 27, 2024, from `https://en.wikipedia.org/wiki/Ising_model`