UCSB, Physics 129AL, Computational Physics: Section Worksheet, Week 8A

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Section Participation and Submission Guidelines

Section attendance is required, but you do not need to complete all the work during the section. At each section, the TA will answer any questions that you might have, and you are encouraged to work with others and look for online resources during the section and outside of sections. Unless otherwise stated, the work will be due one week from the time of assignment. The TA will give you 1 point for each task completed. You can see your grades on Canvas.

We will use GitHub for section worksheet submissions. By the due date, you should have a single public repository on GitHub containing all the work you have done for the section work. Finally, upload a screenshot or a .txt file to Canvas with your GitHub username and repository name so the TA knows who you are and which repository you are using for the section.

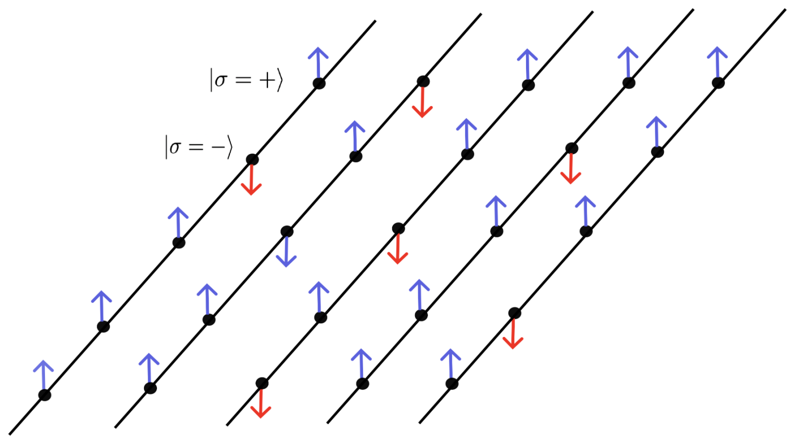
Remember: talk to your fellow students, work together, and use GPTs. You will find it much easier than working alone. Good luck! All work should be done in the Docker container, and don't forget to commit it to Git!

Task 1: 2D Classical Ising Model with MCMC

Depending on the arrangement of spins, the Hamiltonian for the classical Ising model is given by the following expression:

$$H = -J \sum_{\langle i,j \rangle} S_i S_j - B \sum_i S_i \tag{1}$$

where J is the coupling constant, representing the strength of the interaction between neighboring spins. $\langle i, j \rangle$ denotes a sum over pairs of nearest-neighbor spins, S_i represents the spins in z directions, and B represents an external magnetic field. You can see this is the classical Ising model: the Hamiltonian has no exchange interactions.



2D Lattice generation and Ising Hamiltonian

We can treat spins lattice as random variables, denoted as $\{S_{x,y}\}$. Let's define a function to initialize a random spin configuration. When working with a numpy array, we can naturally assign its dimensional index to be its special location, with value -1 or 1.

Statistical Description of the Ising Model

Let's look at various thermodynamic properties and statistical measures. The fundamental quantity is the partition function,

$$Z = \sum_{i,j} e^{-\beta H} \tag{2}$$

where $\beta \equiv \frac{1}{T}$. For the Ising model, we have the partition function,

$$Z = e^{-\beta\left(-J\sum_{\langle i,j\rangle} S_i S_j - B\sum_i S_i\right)}. \tag{3}$$

In particular, the joint distribution is a probability mass function (since we are working on a finite system), and it has the form:

$$P(S) = \frac{1}{Z} e^{-\beta H}, \tag{4}$$

where $S = \{S_1, S_2, \cdots, S_L\}$, and each S defines a unique energy. As one can see, it is very hard to draw samples from this multivariable distribution. It is easy to see that the total number of unique spin configurations exponentially grows with the system's dimension, 2^{L^2}, making computations difficult for large system sizes $L > 20$.

Write a program that sample the exact PDF above for $L = 4, B = 0, J = 1, T = 1$. Visualize the samples as 2D grid, and plot the PDF .

Gibbs Sampler on Ising Model

Calculating the exact partition function and obtaining the exact Boltzmann weight for a spin configuration becomes hard as we increase the system size. Write down the total conditional distribution function: a variable S_i given the rest of the spins.

As we discussed in the class, a Gibbs sampler involves drawing a sample from the total conditional distribution of that variable while fixing the values of all other variables.

Gibbs Iteration

For each variable in the distribution, sample a new value from its conditional distribution given the current values of all other variables (e.g. in our case, we update each spin site sequentially to converge to the posterior distribution). Visualize the posterior statistics with different burn-in periods. Remember, you can parallel Ising chains with different initial spin configurations.

Magnetization, Landau Theory, and Phase Transition of the Ising Model

Magnetization is a measure of the average magnetic moment per spin in a given direction. In the context of the Ising model, the magnetic moment is represented by the sum of the spins. The **magnetization** M is defined as:

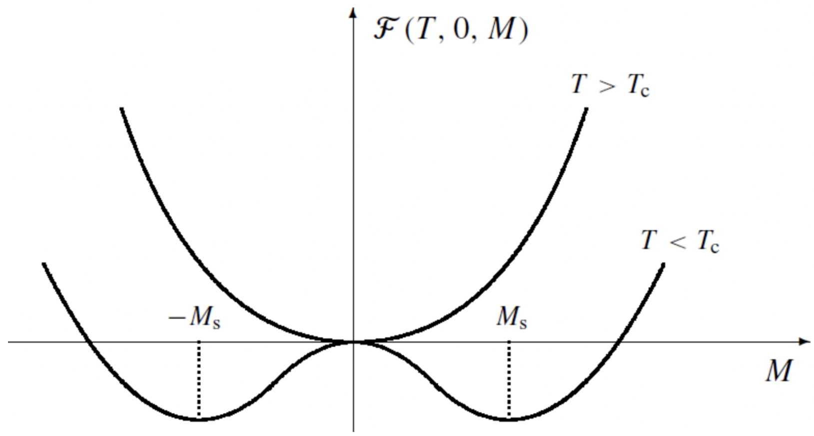
$$M = \frac{1}{N} \sum_i S_i \tag{5}$$

where $N = L^2$ is the total number of spins. In the absence of an external magnetic field ($B = 0$), the Ising model exhibits a spontaneous magnetization at low temperatures, where most spins tend to align in the same direction. In the Ising model, the magnetization serves as an **order parameter** that indicates the presence of a magnetic order in the system. The order parameter is often used to characterize the different phases of the model, especially in the study of phase transitions.

Landau theory, in the context of phase transitions, is a phenomenological approach that describes the free energy of a system near a critical point. It provides a framework for understanding symmetry-breaking mechanisms and the emergence of order parameters. Near a second-order phase transition, the **Landau free energy** can often be written as a Taylor expansion in terms of an order parameter, typically the magnetization:

$$F = F_0 + a(T - T_c)M^2 + bM^4 + \dots \tag{6}$$

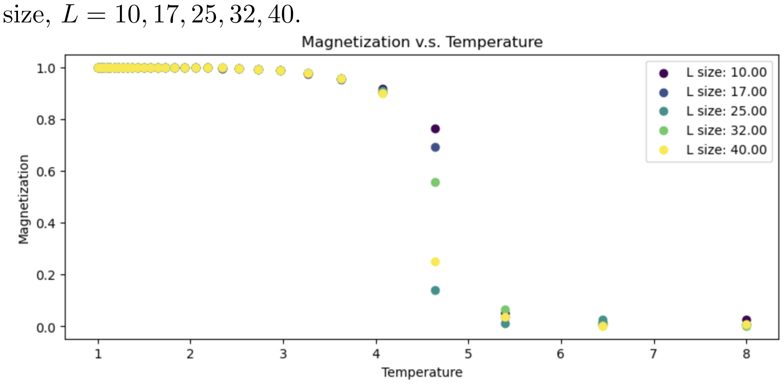
where F_0 is the free energy at the critical temperature (T_c), a and b are phenomenological coefficients, and T is the temperature.



magnetization at different temperature

Using your Gibbs sampler, visualize the ferromagnetic to paramagnetic phase transition, captured by the vanishing order parameter with increasing T.

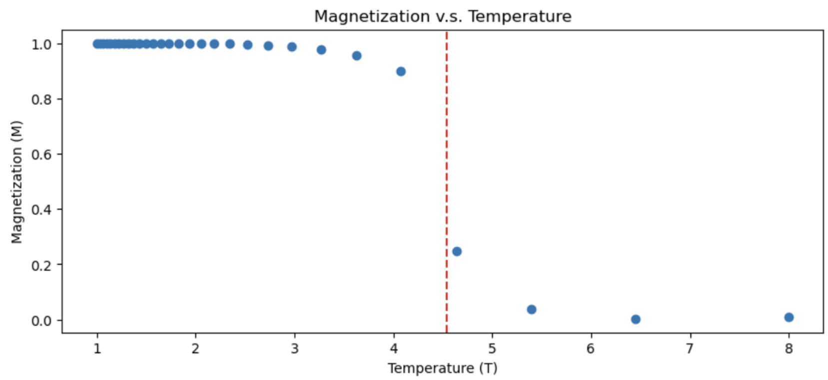
Reproduce the following posterior distribution convergence at different lattice size, $L = 10, 17, 25, 32, 40$.



In 2D Ising model, the critical temperature can be calculated via the following,

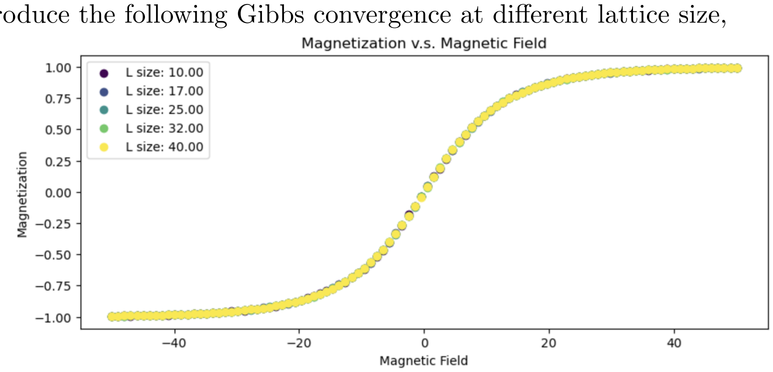
$$T_C = \frac{2J}{\log(1+\sqrt{2})}, \tag{7}$$

and it is labeled as the red vertical dash-line in the following figure. Verify your 2D Ising phase transition with the above fomula. You should see something below,



Classical Magnetic Field dependence: magnetization of the 2D Ising model

Reproduce the following Gibbs convergence at different lattice size,

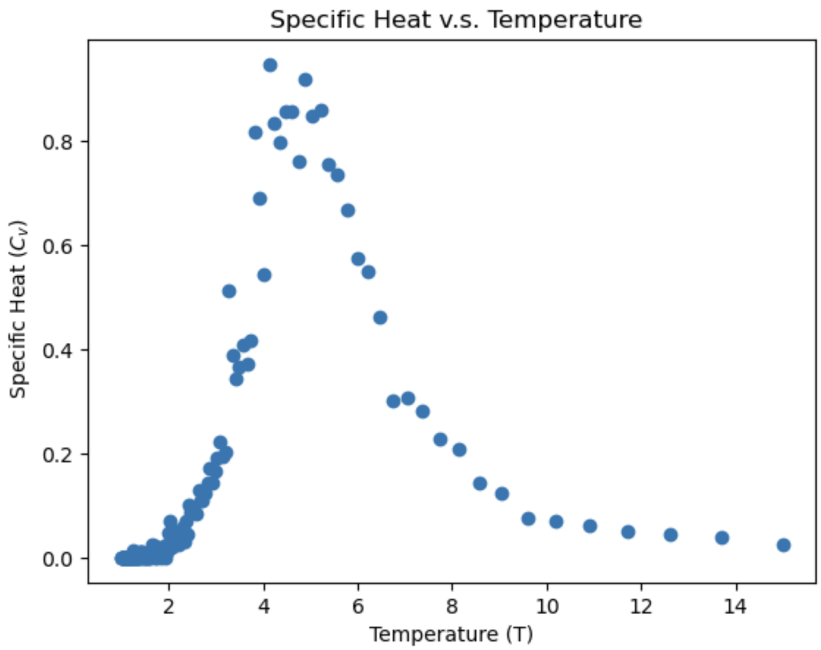


Specific Heat of the 2D Ising Model

The specific heat (C_v) measures the amount of heat energy required to change the temperature of a substance by a unit temperature. It can be related to the variance of the energy in the 2D Ising model as:

$$C_v = \frac{\beta^2}{N}\left(\langle E^2\rangle - \langle E\rangle^2\right), \tag{8}$$

where N is the total number of spins. Reproduce the following temperature dependence of C_V.

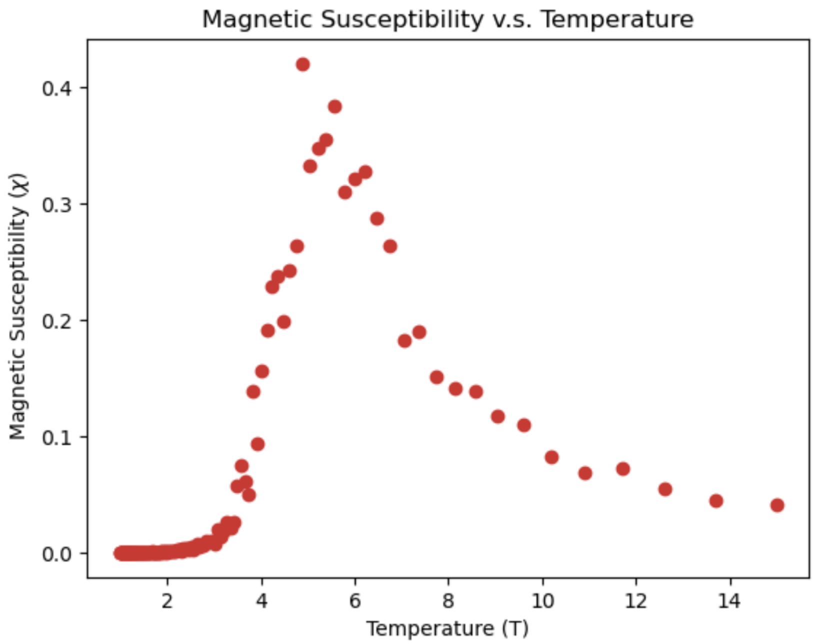


Magnetic Susceptibility of the 2D Ising model

The magnetic susceptibility quantifies the material's ability to become magnetized per unit change in the external magnetic field strength,

$$\chi = \frac{\beta}{N}\left(\langle M^2\rangle - \langle M\rangle^2\right). \tag{9}$$

Reproduce the following magnetic field susceptibility at a given temperature at different magnetic field strength,


Magnetic Susceptibility v.s. Temperature
Magnetic Susceptibility (χ)
Temperature (T)
0.0
0.1
0.2
0.3
0.4
2
4
6
8
10
12
14