

# Homework 9

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## 1 Problem1: Volume of hypersphere using MC

### 1.1 problem description

The interior of a d-dimensional hypersphere of unit radius is defined by the condition  $x_1^2 + x_2^2 + \dots + x_d^2 \leq 1$ . Write a program that finds the volume of a hypersphere using a Monte Carlo method. Test your program for d=2 and d=3 and then calculate the volume for d=4 and d=5, compare your results with the exact results.

### 1.2 algorithm description

First generate uniform random points in  $[-1, 1]$  for each dimension  $x_i$  with Linear Congruential Generator.

$$M_i = (aM_{i-1} + c) \mod m \quad (1)$$

we simply choose a initial  $M_0$ , and then generate a sequence of pseudo-random integers  $M_i$ . The parameters are chosen such that  $m$  is a large prime number,  $a$  is a small integer, and  $c$  is an integer relatively prime to  $m$ . The random number in  $[0, 1)$  can be obtained by dividing  $M_i$  by  $m$ .

Then get  $x_i = 2Y_i - 1 \in [-1, 1]$  from the uniform distribution  $Y_i \in [0, 1)$ , check if the point lies within the hypersphere by evaluating the condition  $x_1^2 + x_2^2 + \dots + x_d^2 \leq 1$ . Count the number of points that satisfy this condition and divide it by the total number of points generated.

The exact volume  $V_d$  of a d-dimensional hypersphere of radius  $r$  is given by the formula:

$$V_d = \frac{\pi^{d/2}}{\Gamma(\frac{d}{2} + 1)} r^d \quad (2)$$

where  $\Gamma$  is the Gamma function. In my code, I use `math.gamma()` to calculate the Gamma function value.

### 1.3 output

run `problem1.py`

Dim	MC Volume	Exact Volume	Error (%)
2	3.14042	3.14159	0.04
3	4.18901	4.18879	0.01
4	4.94266	4.93480	0.16
5	5.28381	5.26379	0.38

Figure 1: Volume of hypersphere

## 2 Problem2: 3D Heisenberg model MC

### 2.1 problem description

Write a MC code for a 3D Face-Centered Cubic lattice using the Heisenberg spin model (adopt periodic boundary condition and only consider nearest neighbour interaction). Estimate the ferromagnetic Curie temperature  $T_c$ .

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j \quad J = 1, \quad |\vec{S}_i| = 1 \quad (3)$$

### 2.2 algorithm description

Metropolis algorithm is used to simulate the Heisenberg model on a 3D Face-Centered Cubic (FCC) lattice. The key steps of the algorithm are as follows:

- **Lattice Initialization:** Create a 3D supercell FCC lattice of size  $L \times L \times L$  with periodic boundary conditions. Each lattice site contains a spin vector  $\vec{S}_i$  initialized randomly on the unit sphere with uniform distribution.
- **Monte Carlo Steps:** For each Monte Carlo step, randomly select a lattice site and propose a new spin orientation by generating a random vector on the unit sphere. Calculate the change in energy  $\Delta E$  due to the proposed spin change using the Hamiltonian:

$$\Delta E = -J \sum_{\langle ij \rangle} (\vec{S}'_i - \vec{S}_i) \cdot \vec{S}_j \quad (4)$$

where  $\vec{S}'_i$  is the proposed new spin and the sum is over nearest neighbors, 12 in total.

- **Acceptance Criterion:** Accept the proposed spin change with probability:

$$P = \min\{u, e^{-\Delta E/k_B T}\} \quad (5)$$

where  $k_B$  is the Boltzmann constant and  $T$  is the temperature.  $u$  is a uniform random number in  $[0, 1]$ .

- **Measurement:** After reaching equilibrium, measure physical quantities such as magnetization, specific heat  $C_v$ , and magnetic susceptibility  $\chi$  by sampling over many Monte Carlo steps. Repeat the above steps for a range of temperatures to observe phase transitions and estimate the Curie temperature  $T_c$ .

## 2.3 output

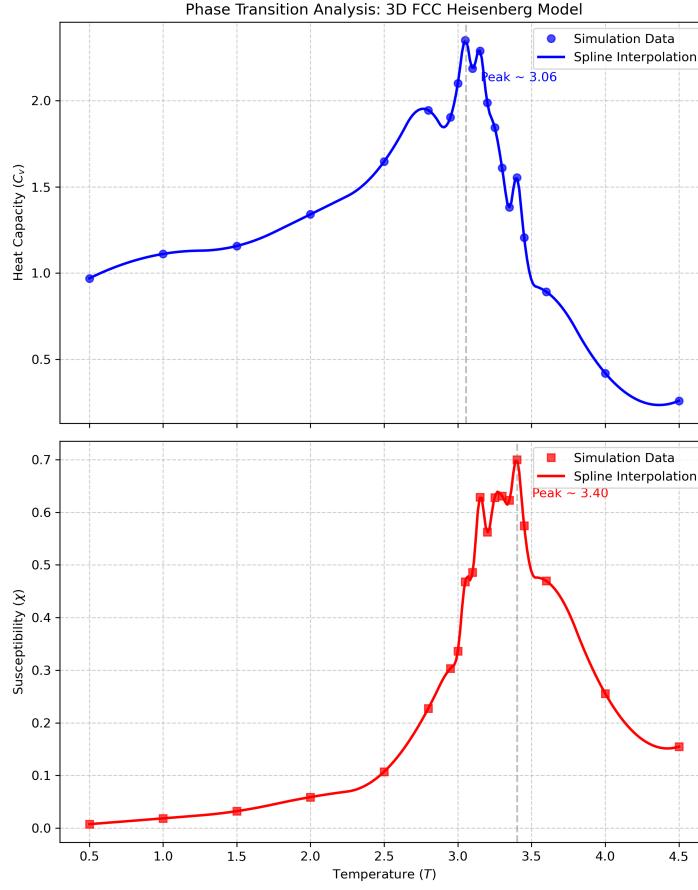


Figure 2:  $C_v$  and Magnetic susceptibility  $\chi$  vs Temperature

It can be seen from the figure that  $C_v$  and  $\chi$  both show an unstable peak at around  $T = 3.1$ , indicating the transition temperature  $T_c \approx 3.1 k_B^{-1}$ .