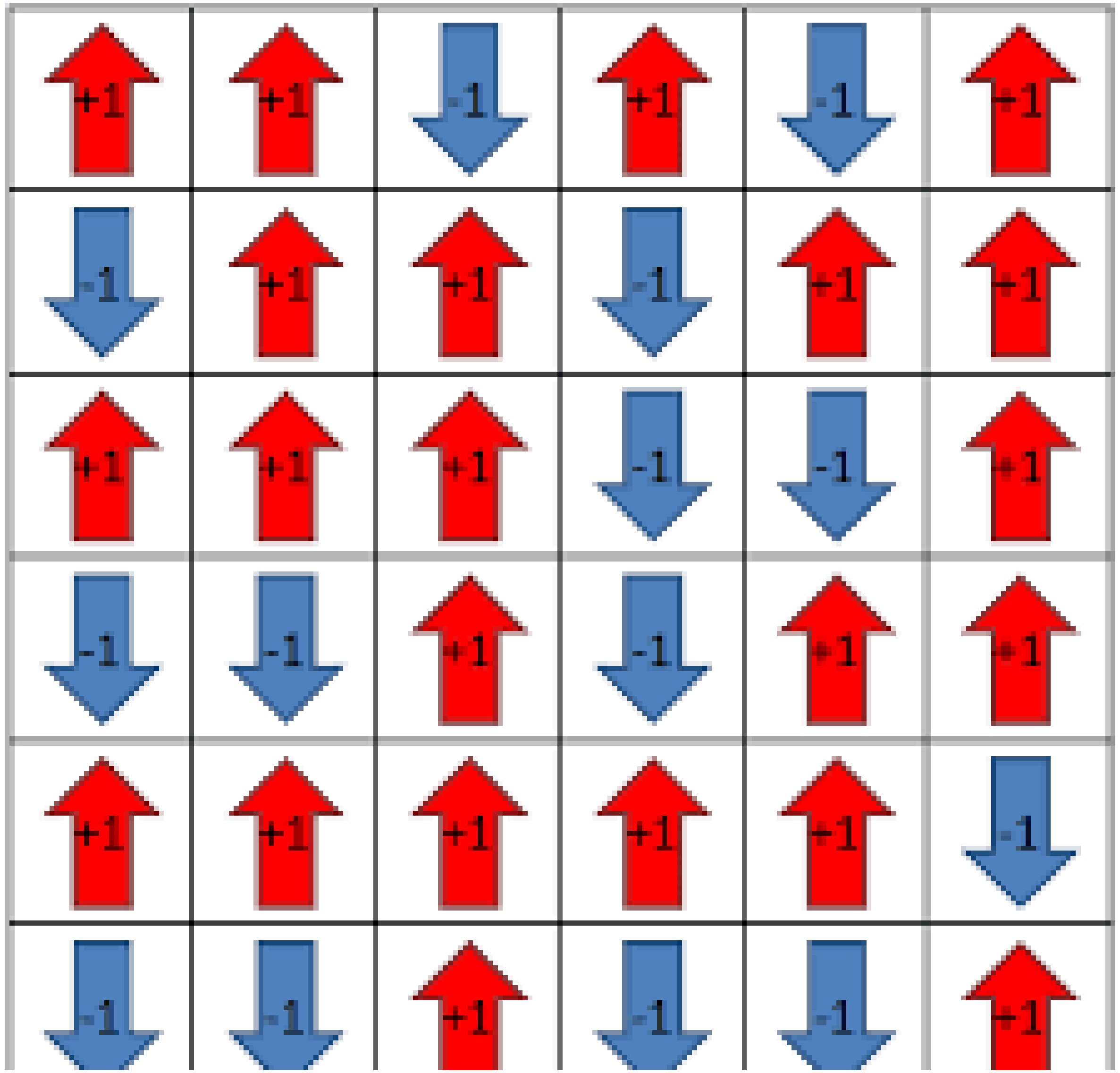
Ising Model

A phase transition simulation

Shriram Pragash M (EP23BTECH11028),
Siddharth Pamidi (EP23BTECH11029) &
Vedant Mokal (EP23BTECH11034)



What is it?

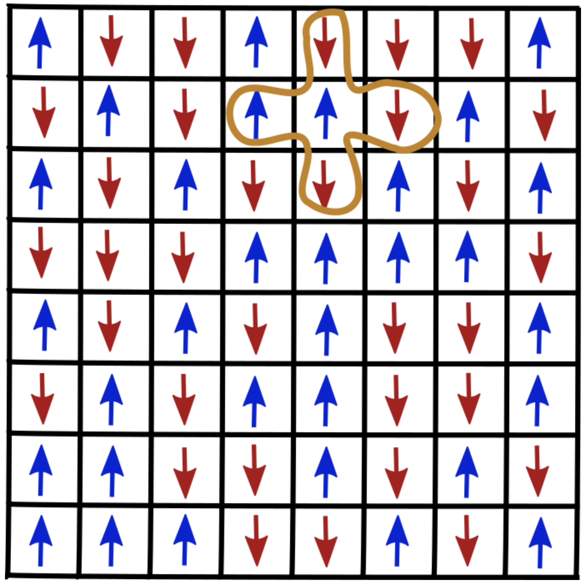
We know how ferromagnetism is a result of magnetic moments aligning within a material.

We also know that at high temperatures, these domains lose their alignment and hence a ferromagnetic material can become paramagnetic.

But we've never qualitatively analysed this transition.

- The simplest theoretical description of ferromagnetism is called the *Ising model*.
- This model was invented by Wilhelm Lenz in 1920: it is named after Ernst Ising, a student of Lenz who chose the model as the subject of his doctoral dissertation in 1925.
- The Ising Model is a *mathematical* model that doesn't correspond to an actual physical system.

- It's a huge (square) lattice of sites, where each site can be in one of two states.
- For the Ising model, we make the simplest possible assumption for the nature of this spin-spin interaction: nearest neighbour interaction.



- The total energy of the system is written as:

$$E = -J \sum_{<ij>} s_i s_j - \mu H \sum_{i=1,N} s_i .$$

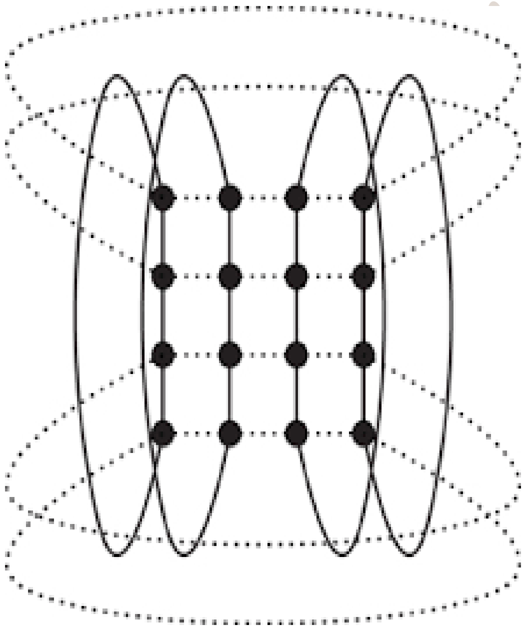
- The magnetization is defined as:

$$M = (\sum_i \sigma_i)/(N^2)$$

Periodic Boundary Conditions

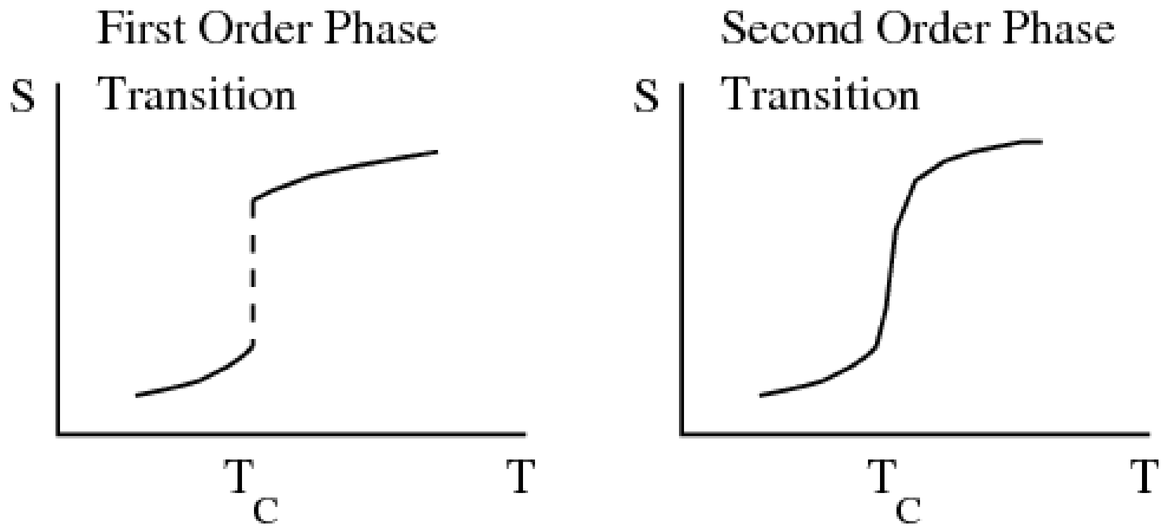
Since we are simulating the Transition using a small Lattice we observe that atoms on the edges of the lattice will have either 3 neighbours (Non Corner Atoms on the edge) or 2 neighbours (Corner Atoms) therefore we consider that the edge atoms are connected to the other edge, as shown in the figure.

We can say that the entire lattice is interconnected and the shape can be imagined as a toroid instead of a square lattice



First order vs Second order phase transitions

- A transition is *first-order* if the energy is discontinuous with respect to the order parameter (*i.e.*, in this case, the temperature), and *second-order* if the energy is continuous, but its first derivative with respect to the order parameter is discontinuous, *etc.*



Metropolis Algorithm

The Historical Background

- The Metropolis algorithm was introduced in 1953 by Nicholas Metropolis
- It was originally designed to solve problems in statistical mechanics, particularly to simulate the behavior of particles in physical systems.
- The method leveraged the new MANIAC computer, one of the earliest programmable supercomputers, to perform large-scale simulations.
- The algorithm's impact grew over time, becoming a foundational tool in physics, statistics, machine learning, and beyond.

The Core Idea

- The Metropolis algorithm generates a sequence of states by proposing random moves and accepting or rejecting them based on how likely they are under the target distribution.

Key steps:

- Start at an initial point x_0.
- Propose a new point x_1= x_0 +Δx.
- Compute the acceptance ratio= a = min(1,$\frac{\phi(x_1)}{\phi(x_0)}$)
- Repeating this process allows the algorithm to explore the space, spending more time in regions where the target distribution is higher

The Goal

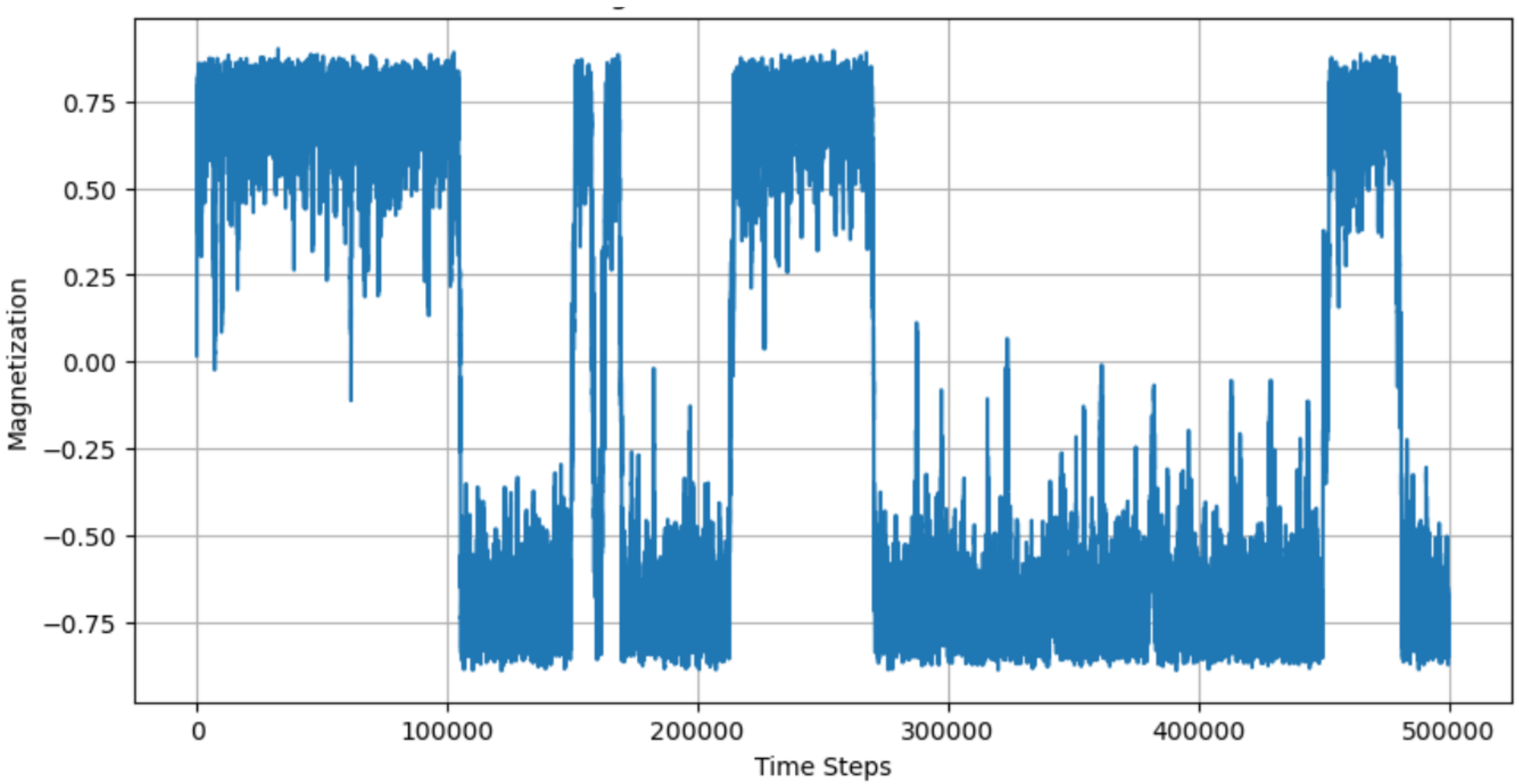
- Objective: Find the equilibrium state of a magnetic lattice (Ising model) at a given temperature.
- Each site (spin) can be up (+1) or down (−1).
- Start with a random arrangement of spins.
- The system evolves until it reaches equilibrium, showing the typical pattern for that temperature.

The Metropolis Steps in Ising model

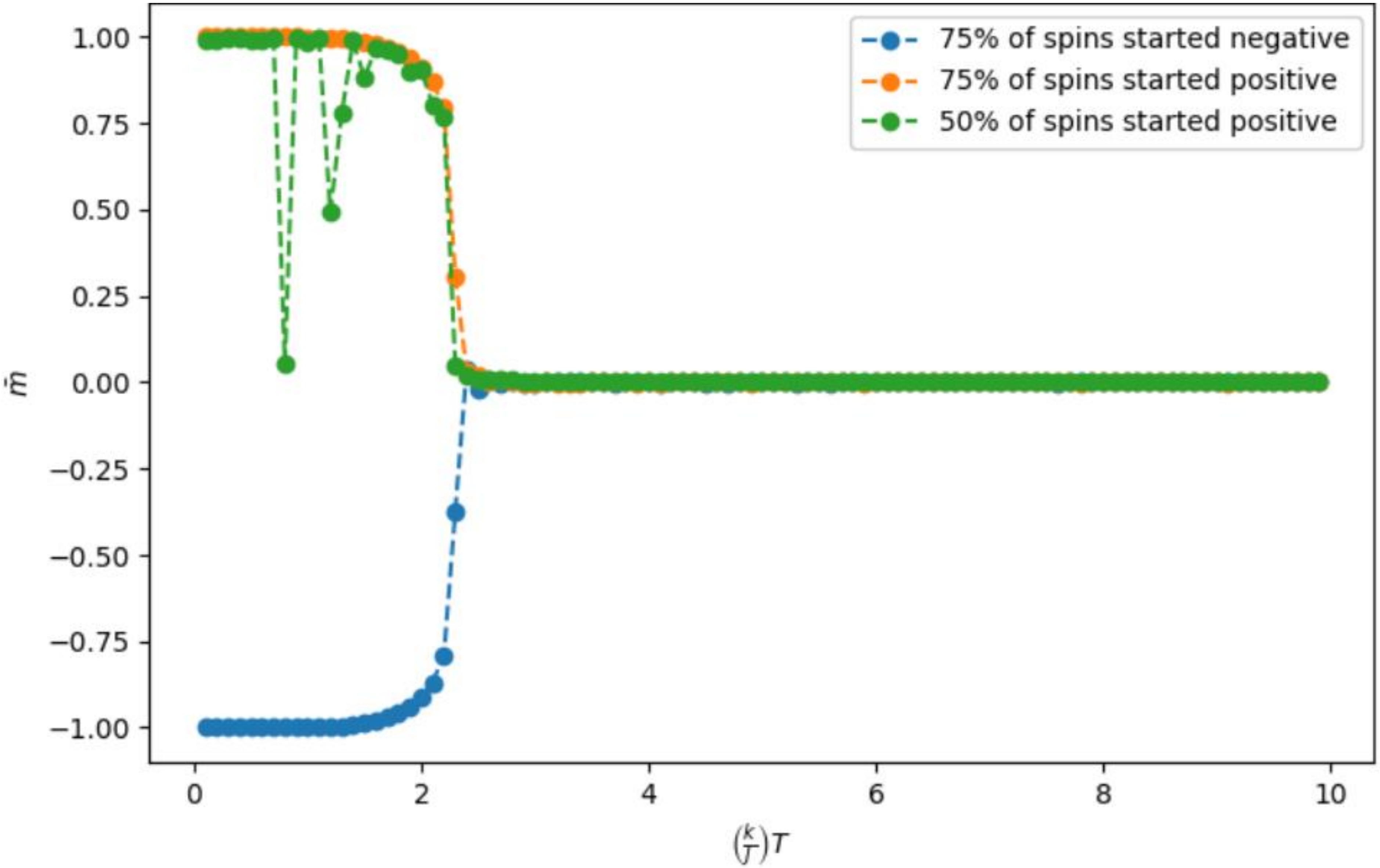
- Pick a random spin and flip its sign to propose a new state (ν) from the current state (μ).
- Calculate the energy difference: E_ν-E_μ
- $\frac{\mathrm{P}(\mu \rightarrow \nu)}{\mathrm{P}(\nu \rightarrow \mu)}$ = exp[−β(E_ν-E_μ)].
- Acceptance Rule:
  - If the new state has lower energy, always accept the flip.
  - If the energy increases, accept the flip with probability exp[−β(E_ν-E_μ)].
- Repeat these steps many times—the system will eventually settle into its equilibrium state.

Results

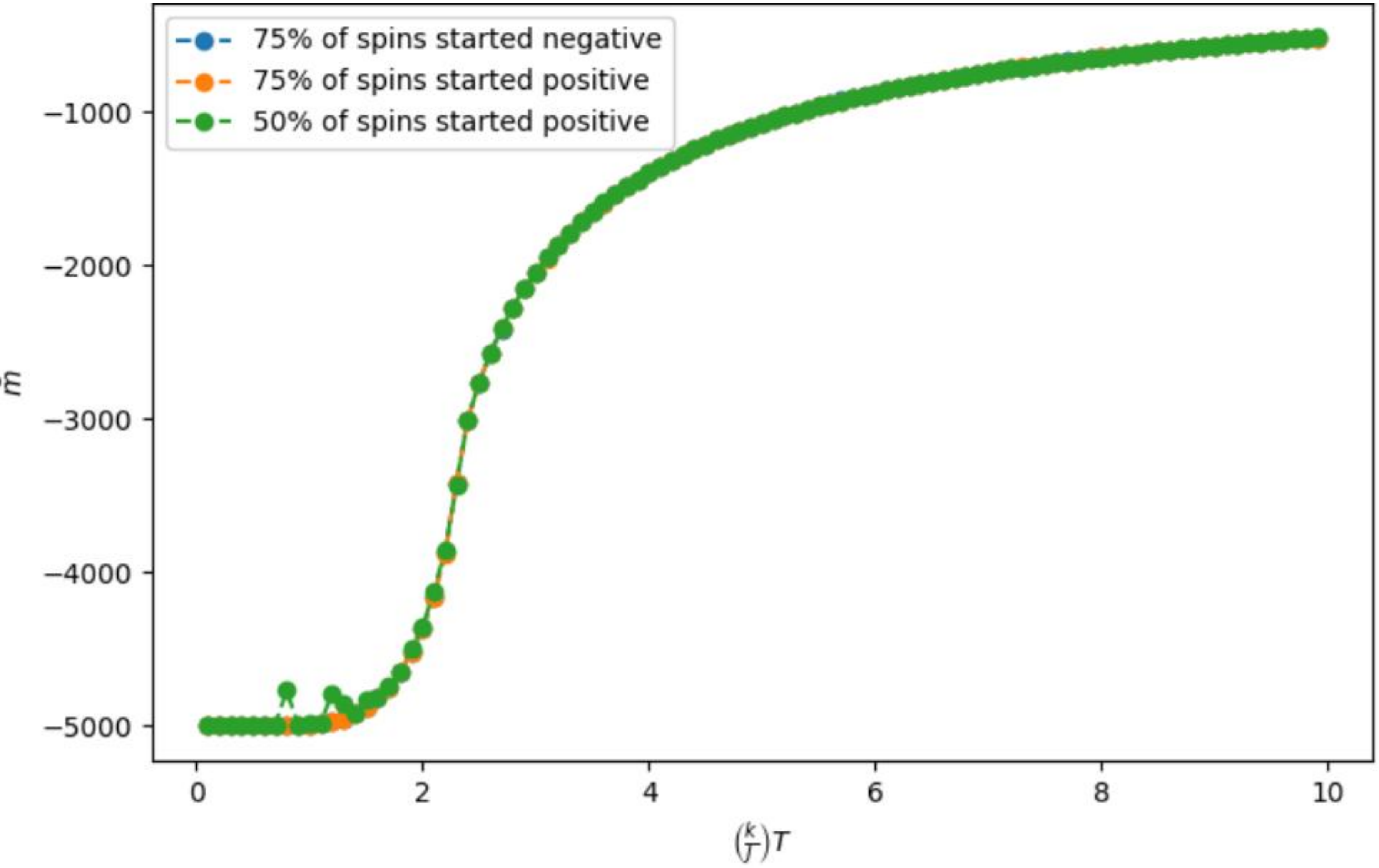
- Magnetization vs Time Steps at T = 2.25 (Kb = 1,J=1)



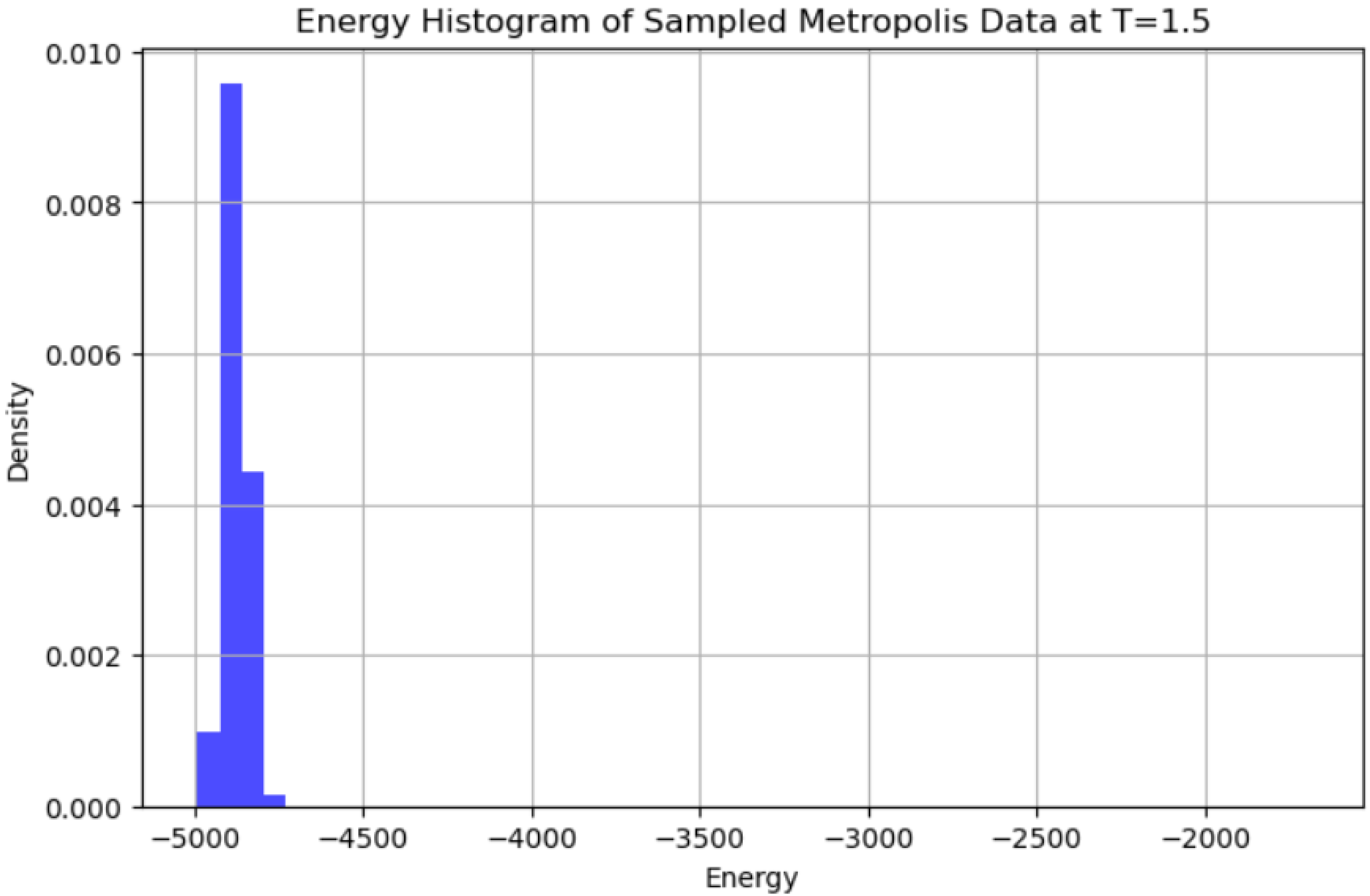
Average Magnetization vs Temperature:

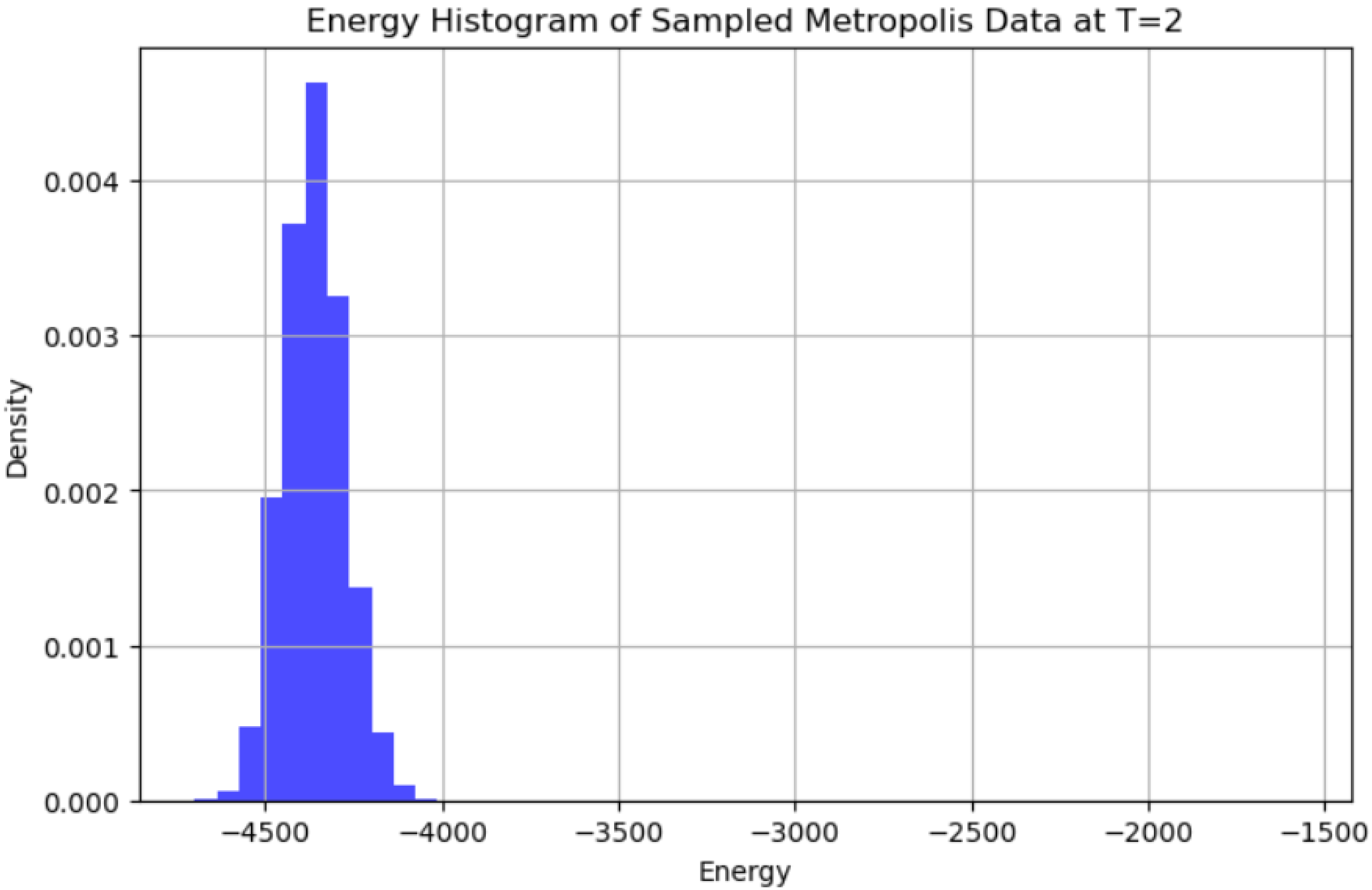


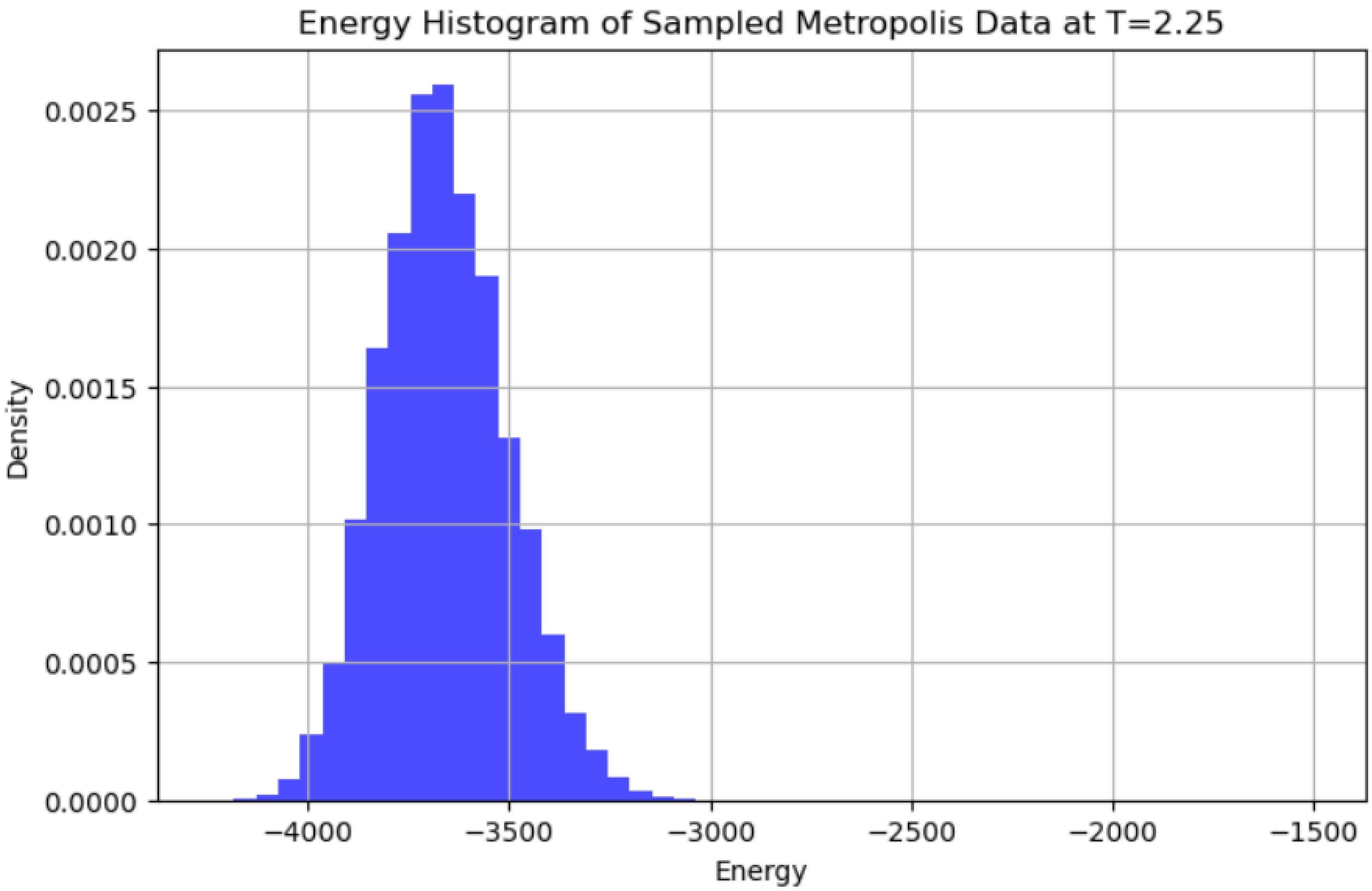
Average Energy vs Temperature

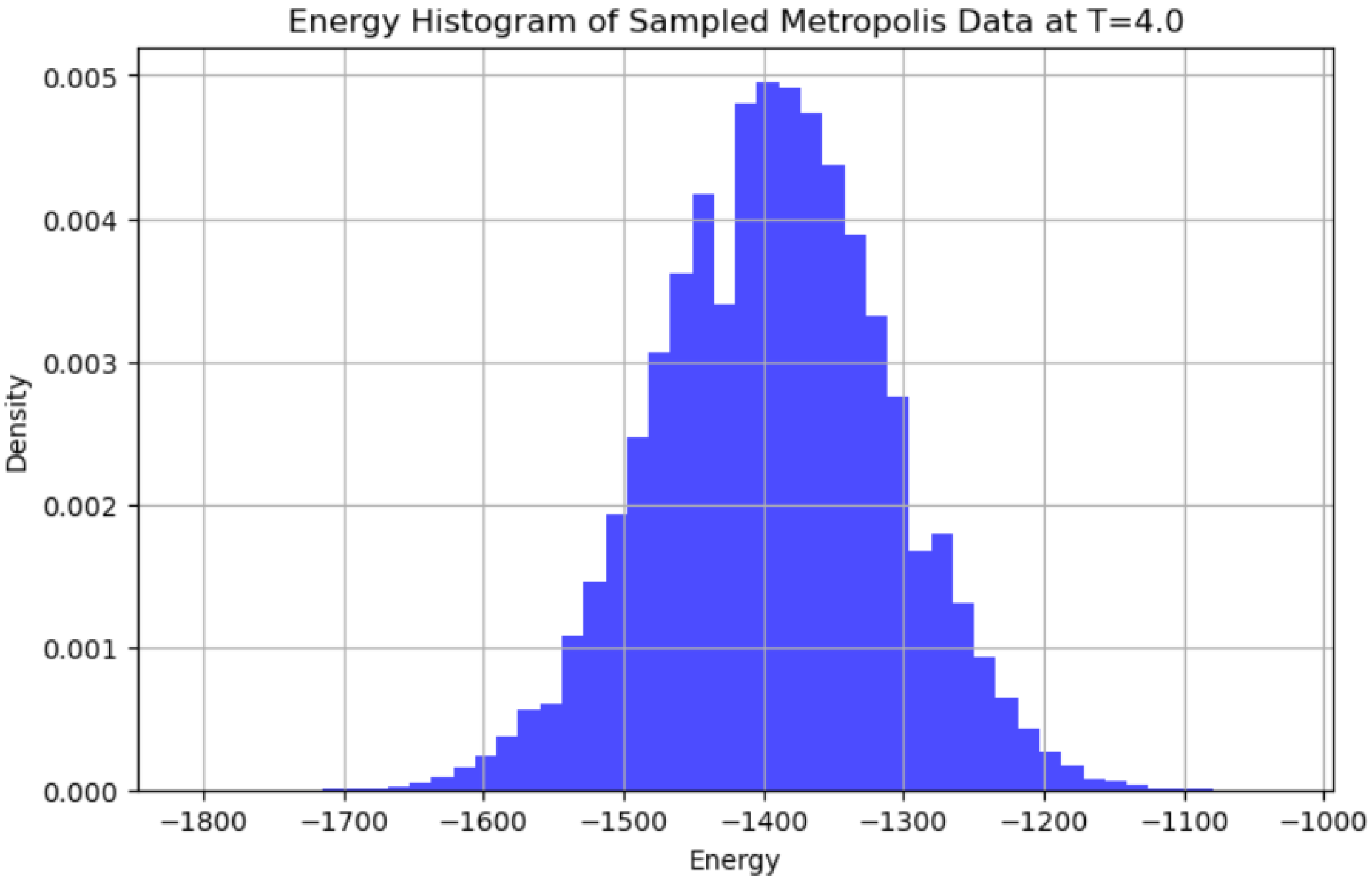


Energy Histograms at different temperatures:




Energy Histogram of Sampled Metropolis Data at T=2
Density
0.004
0.003
0.002
0.001
0.000
−4500
−4000
−3500
−3000
−2500
−2000
−1500
Energy


Energy Histogram of Sampled Metropolis Data at T=2.25
Density
0.0025
0.0020
0.0015
0.0010
0.0005
0.0000
−4000
−3500
−3000
−2500
−2000
−1500
Energy


Energy Histogram of Sampled Metropolis Data at T=4.0
Density
0.005
0.004
0.003
0.002
0.001
0.000
−1800
−1700
−1600
−1500
−1400
−1300
−1200
−1100
−1000
Energy