In this project we considered two methods for qualitatively and quantitively analyzing a system. These methods were The Mean Field Approximation Method and the Monte-Carlo Simulation Method. For our case, we considered the interaction of the spins of many atoms in the system, where the spins could only take two states – up and down. The goal of the analysis was to calculate the average spin alignment of the atoms in the material. We derived the Energy function for the system of N particles describing the total energy influenced by the alignment of the spin of each particle:

$$E = -J \sum_{\langle ij \rangle} s_i s_j - \mu H \sum_i s_i$$

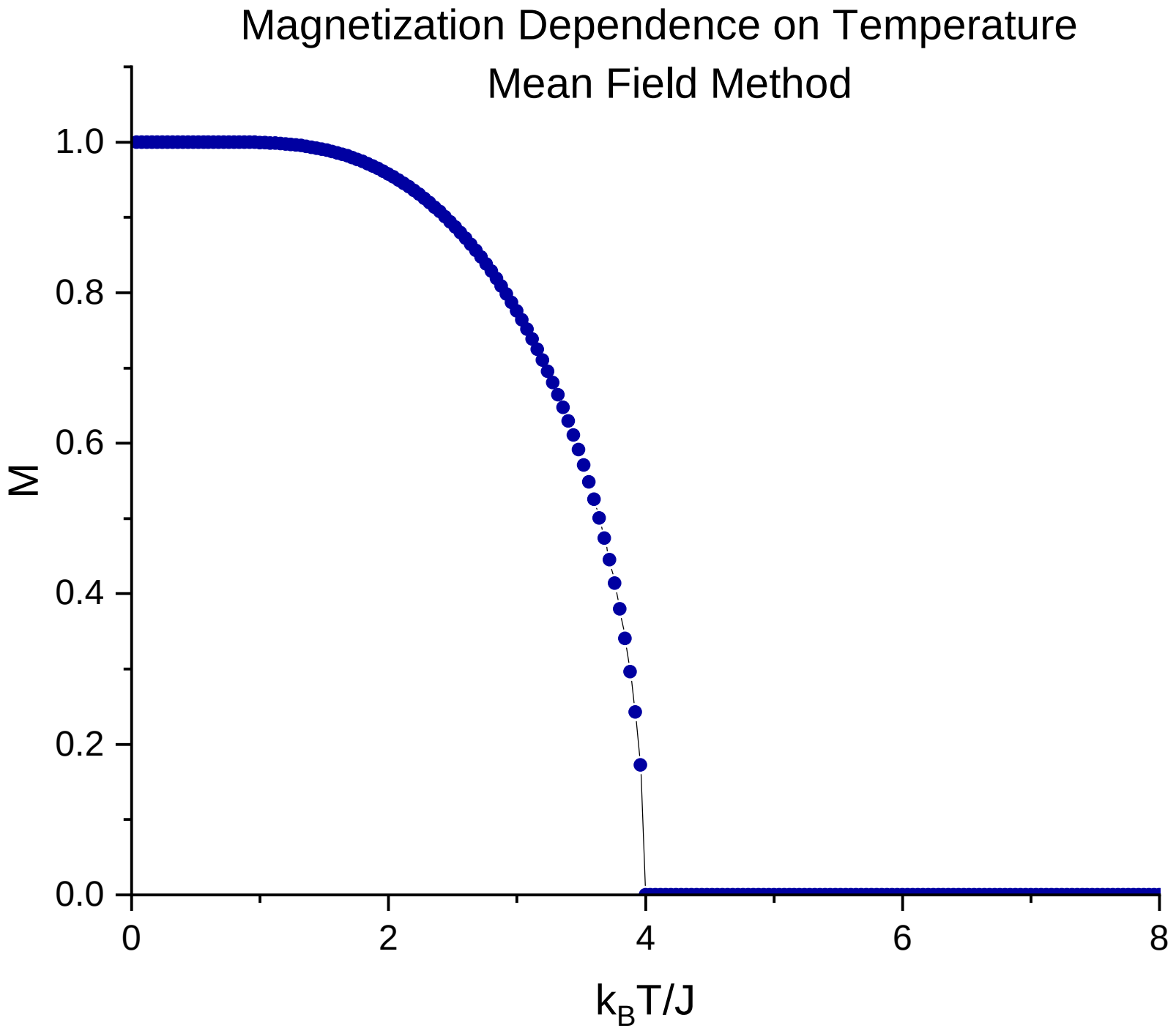
Where H is the magnetic field and μ is the magnetic field moment associated with each particle.

The first method of analyzing the statistics of a large system consisting of many connected particles that we studied in this project is the Mean Field Approximation. The Mean Field Approximation replaces the interaction between each of the terms by a general effective field, takes as an average of the interactions from each of the particles. Therefore, replacing the term for magnetic field moment by the mean magnetic field created from the average spin of the particles in the system:

$$H_{\text{eff}} = \frac{J}{\mu} \sum \langle s \rangle = \frac{z J}{\mu} \langle s \rangle$$

This approximation of the solution let's us obtain a transcendental equation that we then solve numerically and obtain Graph 1.

In the Graph1 we see that as the temperature increases, we expect the average of the spins to fall to zero due to the increased disorder and thermal fluctuations, therefore, our model shows this falloff of the mean magnetization.

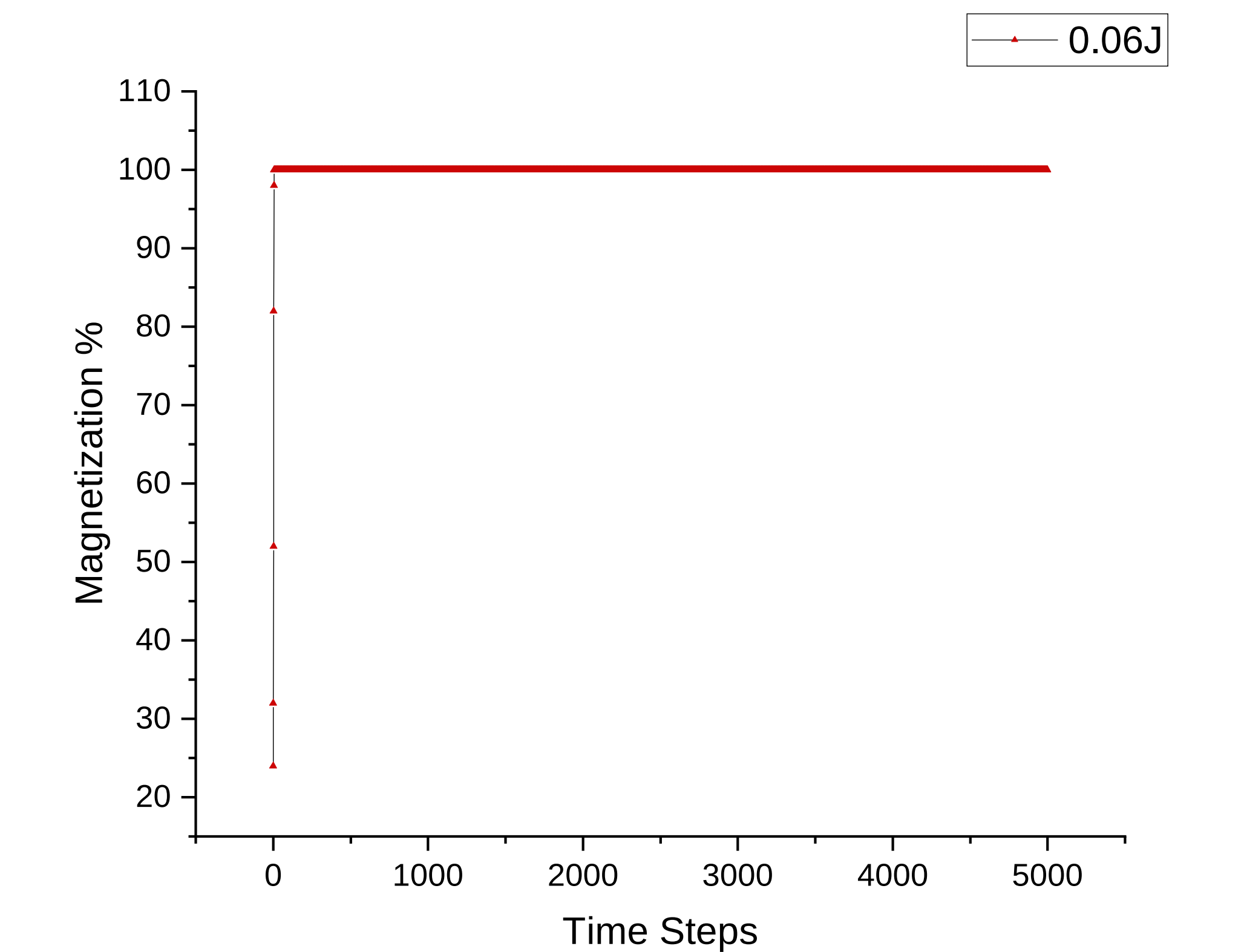

Magnetization Dependence on Temperature
Mean Field Method
M
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
8
k_BT/J

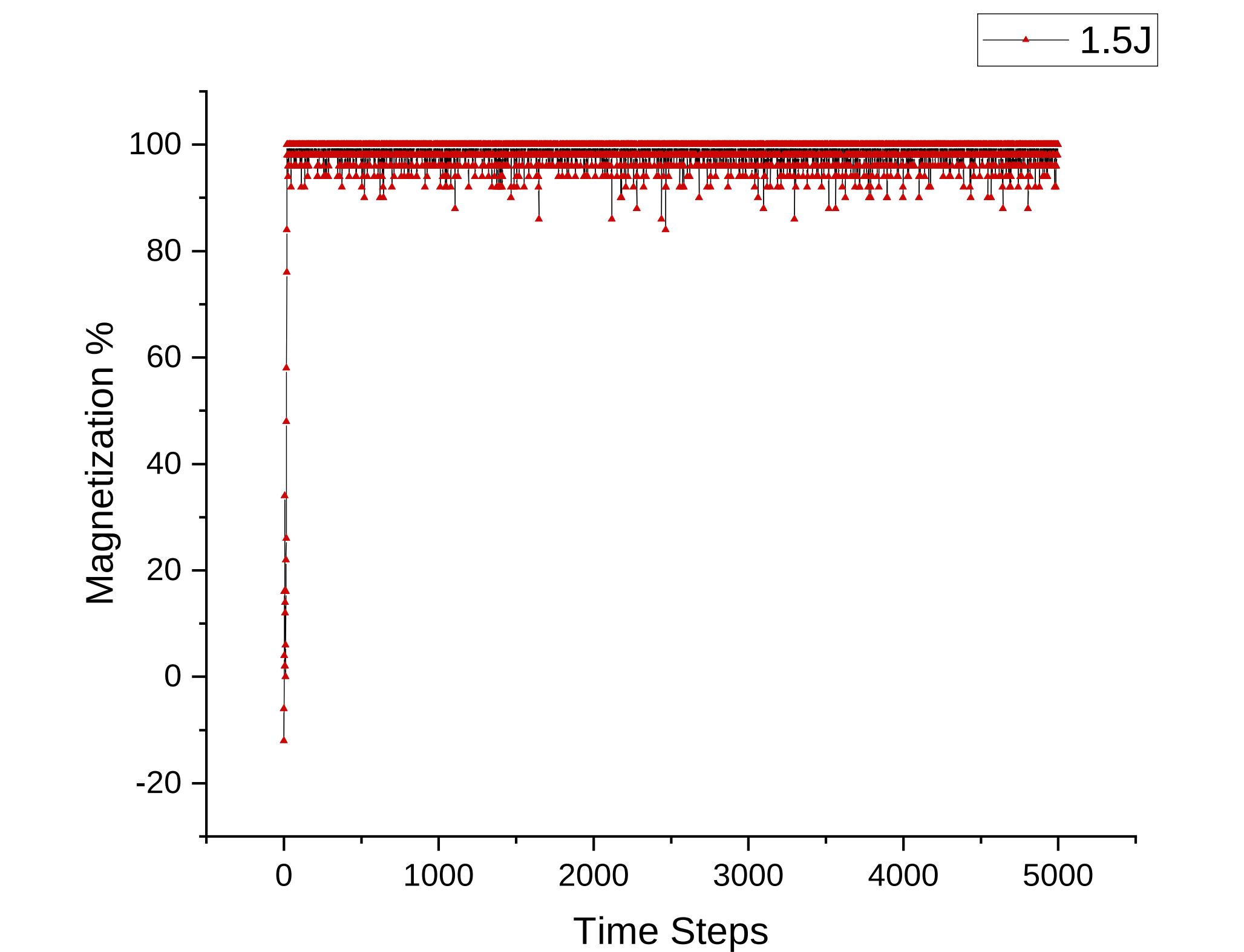
The second method for predicting the behavior of a collection of a large number of interacting particles is the Monte-Carlo Method. In principle, Monte-Carlo method relies on random sampling of the particles in the system, and, after calculating the state for each of the selected particles, a new particle is randomly selected. It is then said that the more random samples we preform, the closer approximation of the actual system we get. However, in our project we only considered a square 10X10 lattice of atoms, so the selection of particles could be done iteratively. The selection was done 5000 time to ensure a good convergence of results.

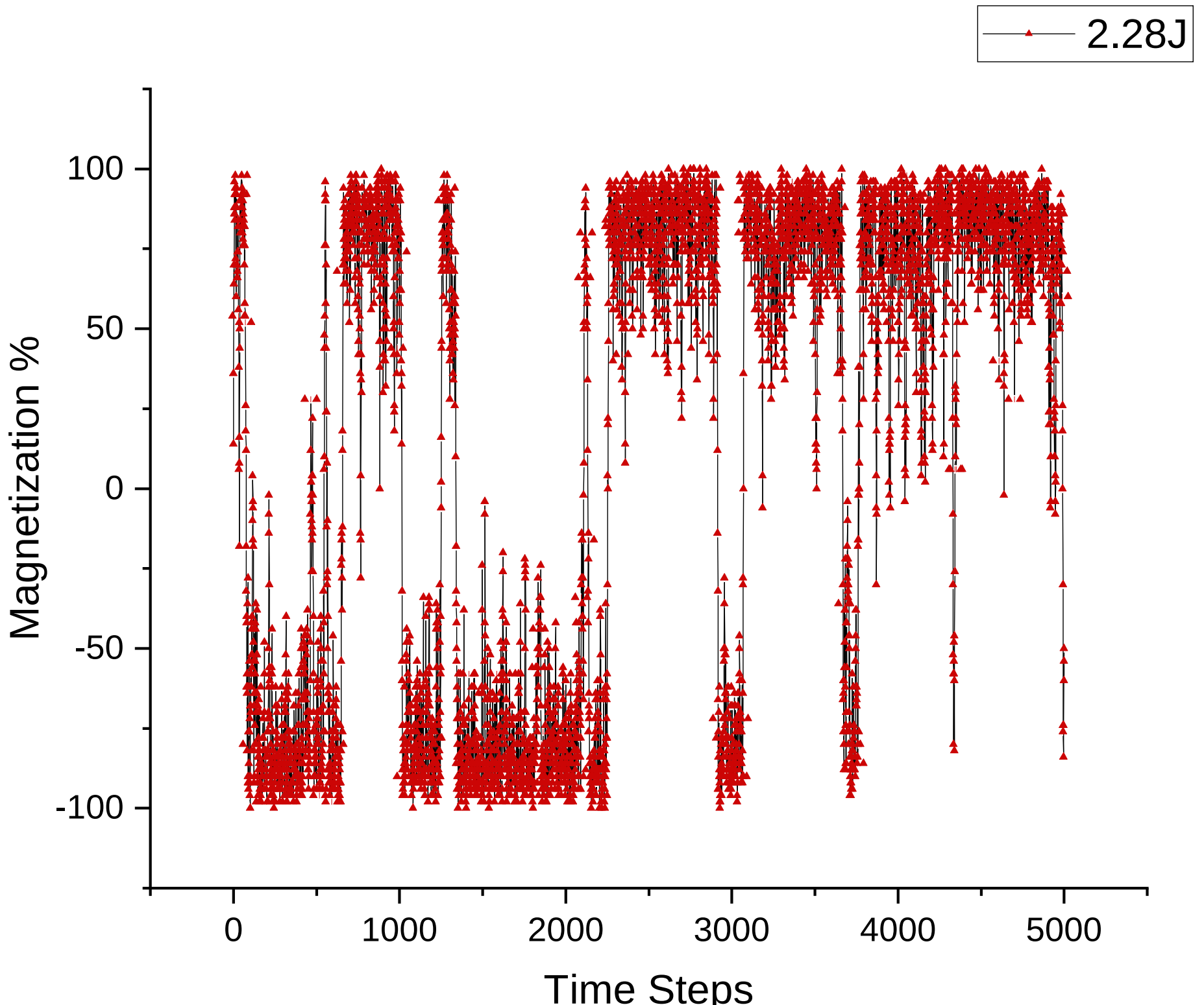
Another crucial difference from the Mean Field Approximation also lied in the fact that we considered the probability for the spin of each particle to flip from the probabilistic point of view. We calculated the average energy state of the four neighboring spins to the selected particle (diagonal neighbors excluded). Then if flipping the spin of the selected particle led to the lowering of the energy state of the five spins, the spin of the selected particle was flipped to align the particle with the majority spin of its neighbors. Otherwise, we calculated the probability of the selected spin to flip using the Boltzmann distribution. If the Boltzmann factor was less then 0.5 the spin was flipped to align with the spin of the majority, otherwise the spin remained the same.

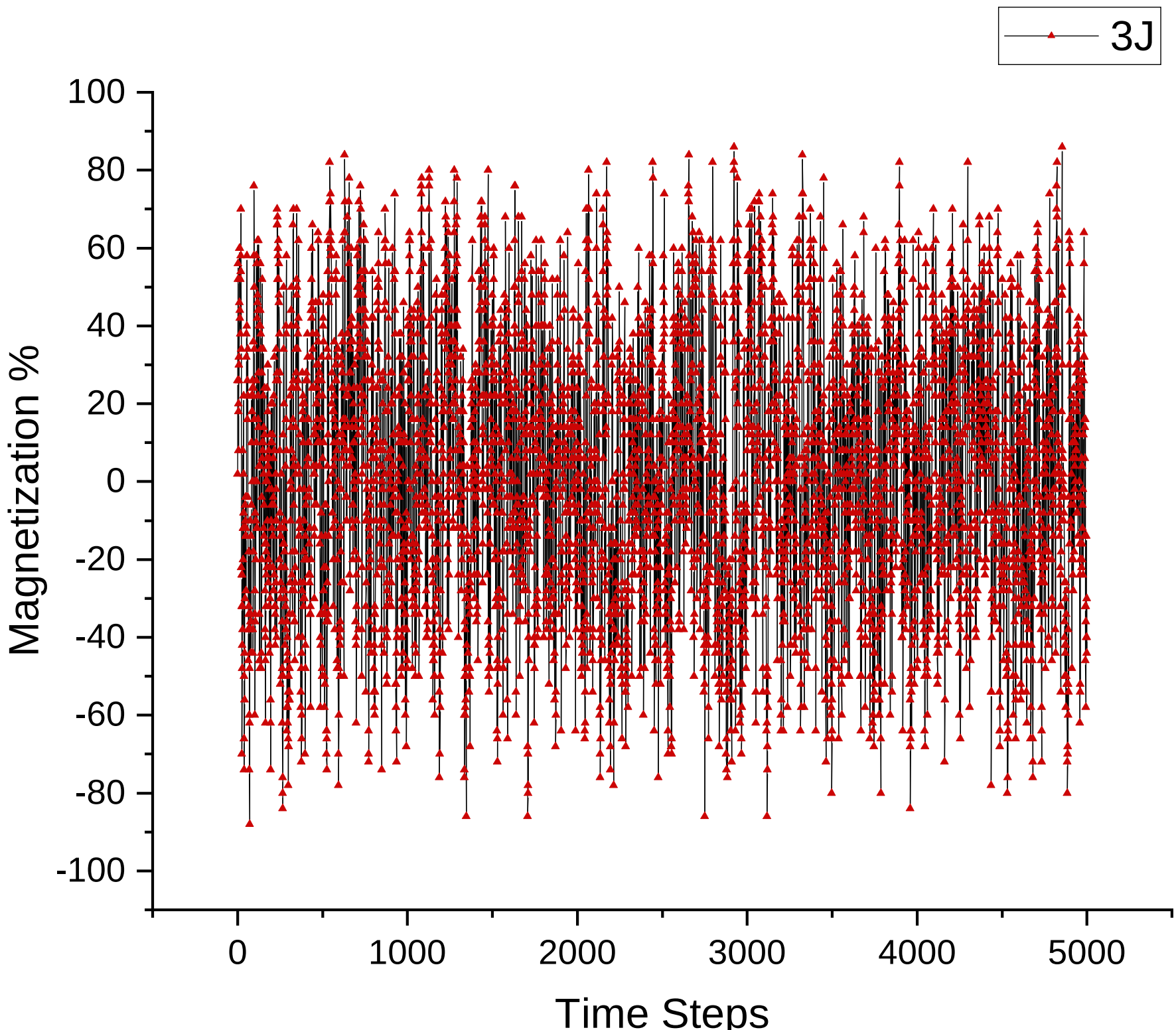
We then preformed this simulation for five different temperatures given in terms of Energy over the Boltzmann constant. W can see that as the temperature is increased, the average magnetization tends to oscillate, asymptotically falling to zero as the temperature increases. This can be seen in the final graph, where the average magnetization was plotted against a range of temperatures from 1 to 200 given in terms of energy over the Boltzmann factor.

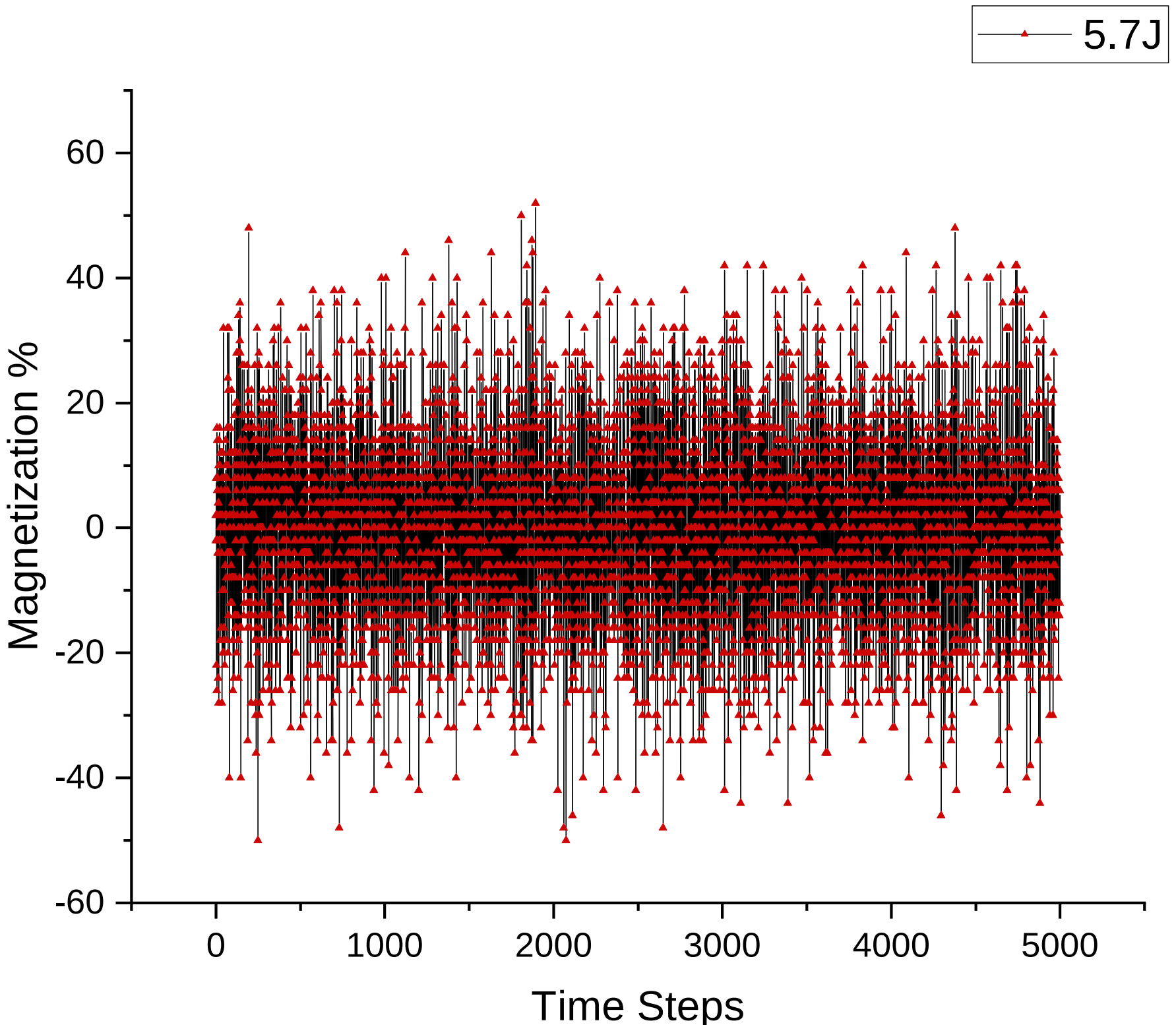
In the final graph the two methods were plotted side by side for comparison. We can see that the Monte-Carlo method predicts a quicker decay of the spin average, however the Mean Field method still offers good quantitative results.

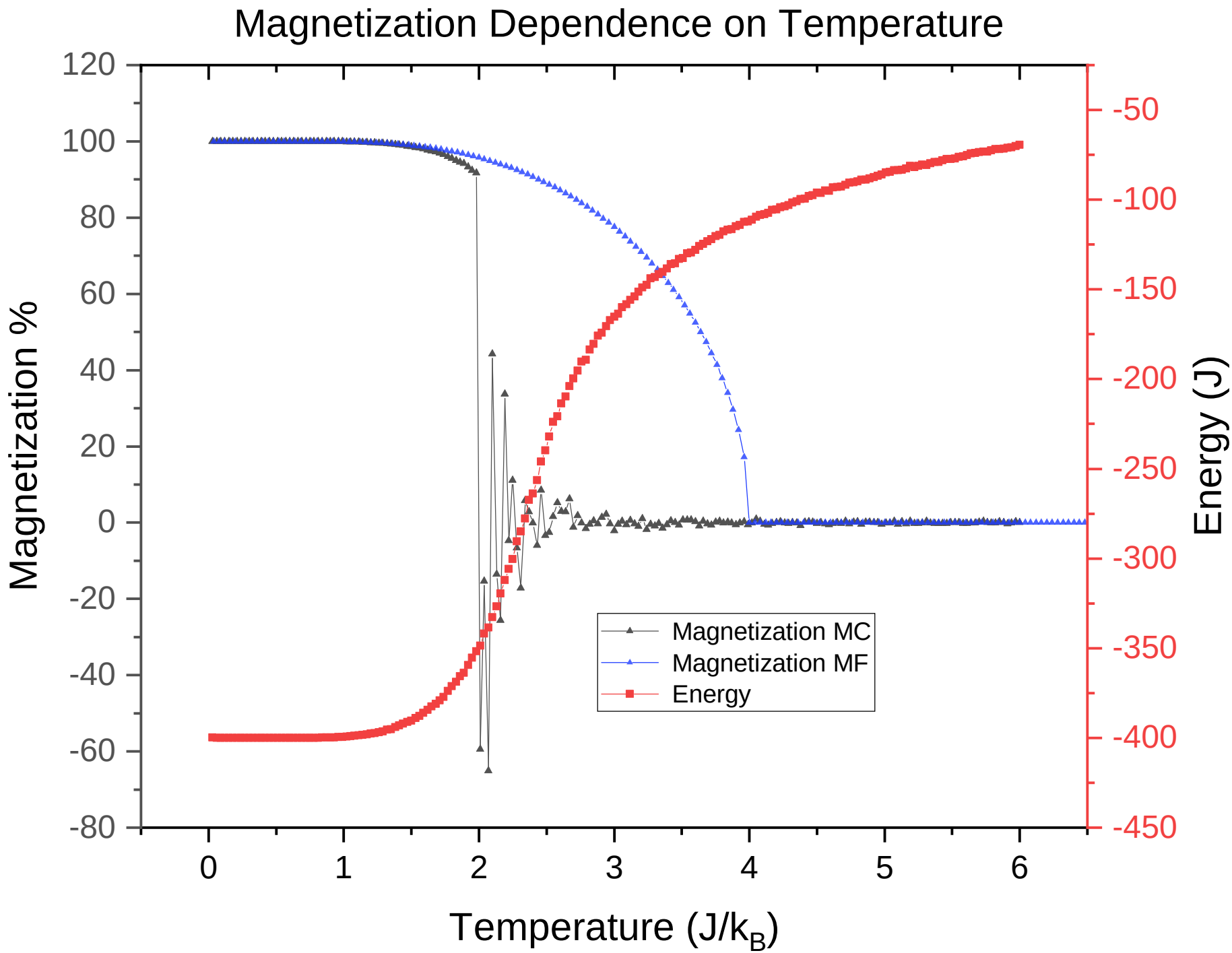

0.06J
110
100
90
80
70
60
50
40
30
20
Magnetization %
0
1000
2000
3000
4000
5000
Time Steps


1.5J
Magnetization %
100
80
60
40
20
0
-20
0
1000
2000
3000
4000
5000
Time Steps


2.28J
Magnetization %
100
50
0
-50
-100
0
1000
2000
3000
4000
5000
Time Steps


3J
100
80
60
40
20
0
-20
-40
-60
-80
-100
Magnetization %
0
1000
2000
3000
4000
5000
Time Steps


5.7J
60
40
20
0
-20
-40
-60
Magnetization %
0
1000
2000
3000
4000
5000
Time Steps


Magnetization Dependence on Temperature
Magnetization %
Energy (J)
Temperature (J/k_B)
Magnetization MC
Magnetization MF
Energy
120
100
80
60
40
20
0
-20
-40
-60
-80
-50
-100
-150
-200
-250
-300
-350
-400
-450
0
1
2
3
4
5
6