Physics Assignment 6

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Introduction

The Ising model serves as a foundational pillar in statistical mechanics, offering invaluable insights into ferromagnetism. Especially intriguing is its two-dimensional representation, which has been allows us to better our understanding of phase transitions. This report documents a simulation of the 2D Ising model via the Metropolis algorithm, delving into the resulting physical phenomena.

Data Capture

We make use of the metropolis algorithm. We start with the intial state with all spins up and from there we effectively select a spin at random and then flip the spin based on the metropolis acceptance probability according to the change in energy. If the $\Delta E < 0$ then the flip is accepted, else if $\Delta E > 0$ then the flip is accepted with probability of $e^{-\beta \Delta E}$. We continue this process for a large number of steps allowing the system to evolve. From there we can investigate different physicsal properties of the system after a period of equilibriation

In The Context of Random Walks

Random Walks

The Metropolis algorithm can be viewed as a random walk in the configuration space (or state space) of the system. Each spin flip proposal corresponds to taking a step in this space. Whether or not the step is accepted depends on the energy change, as dictated by the Metropolis criterion. Over time, the system wanders through various configurations, thus "exploring" the state space. We will revisit the equilibriation and ergodicity later on.

Exploring State Space

The state space of the Ising model is vast, especially for large lattice sizes. For a $L \times L$ lattice, there are 2^{L^2} possible configurations. The Metropolis algorithm allows efficient exploration of this space by preferentially sampling configurations that contribute most to the partition function (i.e., those with lower energy at low temperatures and a broader range of energies at high temperatures). This is more efficient than a naive approach that would sample configurations uniformly.

Initial Probability Distributions

When the simulation starts, the system might be in a configuration determined by some initial probability distribution. For instance, we start with all spins up . The choice can affect how long it takes for the system to equilibrate, but given enough time, the Metropolis algorithm should lead the system to sample from the Boltzmann distribution, regardless of the initial configuration.

Stationary Probability Distributions

The stationary probability distribution for the Ising model at a given temperature is the Boltzmann distribution:

$$P(s) = \frac{e^{-\beta E(s)}}{Z}$$

The Metropolis algorithm, after equilibration, samples states according to this distribution. That is, the probability of observing the system in a particular state s becomes proportional to $e^{-\beta E(s)}$. This is the primary goal of the algorithm: to get the system to a point where it's sampling from the stationary distribution.

Part I: Equilibration and Ergodicity

With lattice dimensions set at $L = 4, 10, 50$, the simulation was initialized in an all-up state. The βJ parameter was varied between 0.2 to 0.6, offering a comprehensive view of system behavior. *In this section we refer to the figures in the appendix; note further that $J = 1$ for all figures.

Findings

On observing the magnetization per unit area $\frac{M}{L^2}$: *Note that when we refer to M or $|M|$ we mean $\frac{M}{L^2}$ and $\frac{|M|}{L^2}$ respectively.

In Figures 3 through 5 we investigate the average magnetization per spin for Ł = 4. For figure 3 we have $\beta = 0.2$. Interestingly we see that the running average of M is approximately zero while the $|M|$ is not; from this we can conclude that the system must be flipping between a net positive and a net negative magnetization. This effect continues and increases in severity in figure 4 where $\beta = 0.4$, the increase in $|M|$ suggests that there is greater dependence between spins at this lower energy state which leads to a clustering of aligned spins.

Furthermore, we see the first signs of equilibration rearing its head; it takes a about 2000 sweeps for the running average of M to settle around 0. Moving to figure 5 we have $\beta = 0.6$

In figures 6 through 8 we do the same for the $L = 10$ case. We see a similar story but here there is very little clustering at high temperatures, and then more clustering as the temperature approaches the critical temperature which we see in figures 6 and 7 respectively. We can see the severity of the clustering via the magnitude of the running average of $|M|$. However, in figure 8 we see that the running averages are almost exactly the same which indicates that all or almost all the spins are aligned in the same direction, which in this case is up. This is the behaviour we would expect to see when $T < Tc$

In figures98 through 11 we continue for the $L = 50$ case. Here we have the same story, the only difference being that the variations in M and $|M|$ are smaller. We see that larger values of L produce a better model for our system.

- For $L = 4$: The system takes longest to reach equilibrium. The magnetization displayed major fluctuations. We put this down to the small size of the system.
- For $L = 10$: A less pronounced equilibration time was observed. The fluctuations in magnetization were moderate, suggesting the system's slightly increased complexity.
- For $L = 50$: Here, the equilibration process was the shortest. Post-equilibration, the magnetization depicted small oscillations.

These observations are counter-intuitive as we might expect the larger L values to have larger equilibration values. This could be due to the smearing and other effects which make smaller systems less reliable; hence we might expect to see this behaviour (longer equilibration for larger values of L) with values of L that are much larger. I try to illustrate this with figure 12 where I set $L = 200$, however there is no clear indication of a longer equilibration period, this is something interesting that will require further analysis to decipher. We see that the behaviour of the system is more clear for $L = 50$ post-equilibriation compared to the smaller L values, this is clear in the $\beta = 0.6$ graphs where we would expect the the spins to align due to $T < T_c$ and lead to a consistent running average for M, but for the $L = 4$ case the running average magnetization varies tremendously. To illustrate my point in figure 12 where $\beta = 0.7$,which is a temperature range where we would most definitely expect alignment, we see that it is most definitely not happening. This indicates that the $L = 4$ case is not reliable as a model for our system; this is most probably due to Finite-Size Effects, meaning the effects of the phase transition are smeared out over a range of temperatures. Further the boundary effects due to the periodic boundary conditions could be playing a role. The smaller the system, the more significant this smearing. For larger lattices, the transition becomes sharper.

Equilibration Period

Looking at the plots, there is a clear equilibration period where the magnetization fluctuates significantly before stabilizing. This is most pronounced for smaller values of L . For $L = 4$, equilibration is quite slow, while for $L = 50$, it takes less sweeps for the system to equilibrate. An estimate of this period can be made by observing where the running average starts to flatten or change at a reduced rate. For $L = 50$, this appears to be around only a few hundred sweeps for temperatures not near the T_c, although this depends on the temperature. It is also important to note that near the transition point the equilibration period is longer for all values of L.

Ergodicity

The ergodic hypothesis suggests that, given enough time, a system will visit all accessible states. If our simulation were perfectly ergodic, the running average would converge to a stable value and remain there. Given the fluctuations we see, especially at larger system sizes, it suggests that the simulation might not be fully exploring all the relevant parts of the system's state space within the given number of sweeps. However, the running averages do seem to stabilize, indicating a degree of ergodicity.

Role of Temperature

Temperature plays a significant role in the behavior of the Ising model. At low temperatures (e.g., $\beta J = 0.6$), the system tends to order (all spins aligned), while at higher temperatures (e.g., $\beta J = 0.2$), it is more disordered. This is evident in the plots, where the magnetization at lower temperatures stabilizes at a higher value compared to higher temperatures.

Change in Behavior at Specific Temperature

While we didn't explicitly plot a phase transition graph here, the Ising model has a critical temperature at which a phase transition from ordered to disordered state occurs. This can be inferred from the behavior seen in the plots, especially for larger system sizes. The temperature at which this change becomes pronounced would be close to the critical temperature.

Part II: Probing Average Magnetisation

Experimental Setup

For this portion of the investigation, the lattice size was expanded to $L = 200$, providing a sufficiently large system to capture emergent macroscopic phenomena. Our primary aim was to understand how the average magnetization metrics

$m = \langle M \rangle / L^2$ and $m_{\text{abs}} = \langle |M| \rangle / L^2$ behave as functions of βJ, the inverse temperature scaled by the coupling constant J; and what we can infer about the phase transition of the system. I made sure that the equilibration period was larger for the simulation at β values close to the transition.

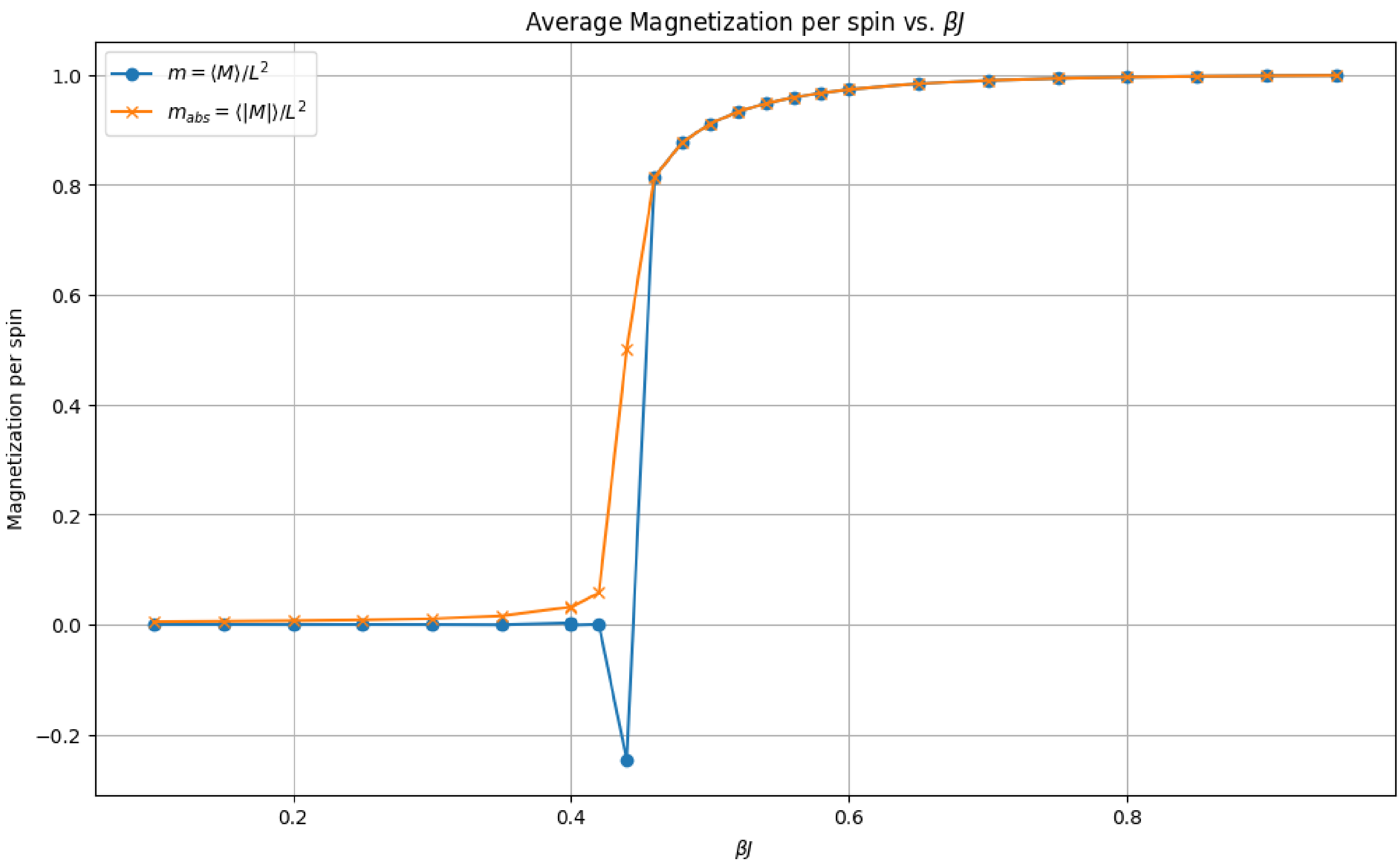


Figure 1: Average Magnetization

Findings

We see that the average magnetization starts at 0 for small values of β i.e. high temperatures , which is what we expect as we know that at high temperatures the spins should be orientated randomly and independently of one another, since the energy cost of misaligned spins is irrelevant - this is the ferromagnetic state. Thus the average magnetization should be zero or close to zero as β increases.

Once β reaches aprroximately 0.42 the phase transition occurs which we see manifested in the sudden and drastic change in the average magnetization. The average magnetization very rapidly tends to 1 which indicates that almost all the spins are aligned in the same direction. This occurs in order to minimize the system's energy . This is the paramagnetic state.

- **Phase Transition**: A distinct phase transition was observed around $\beta J \approx 0.42$. This is a significant result, as it marks the temperature below which spontaneous magnetization manifests, indicative of ferromagnetic ordering. Above this point, the system remains largely disordered.
- **Disordered Region ($\beta J < 0.42$)**: Within this temperature range, the system exhibited behaviors characteristic of a paramagnet. The spins were largely uncorrelated, resulting in a near-zero net magnetization. This is consistent with the high-temperature behavior of the Ising model, where thermal energy dominates over spin-spin interactions.
- **Ordered Region ($\beta J > 0.42$)**: As the temperature was lowered (or equivalently, βJ was increased), a sharp rise in m and m_{abs} was observed, indicative of spontaneous alignment of spins. This ferromagnetic ordering is emblematic of the Ising model's low-temperature phase, where spin-spin interactions result in large domains of aligned spins.

Discussion

The phase transition observed at $\beta J \approx 0.42$ stands testament to the Ising model's prowess in capturing real-world physical phenomena, such as ferromagnetism. The sharpness of the transition, especially in a large system like ours ($L = 200$).

Furthermore, the regions on either side of this critical point (βJ_c) offer valuable insights:

- The disordered phase at higher temperatures mirrors the behavior of real materials that lose their magnetic ordering when subjected to significant thermal agitation.
- The ordered phase, with its pronounced magnetization, mirrors the behavior of ferromagnetic materials below their Curie temperature, where domains of aligned spins contribute to a net magnetic moment.

Side Note About Spontaneous Symmetry

In the context of the Ising model, there's a natural symmetry in the system's Hamiltonian. It's invariant to flipping all the spins. This means that the Hamiltonian does not favor one direction of magnetization over the other. If you flip all the spins, the energy remains the same. The canonical ensemble predicts that the expected value of M should be zero when $h = 0$, irrespective of the temperature, due to the mentioned symmetry. However, in practice and in our case, for an ergodic system, the ensemble average of an observable should match the long-time average. If the system is not ergodic, the ensemble average may not represent the actual physical state of the system. In the case of magnetization, once a direction is chosen, it persists for a long time, rendering the system effectively non-ergodic. Hence, the time average of magnetization is non-zero, breaking the spin-flip symmetry.

Part III: Delving into Specific Heat and Magnetic Susceptibility

The metrics of specific heat c and magnetic susceptibility χ were computed using:

$$\frac{c}{k} = \beta^2 \frac{\langle E^2 \rangle - \langle E \rangle^2}{N}$$
$$\chi = \beta \frac{\langle M^2 \rangle - \langle M \rangle^2}{N}$$

Findings

The specific heat c/k and the magnetic susceptibility χ are two critical thermodynamic quantities that provide insights into the behavior of a system close to a phase transition.

* Find figure 16 in appendix

- **Specific Heat** $\left(\frac{c}{k}\right)$:
  - This quantity tells us about the system's response to a change in temperature. Specifically, it measures the amount of energy required to change the temperature of the system by a small amount.
  - Near a phase transition, the specific heat typically shows a peak, indicating increased fluctuations in energy.
- **Magnetic Susceptibility** (χ):
  - The magnetic susceptibility quantifies how much the system responds to an applied magnetic field. A large χ indicates that the system is very responsive to magnetic fields.
  - Near a phase transition, χ typically diverges, reflecting increased fluctuations in magnetization.

Part IV: Insights from Two-point Function and Correlations

The spin-spin correlation function $g(r)$ serves as a window into the underlying correlations of the system. For large distances, $g(r)$ tends to decay exponentially, revealing the system's inherent correlation length ξ. // // *Note figures can be found in appendix

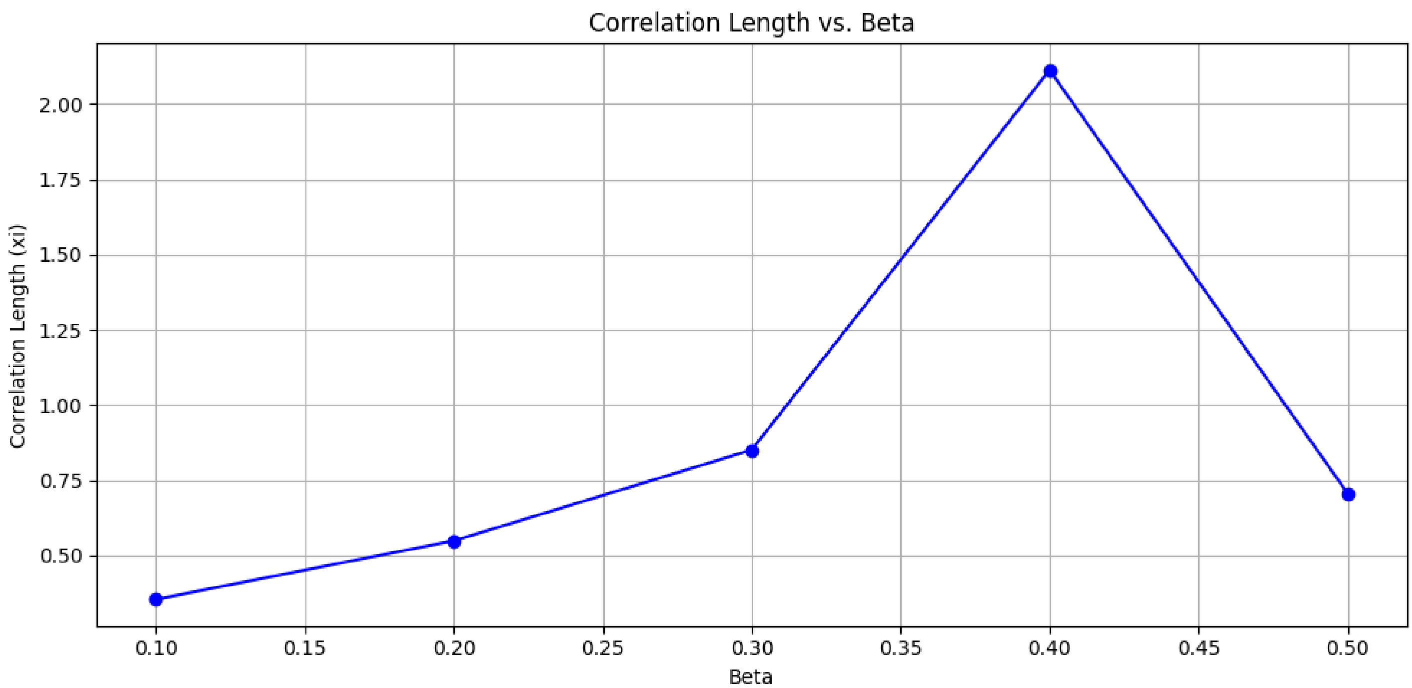


Figure 2:

We see that the correlation length is greatest near the transition point.

$G(r)$ vs r

- As r increases, $G(r)$ decreases. This indicates that the correlation between spins decreases with increasing distance, which is expected.
- For lower β values (higher temperatures), the correlation function drops to zero more quickly, indicating that spins are less correlated over distances. This is consistent with the high-temperature disordered phase of the Ising model.
- As β increases (temperature decreases), the correlation length (the distance over which spins are significantly correlated) seems to increase, suggesting a transition towards a more ordered phase.

$g(r)$ vs r

- The deviation $g(r)$ also decreases with increasing r, consistent with the behavior of $G(r)$.
- The deviation is larger at smaller β values, indicating stronger fluctuations in the spin-spin correlations at higher temperatures.

Conclusion

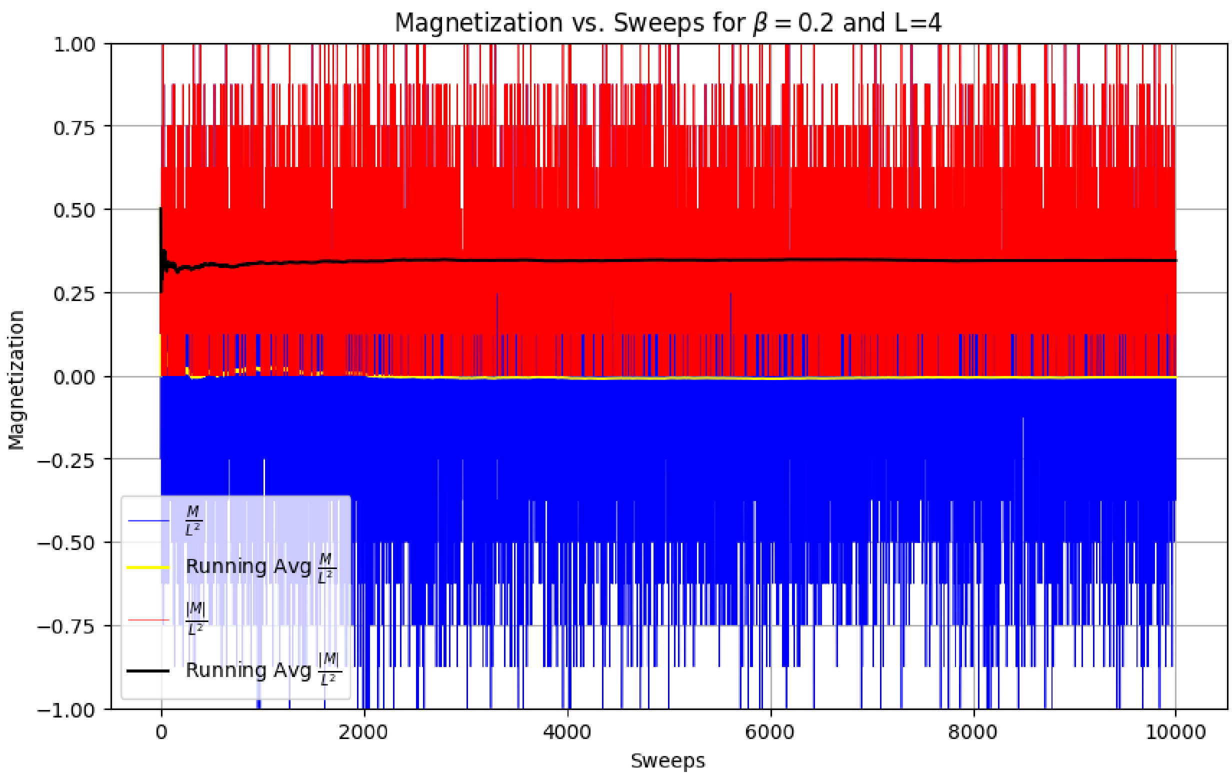
The Ising model, simulated using the Metropolis algorithm, provides valuable insights into phase transitions and critical phenomena. Through our simulations, we observed the behavior of the Ising model across different temperatures and system sizes.

The visualizations clearly demonstrated the equilibration process and highlighted how temperature affects system order. At high temperatures, the system tends to be disordered due to increased thermal fluctuations, while at lower temperatures, the system leans towards an ordered state because of stronger spin-spin interactions.

However, one challenge that became evident was achieving ergodicity in larger systems. Larger lattices have a broader range of possible configurations, making it difficult to sample all states in a practical timeframe. This highlights some computational limitations when simulating larger systems.

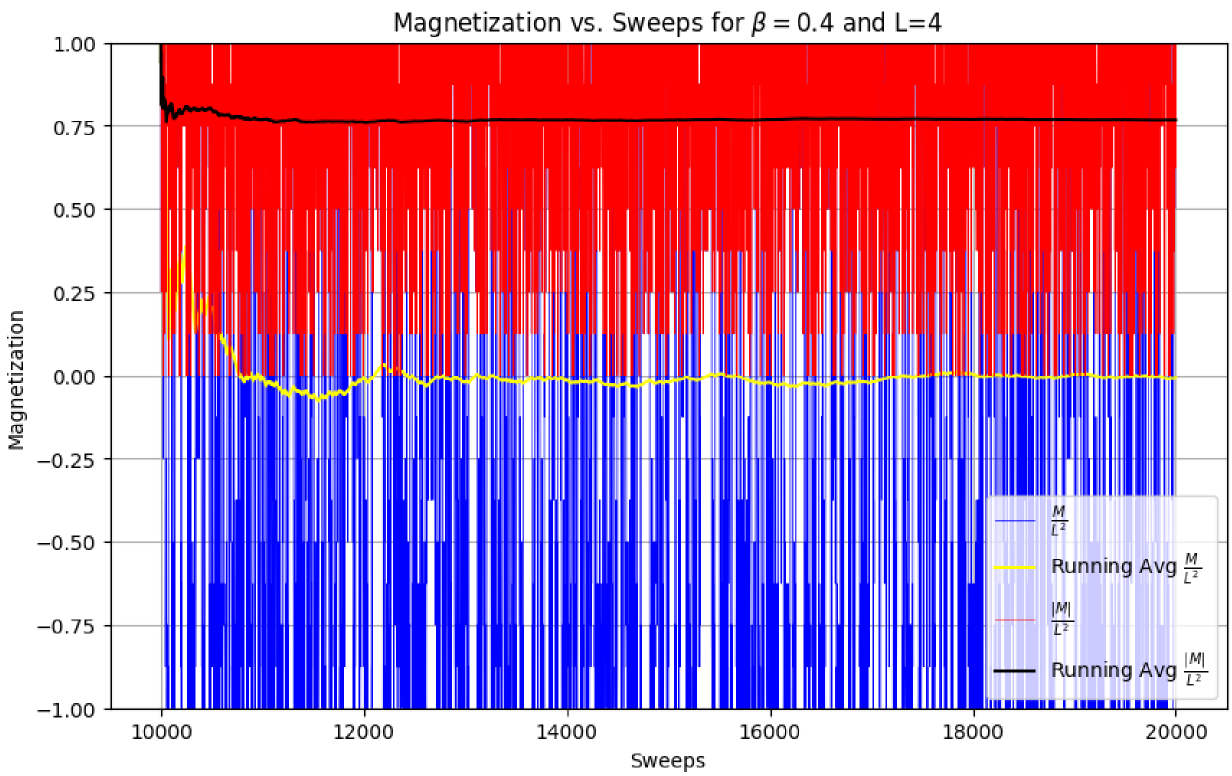
In summary, the Ising model, combined with the Metropolis algorithm, is a powerful tool for understanding complex physical systems. It emphasizes the importance of computational methods in complementing theoretical understanding.

Appendix



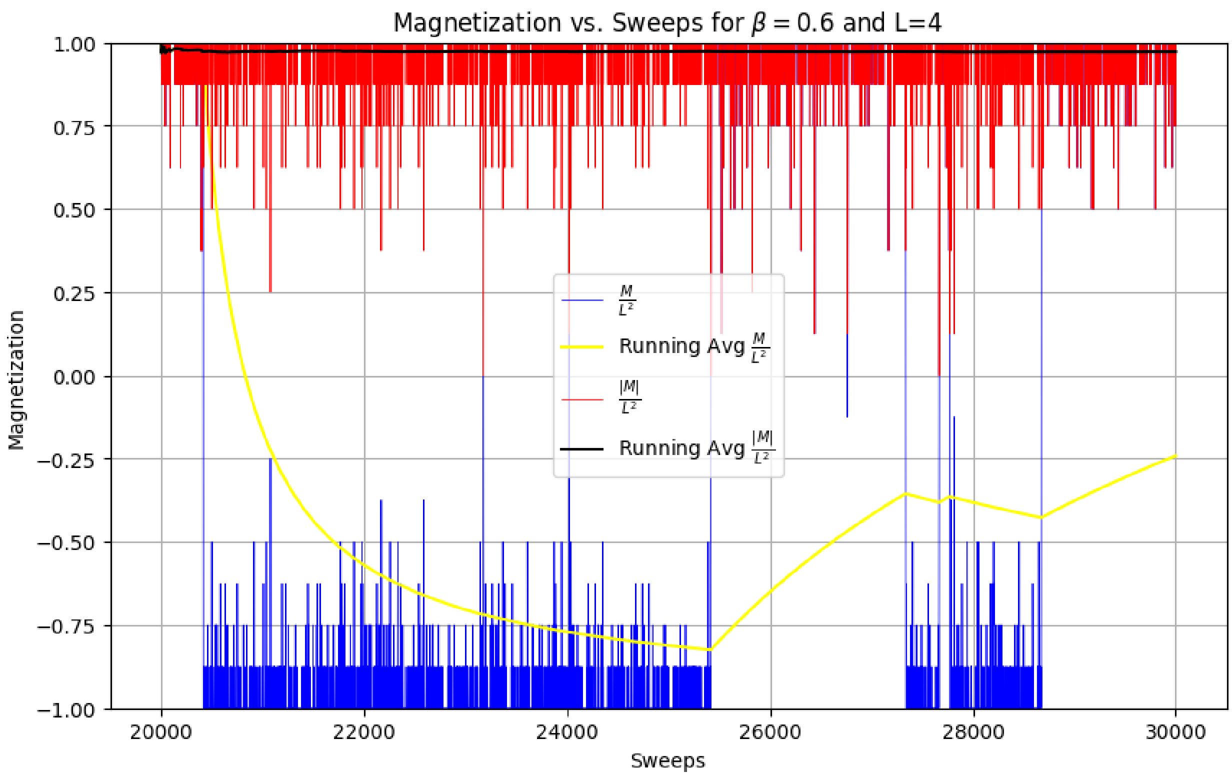
Magnetization vs. Sweeps for $\beta = 0.2$ and L=4
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Magnetization
0
2000
4000
6000
8000
10000
Sweeps
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 3:



Magnetization vs. Sweeps for $\beta = 0.4$ and L=4
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Magnetization
10000
12000
14000
16000
18000
20000
Sweeps
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 4:



Magnetization vs. Sweeps for $\beta = 0.6$ and L=4
Magnetization
Sweeps
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
20000
22000
24000
26000
28000
30000
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 5:

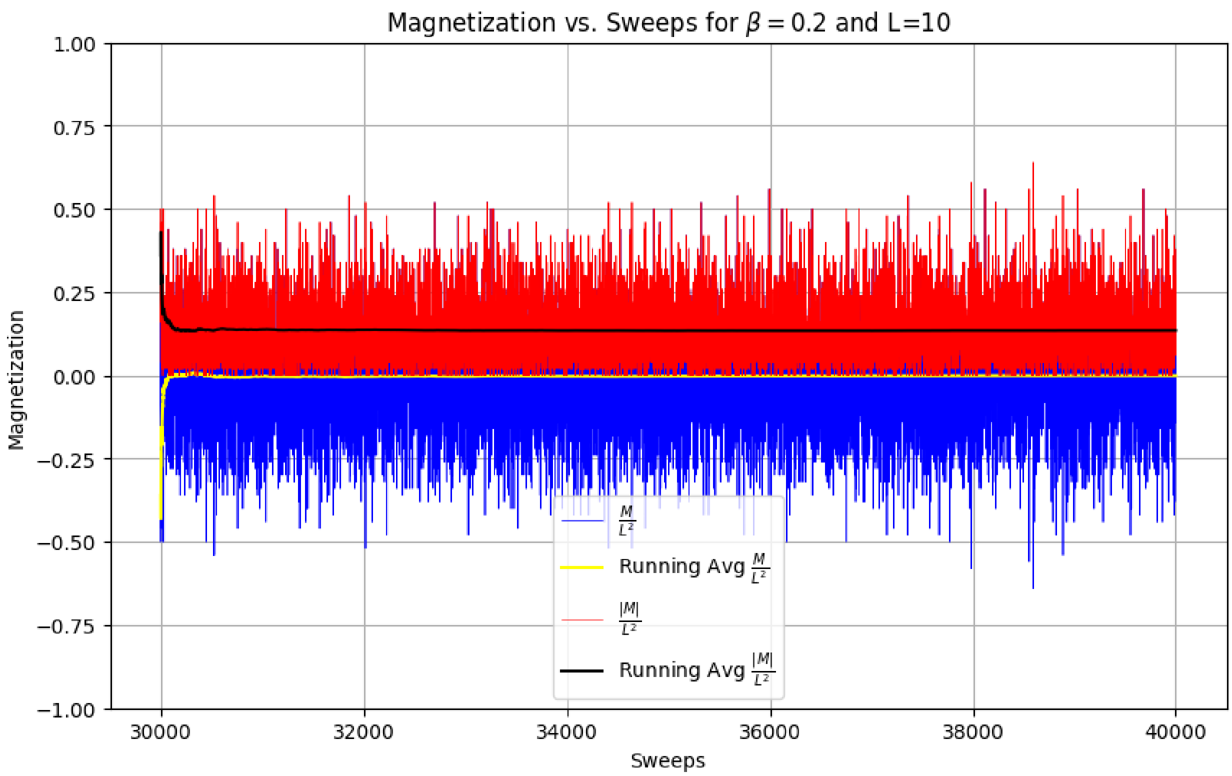
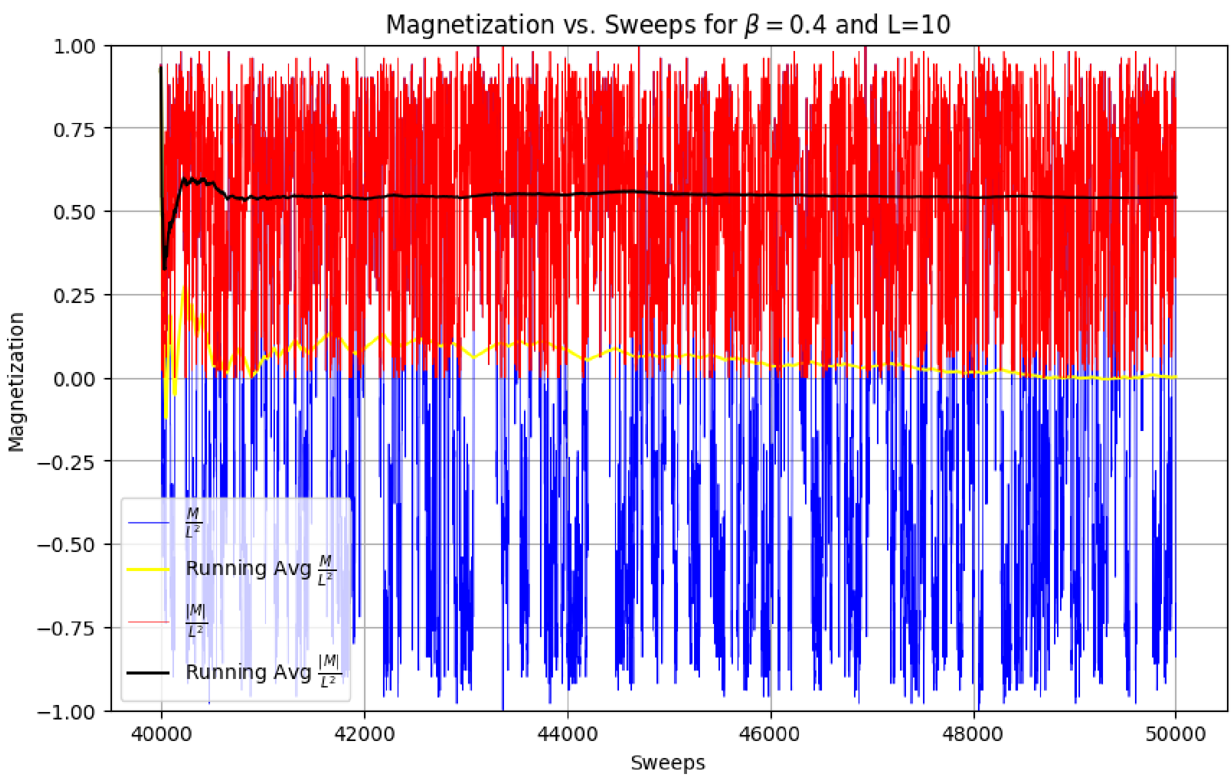

Magnetization vs. Sweeps for $\beta = 0.2$ and L=10
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Magnetization
30000
32000
34000
36000
38000
40000
Sweeps
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 6:



Magnetization vs. Sweeps for $\beta = 0.4$ and L=10
Magnetization
Sweeps
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
40000
42000
44000
46000
48000
50000
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 7:

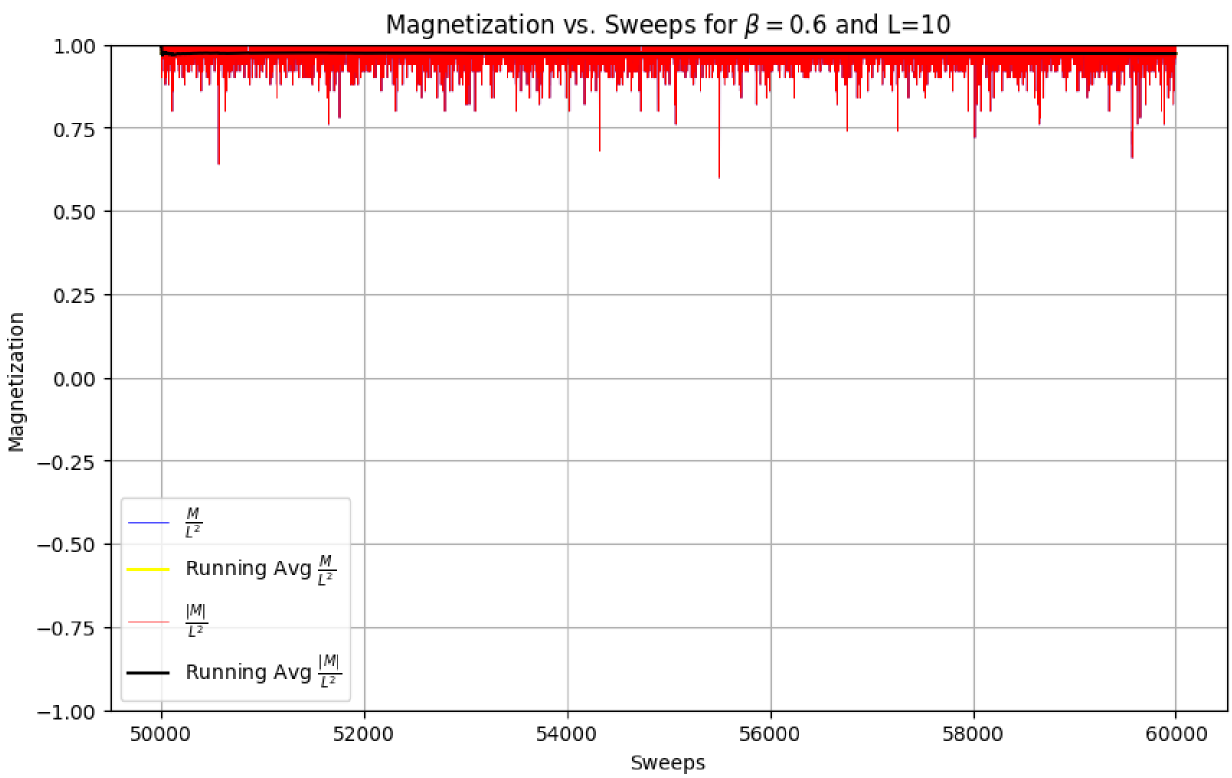
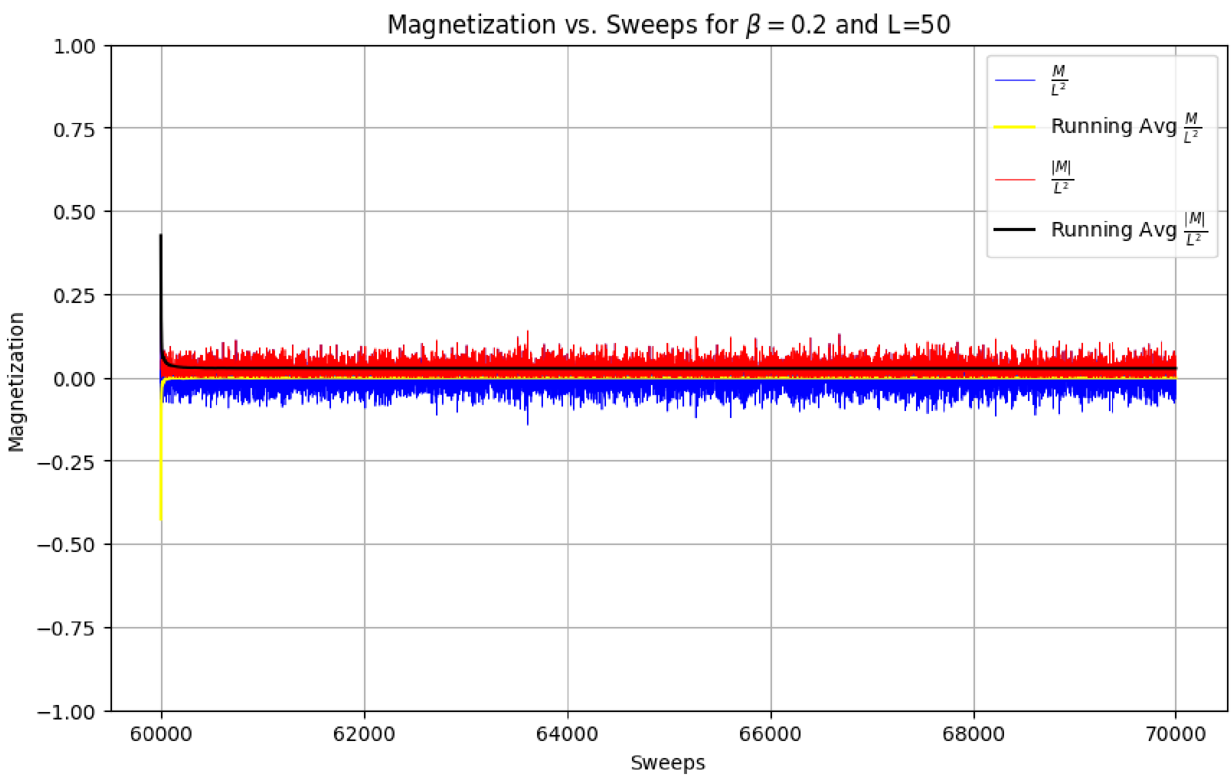
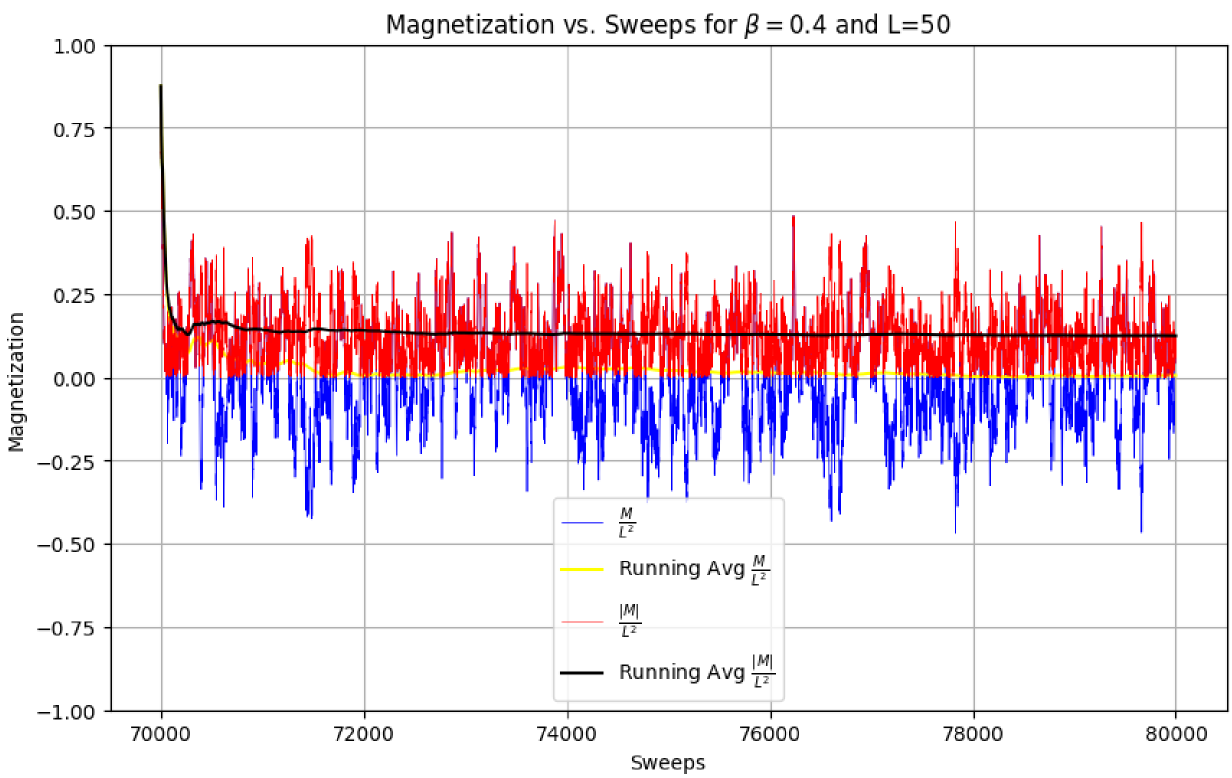

Magnetization vs. Sweeps for $\beta = 0.6$ and L=10
Magnetization
Sweeps
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
50000
52000
54000
56000
58000
60000
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 8:



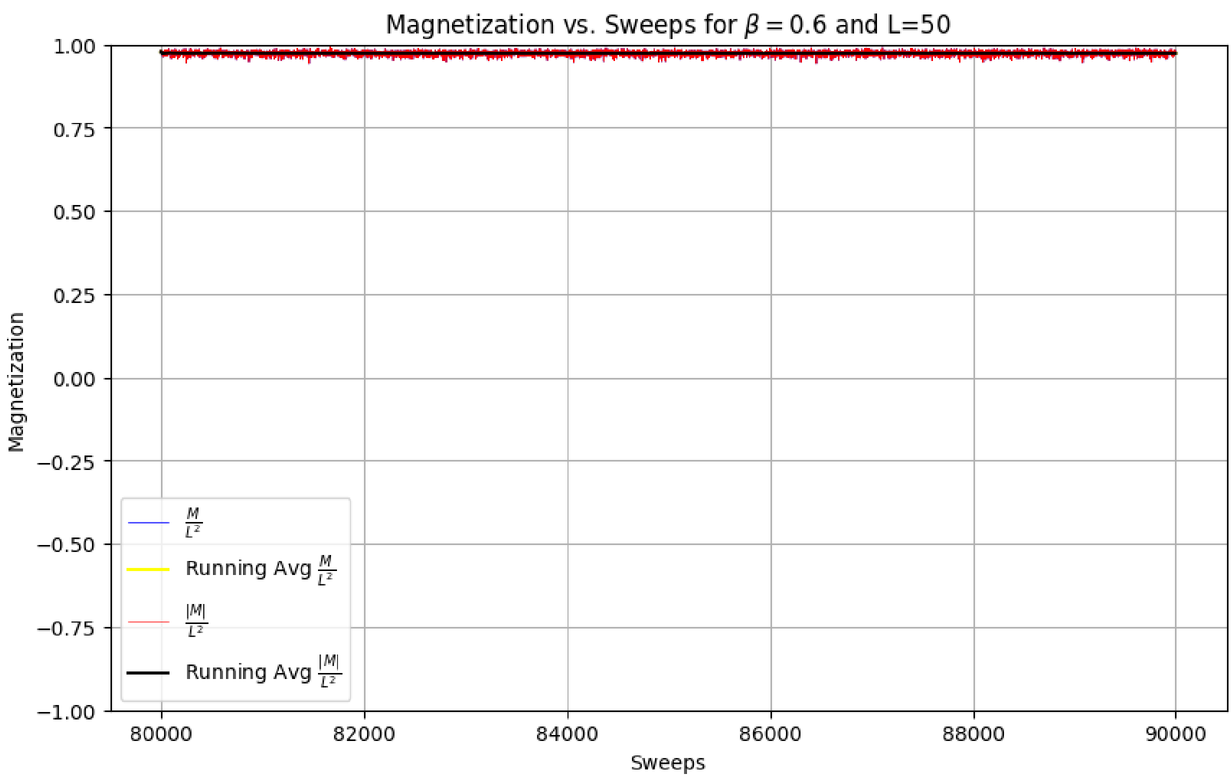
Magnetization vs. Sweeps for $\beta = 0.2$ and L=50
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Magnetization
60000
62000
64000
66000
68000
70000
Sweeps
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 9:



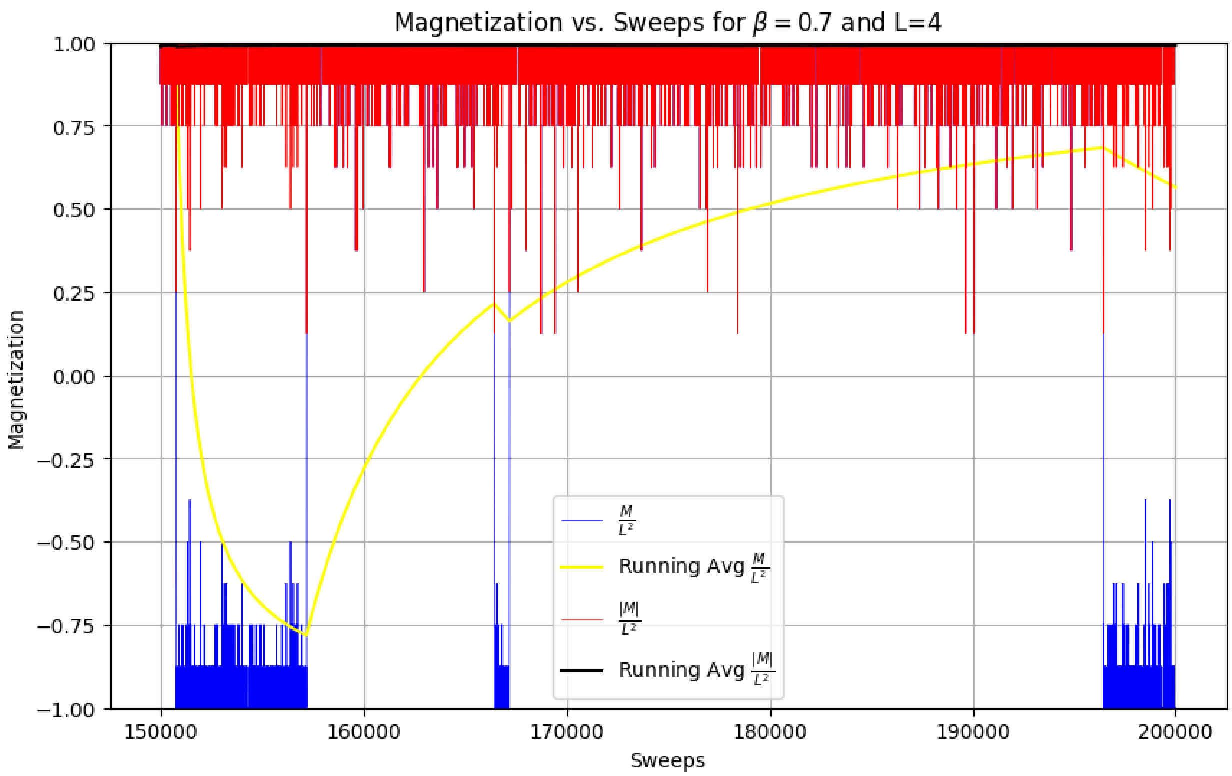
Magnetization vs. Sweeps for $\beta = 0.4$ and L=50
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Magnetization
70000
72000
74000
76000
78000
80000
Sweeps
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 10:



Magnetization vs. Sweeps for $\beta = 0.6$ and L=50
Magnetization
Sweeps
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
80000
82000
84000
86000
88000
90000
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 11:



Magnetization vs. Sweeps for $\beta = 0.7$ and L=4
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Magnetization
150000
160000
170000
180000
190000
200000
Sweeps
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 12:

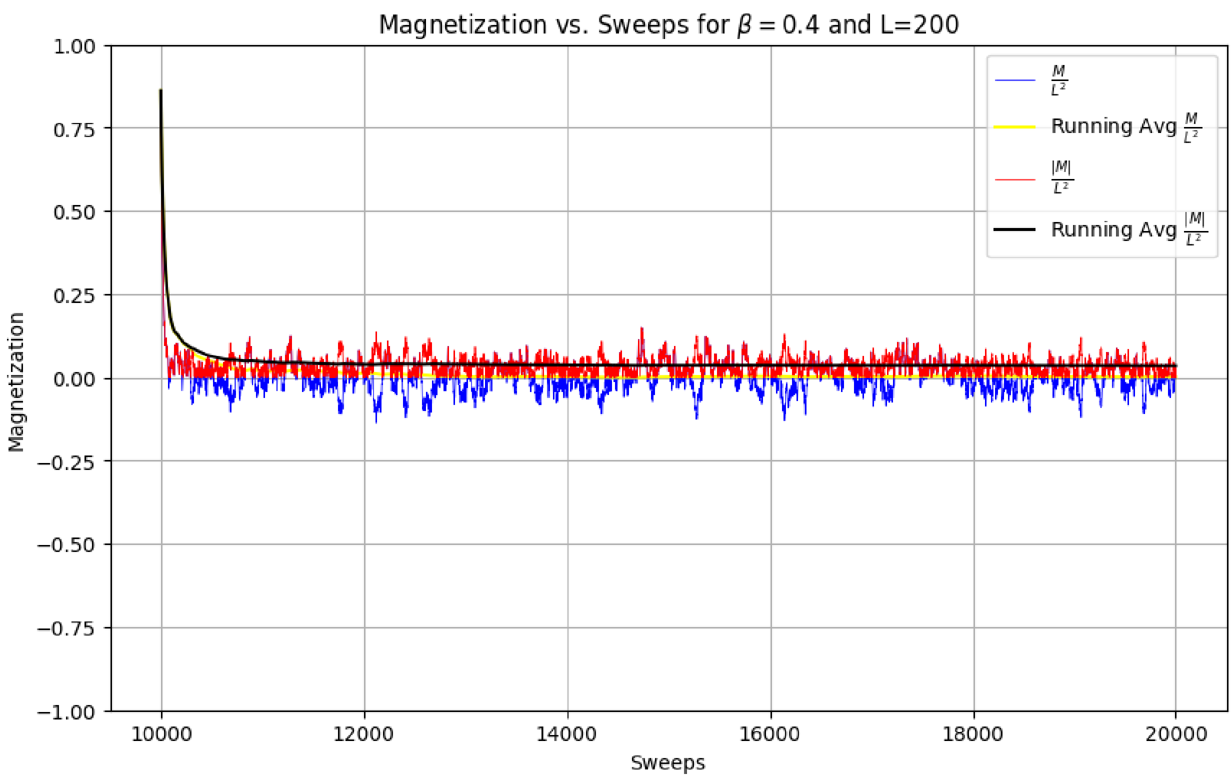
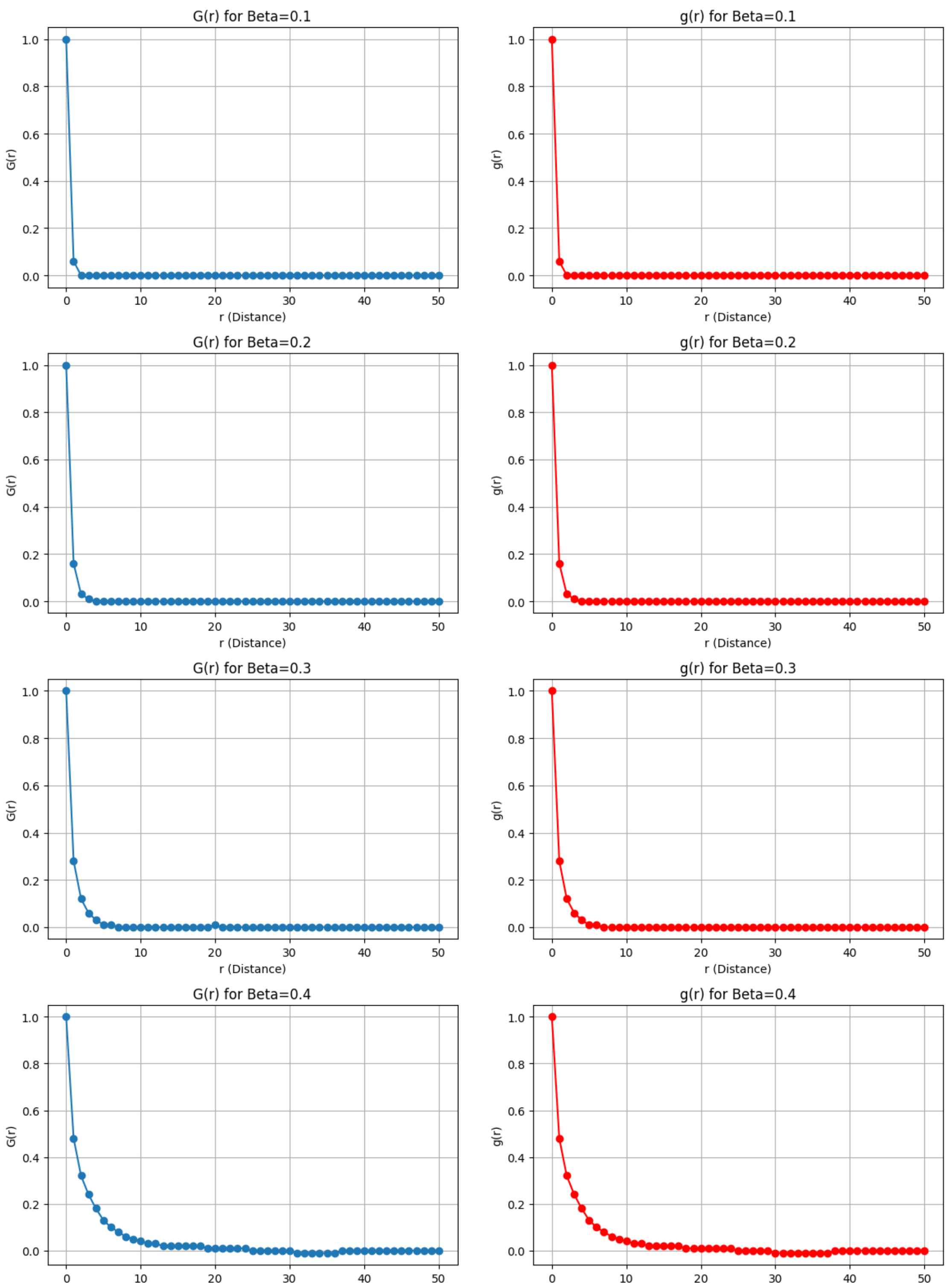
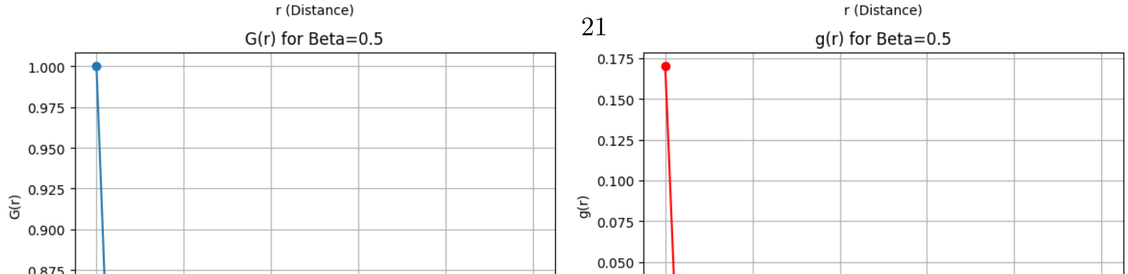
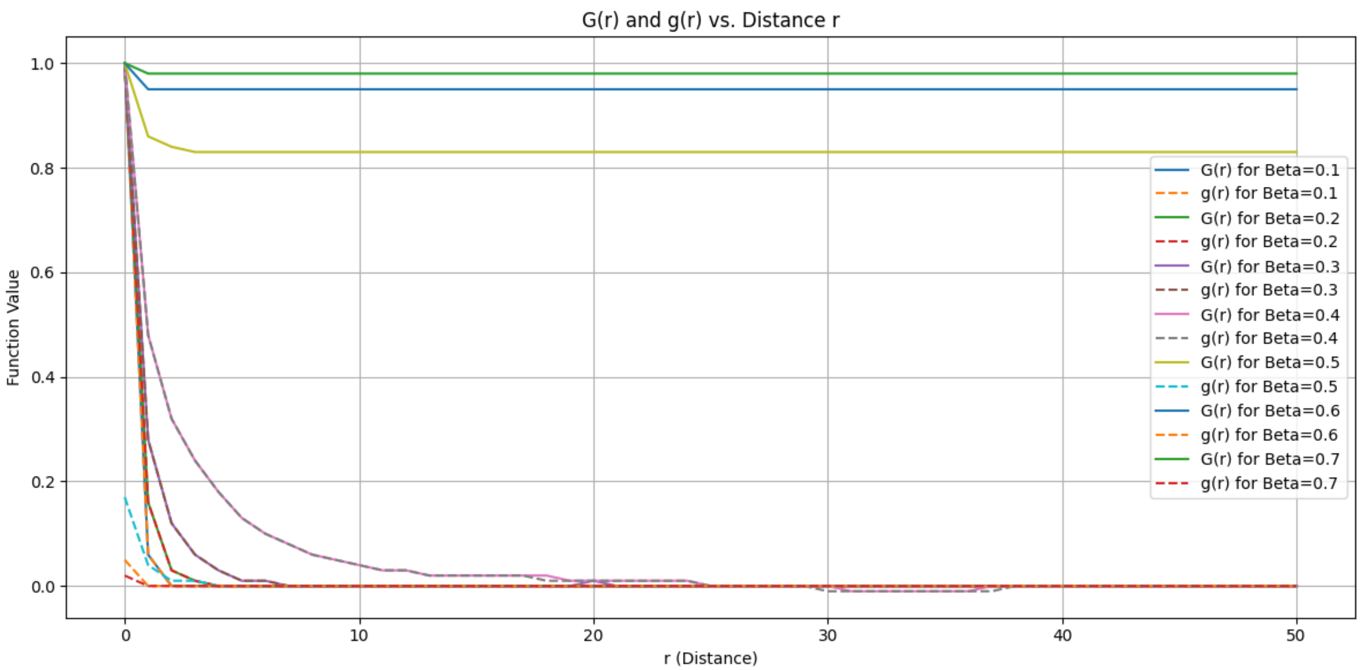

Magnetization vs. Sweeps for $\beta = 0.4$ and L=200
Magnetization
Sweeps
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
10000
12000
14000
16000
18000
20000
$\frac{M}{L^2}$
Running Avg $\frac{M}{L^2}$
$\frac{|M|}{L^2}$
Running Avg $\frac{|M|}{L^2}$

Figure 13:


G(r) for Beta=0.1
g(r) for Beta=0.1
G(r) for Beta=0.2
g(r) for Beta=0.2
G(r) for Beta=0.3
g(r) for Beta=0.3
G(r) for Beta=0.4
g(r) for Beta=0.4
G(r)
g(r)
r (Distance)


G(r) for Beta=0.5
g(r) for Beta=0.5
G(r)
g(r)



G(r) and g(r) vs. Distance r
1.0
0.8
0.6
0.4
0.2
0.0
Function Value
0
10
20
30
40
50
r (Distance)
G(r) for Beta=0.1
g(r) for Beta=0.1
G(r) for Beta=0.2
g(r) for Beta=0.2
G(r) for Beta=0.3
g(r) for Beta=0.3
G(r) for Beta=0.4
g(r) for Beta=0.4
G(r) for Beta=0.5
g(r) for Beta=0.5
G(r) for Beta=0.6
g(r) for Beta=0.6
G(r) for Beta=0.7
g(r) for Beta=0.7

Figure 15:

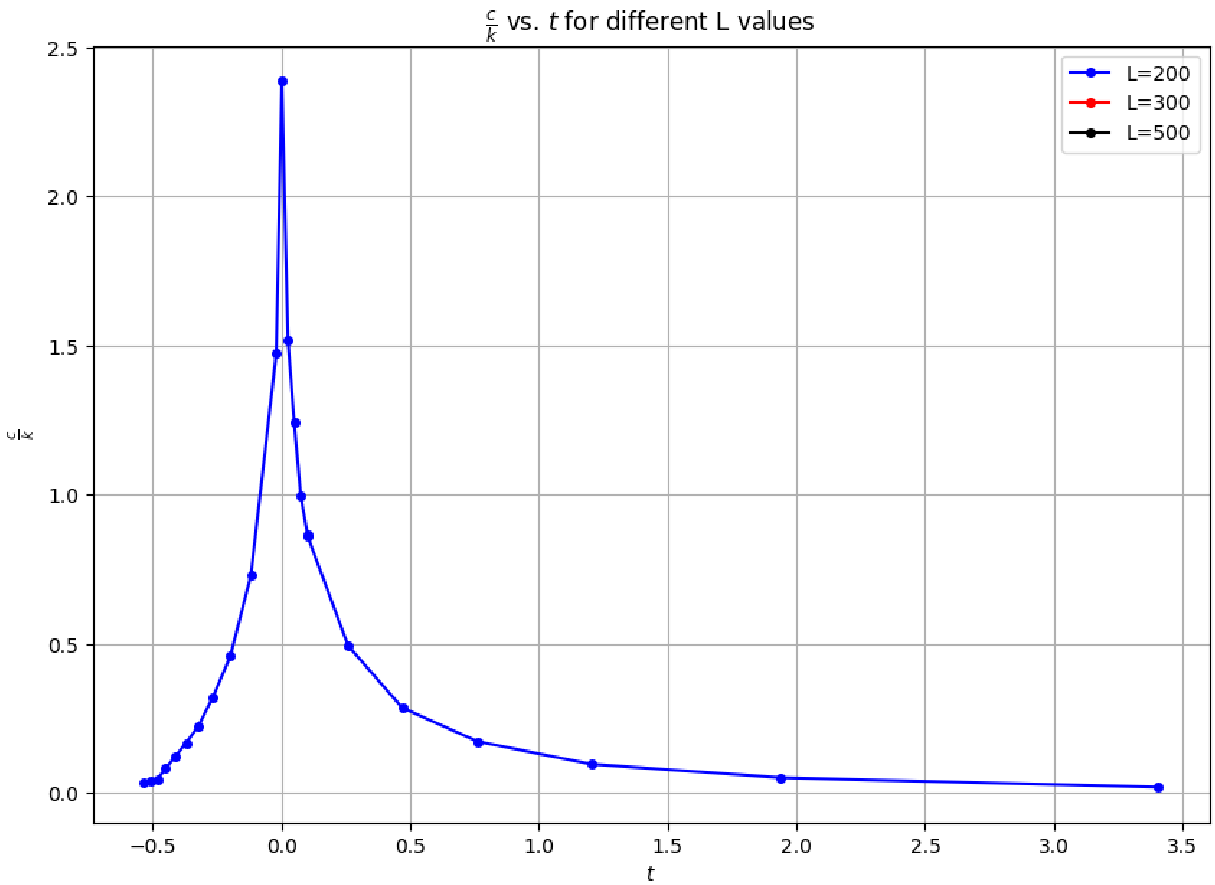

$\frac{c}{k}$ vs. t for different L values
L=200
L=300
L=500
$\frac{c}{k}$
t
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5

Figure 16: