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Numerical study of the 2D Ising Model
Final Report

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1 Ising Model

§1.1 Phase Transition in Ising Model

Phase Transition is a widely studied physical process used to characterise the behaviour of substances when subjected to a change in external conditions, like temperature or pressure.

Different phases of a substance differ in their disorderedness. The more ordered a phase is, the less symmetric it becomes. This disorderedness is quantified by the *order-parameter*. For example, density is an order-parameter for phase transition from solid to liquid, magnetisation is an order-parameter for magnetic systems. The point at which the phase change occurs is called the *Critical Point* and the study of critical phenomenon is an active area of research.

The *Ising Model* is one of the widely studied models for ferromagnetism. The model consists of a lattice with spins, interacting with its nearest neighbours with coupling constant J and an applied external field h. The Hamiltonian for the system is given by:

$$\boxed{\mathcal{H} = -J\sum_{\langle ij \rangle}\sigma_i\sigma_j - h\sum_i \sigma_i}$$

σ_i denotes the i^{th} spin in the lattice and $\sigma_i \in \{-1, +1\}$. $\langle ij \rangle$ denotes the sum over the nearest neighbour of σ_i.

We will consider the study of the zero-field case ($h = 0$) and take $J = 1$. We will take $k_B = 1$, that is, temperature will be measured in units of energy.

In one-dimension, in the absence of external field, Ising Model shows no phase transitions. However, for higher dimensions, it shows a phase transition from a ordered ferromagnetic phase to a disordered paramagnetic phase above a critical temperature T_c, characterised by a continuous change in the magnetisation m which is the order parameter. Exact analytic solution exists for the 1D and 2D case, however no analytic solution exists for 3D case.

The Ising Model is thus an example of a **continuous phase transition**.

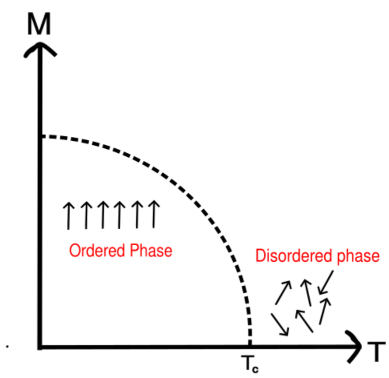


Figure 1.1: Magnetisation variation with temperature for a magnetic system

The figure shows a schematic of the variation of magnetisation with temperature. The critical point has been denoted by T_c.

When T is large, the average magnetisation is zero, denoting a *disordered phase*. The spins in the lattice are oriented randomly due to high thermal fluctuations and have no correlation among them, thus there is no magnetisation. As T decreases below T_c, we see that magnetisation gradually rises to a finite value, denoting an *ordered magnetic phase*.

The critical temperature for the 2D Ising Model in square lattice, obtained from the analytic solution is: $T_c = \dfrac{2}{\ln(1+\sqrt{2})} \approx 2.27$

§1.2 Spin Dynamics

We consider a one dimension Heisenberg model.

$$\boxed{\mathcal{H} = -J_1 \sum_i^n \sigma_i^z \sigma_{i+1}^z - J_2 \sum_i^n \sigma_i^x \sigma_{i+1}^x - J_3 \sum_i^n \sigma_i^y \sigma_{i+1}^y}$$

Ising model is a special case of the above model where σ^x and σ^y terms are absent. Then, if we consider the time evolution of the spin, we have:

$$\boxed{i\hbar \frac{d\sigma_i^z}{dt} = [\mathcal{H}, \sigma_i^z,]}$$

Since the Ising hamiltonian has only σ^z terms, the commutator is 0 and hence $\dfrac{d\sigma_i^z}{dt} = 0$. Thus, **Ising Model has no intrinsic dynamics**. The dynamical nature is introduced through thermal fluctuations. The dynamics of the system due to these thermal fluctuations are governed by a master equation which follows the two important conditions:

- Ergodicity
- Detailed Balance

From this, we can define different rates by which the system evolves, of which Glauber dynamics is one.

Various algorithms have been developed to simulate the Ising Model. Most of them follow single spin flip dynamics like Metropolis algorithm, Glauber dynamics while Wolff and Swendsen-Wang Algorithm follow cluster flip algorithms. Here, Ising Model is simulated using **Glauber Dynamics**.

1.2.1 Markov Process and Monte-Carlo Simulation

We consider the evolution of states to be a **Markov process**, that is, the evolution to the next state depends only on the present state of the system and not on any previous states. The system goes from the present state μ to ν with some time-independent transition probability $\mathbb{P}(\mu \longrightarrow \nu)$.

The condition of **Ergodicity** is a necessary condition for such evolution. It should be possible for the Markov process to reach any state of the system from any other state.
The master equation governing the transition probability is given by

$$\frac{d}{dt}w_\mu(t) = \sum_\nu w_\mu(t)\mathbb{P}(\mu \longrightarrow \nu) - \sum_\nu w_\nu(t)\mathbb{P}(\nu \longrightarrow \mu)$$

where $w_\mu(t)$ denotes the probability of finding the system in state μ at time t. After long time, $w_\mu(t)$ and $w_\nu(t)$ reaches equilibrium values p_μ and p_ν respectively. Thus, $\frac{d}{dt}w_\mu(t) = 0$ and $\sum\limits_\nu p_\mu\mathbb{P}(\mu \longrightarrow \nu) = \sum\limits_\nu p_\nu\mathbb{P}(\nu \longrightarrow \mu)$. We impose a more stringent condition:

$$\boxed{p_\mu\mathbb{P}(\mu \longrightarrow \nu) = p_\nu\mathbb{P}(\nu \longrightarrow \mu)}$$

This is the condition of **Detailed Balance** and it satisfies the equilibrium condition. We know that the equilibrium probabilities are the respective Boltzmann weights. Substituting in the above equation, we get:

$$\boxed{\frac{\mathbb{P}(\nu \longrightarrow \mu)}{\mathbb{P}(\mu \longrightarrow \nu)} = \frac{p_\nu}{p_\mu} = \frac{e^{-\beta\sigma_i\sum\sigma_j}}{e^{+\beta\sigma_i\sum\sigma_j}} = \frac{1-\sigma_i\tanh\left(\beta\sum\limits_{j\in\langle i\rangle}\sigma_j\right)}{1+\sigma_i\tanh\left(\beta\sum\limits_{j\in\langle i\rangle}\sigma_j\right)}}$$

In the above equation, we have used the identity $e^{As} = \cosh A(1+s\tanh A)$ valid when $s=\pm1$
A suitable rate $\mathbb{P}(\nu \longrightarrow \mu)$ which satisfies the above is the Glauber Rate [5]:

$$\boxed{\mathbb{P}(\nu \longrightarrow \mu) = \frac{1}{2}\left(1-\sigma_i\tanh\left(\beta\sum_{j\in\langle i\rangle}\sigma_j\right)\right)}$$

1.2.2 Glauber Dynamics Algorithm

The following algorithm, derived from the above equation, has been implemented to simulate the 2D Ising Model. For the simulation, we have considered a 2D $L\times L$ lattice with periodic boundary conditions.

1. Start with an initial configuration. We have considered an initial configuration with random spins.

2. Randomly choose a spin σ_i from the lattice.

3. Calculate the energy difference ΔE between the present configuration and the configuration if the spin σ_i is flipped. Since the two configurations differ only in the spin σ_i, the energy difference will result only from the nearest neighbours.

4. Flip the spin with σ_i probability $\dfrac{1}{(1+e^{\Delta E/T})}$

The above steps are to be repeated at least L^2 times. We define 1 *Monte Carlo Step (MCS)* as the completion of L^2 updates. It is done to ensure that on an average, every spin is updated atleast once.

The number of times the steps will be repeated is dependent on the **Equilibriation time** of the system (dependent on lattice size). To have an estimate of the equilibriation time, we generally consider the variation of the order parameter m with time and check the time after which the fluctuations in m becomes limited [7], that is, m takes a almost constant value.

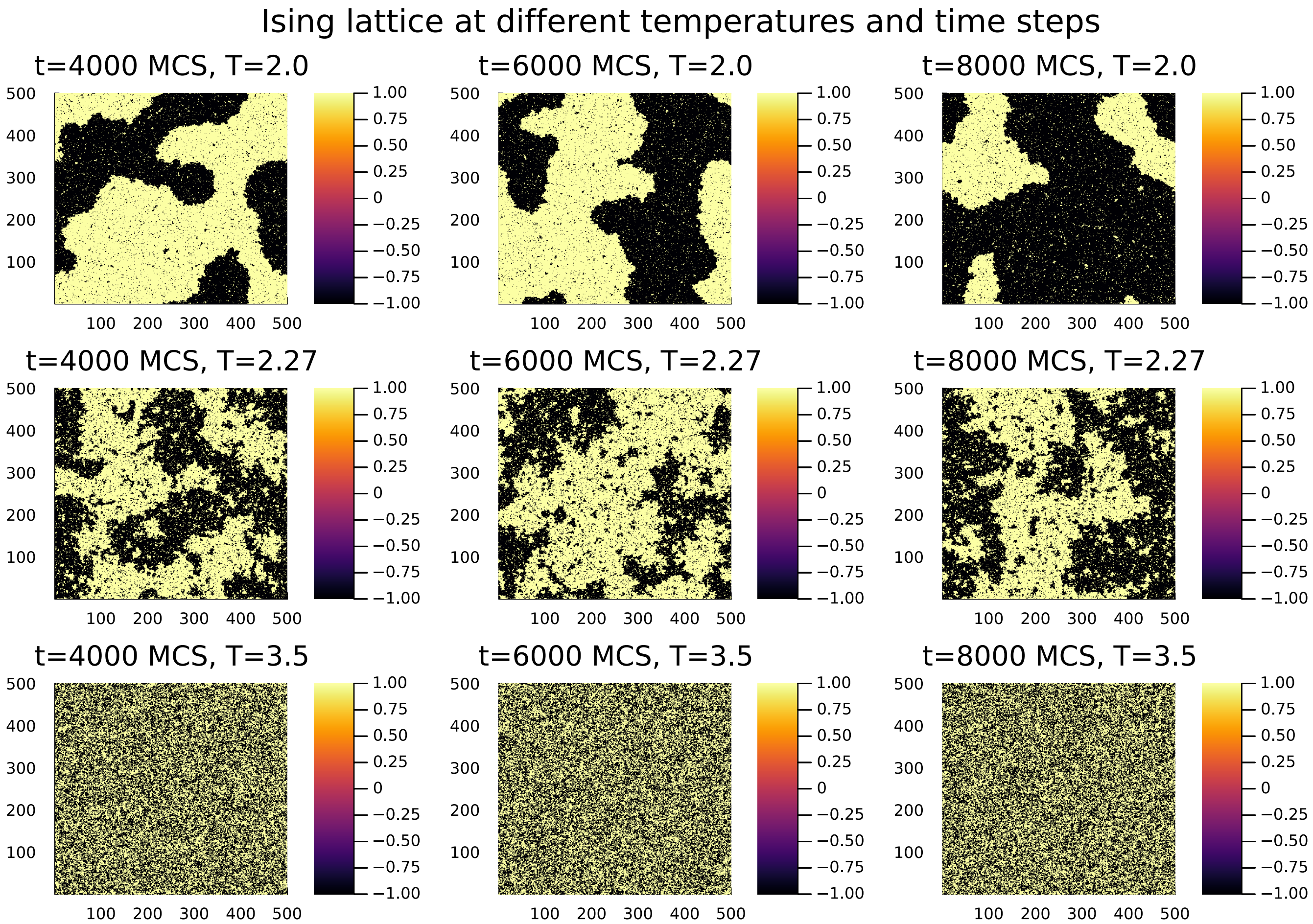


Figure 1.2: Simulation of a 500×500 lattice 2D Ising Model at different time steps and temperatures $T < T_c, T = T_c, T > T_c$. Black squares denote $\sigma = -1$ and yellow square denotes $\sigma = +1$ in the lattice.

The above figure is obtained from the Monte-Carlo Simulation of the Ising Model using Glauber Dynamics. We have taken 3 different temperatures $T < T_c, T \approx T_c$ and $T > T_c$ to demonstrate the different phases.

- When $T < T_c$, we notice the presence of large regions of like spins called *domains*. This signifies the order in the system and thus has a non-zero magnetisation.
- When $T > T_c$, we do not observe any domains. The spins tend to be aligned randomly in the entire lattice and this phase is more symmetric and hence has almost negligible magnetisation.
- When $T \approx T_c$, we see the presence of both domains and random spins. This system is characterised by scale-invariance, that is, the system remains identical when scaled.

2 Equilibrium and Non-Equilibrium Study of Ising Model from Monte Carlo Simulation

We will now consider the study of the equilibrium properties of the Ising Model and verify the critical exponents as reported in literature.

§2.1 Critical Exponents and Finite-Size scaling

We will see how different quantities at equilibrium scale with lattice size and temperature. For this, we will define $\epsilon = \left(\frac{T - T_c}{T_c}\right)$ to quantify the deviation from criticality.
We first consider the **Correlation length** ξ which quantifies the length upto which the spins in the lattice remain correlated. Empirically it has been shown that the correlation length diverges around the critical point as:

$$\boxed{\xi \sim |\epsilon|^{-\nu}}$$

While considering finite system, we cannot have quantities diverging at the critical point. Thus, there must also be a dependence on the lattice size L. As an ansatz, we assume that the free energy scales as:

$$\boxed{f(T, L, h) = L^{-d} F\left(L^{\frac{1}{\nu}}\epsilon, L^c h\right) = L^{-d} F\left(L^{\frac{1}{\nu}}\epsilon, L^c h\right)}$$

where d is the dimension of the lattice and c is some constant. The scaling of all other quantities can be obtained from this ansatz scaling form of the free energy [2].

We will also consider the non-equilibrium studies wherever possible.

§2.2 Magnetisation per spin

The average magnetisation per spin is defined by:

$$\boxed{m = \left\langle \frac{\sum_i \sigma_i}{N} \right\rangle}$$

where the average is over different configurations and N is the total number of spins in the lattice.

We first consider the non-equilibrium study of magnetisation, that is, the time evolution of m.
From the literature, we know that $m \sim \sqrt{t}$ for $T < T_c$. That is, if we start from initial random configuration of spins, m grows as a power-law with time, until it reaches an equilibrium value.

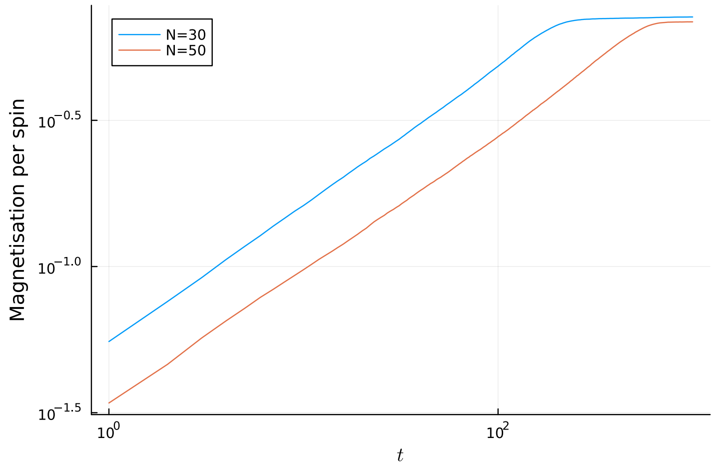


Figure 2.1: Time evolution of magnetisation per spin for different lattice size N=30,50

In the above figure, we have plotted the magnetisation per spin vs. time in log-log scale. We can observe that the intial part of the curve is linear, signifying a power-law growth. The end part of the curve is almost constant, signifying that the magnetisation value has reached equilibrium. The average slope obtained from the linear part of the curve is: 0.46 with an error of order 10^{-4}, which is close to the literature value of 0.5.

We now analyse the equilibrium properties of m. The equilibrium magnetisation value can be obtained from the free energy as:

$$m = \left.\frac{\partial f}{\partial h}\right|_{h=0}$$

$$m = L^{-d}\left.\frac{\partial F}{\partial h}\right|_{h=0} = L^{-d+c}\left.\frac{\partial F}{\partial (L^c h)}\right|_{h=0} = L^{-d+c}\tilde{m}(L^{\frac{1}{\nu}}\epsilon, 0) = L^{-\frac{\beta}{\nu}}\tilde{m}(L^{\frac{1}{\nu}}\epsilon)$$

Thus we obtain a scaling for the magnetisation with lattice size. The average magnetisation per spin was plotted against temperature for various lattice sizes. We can see that at low temperature, m was close to 1, indicating an ordered phase. As temperature decreases, we find the magnetisation decreases towards 0. At around T_c, magnetisation changes steeply but continuously, indicating second-order phase transition.

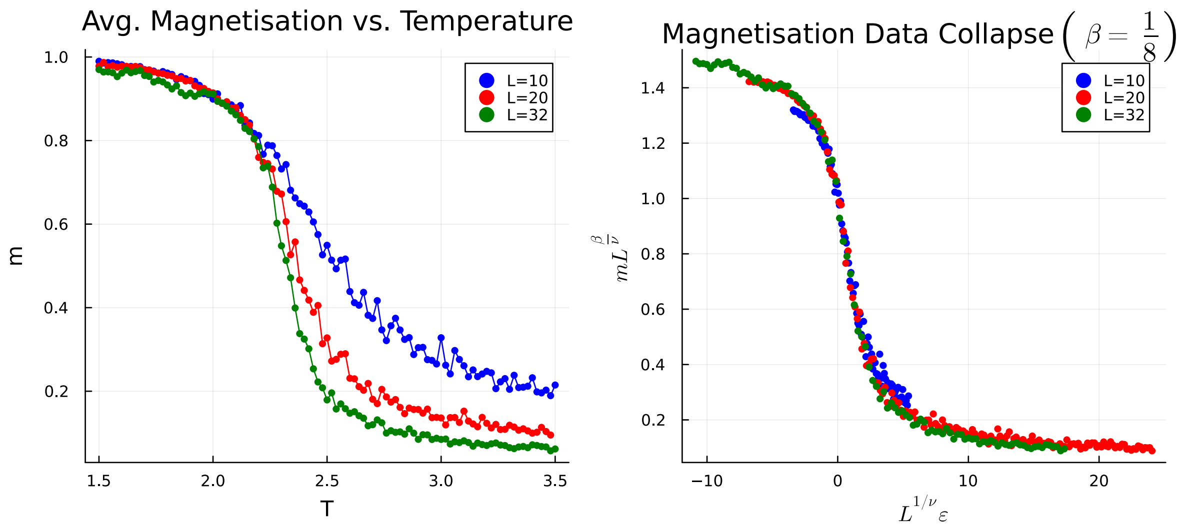


Figure 2.2: Average magnetisation per spin variation with temperature for various lattice sizes at t=1000 MCS (left), Magnetisation data collapse (right)

As shown above, magnetisation per spin m scales as $m = L^{-\frac{\beta}{\nu}}\tilde{m}(L^{1/\nu}\epsilon)$. Thus, we obtained the collapsed magnetisation data after appropriate rescaling with $\beta = 1/8$.

Hence, we verified that the critical exponent $\boxed{\beta = \frac{1}{8}}$ **for a 2D Ising model.**

§2.3 Binder Cumulant

The Binder Cumulant is a dimensionless quantity used to numerically estimate the critical temperature and is dependent on the lattice size L and temperature T. It is defined as the kurtosis of the order parameter m:

$$\boxed{U_L(T) = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2}}$$

$$U_L(T) = 1 - \frac{\langle m^4 \rangle_L}{3\langle m^2 \rangle_L^2} = 1 - \frac{\left\langle (L^{-\frac{\beta}{\nu}}\tilde{m}(L^{1/\nu}\epsilon))^4 \right\rangle}{3\left\langle (L^{-\frac{\beta}{\nu}}\tilde{m}(L^{1/\nu}\epsilon))^2 \right\rangle^2} = 1 - \frac{\cancel{L^{-\frac{4\beta}{\nu}}}\left\langle (\tilde{m}(L^{1/\nu}\epsilon))^4 \right\rangle}{3\cancel{L^{-\frac{4\beta}{\nu}}}\left\langle (\tilde{m}(L^{1/\nu}\epsilon))^2 \right\rangle^2} = \tilde{U}(L^{1/\nu}\epsilon)$$

The Binder Cumulant was plotted against temperature for various lattice sizes. We see that the plots for different L almost intersected at around $T = 2.7$. From this, we can say that $T_c \approx 2.7$, matching with the theoretically obtained value for square lattice, $T_c = \frac{2}{\ln 1+\sqrt{2}} \approx 2.269$

As shown above, Binder Cumulant scales as $U_L \approx \tilde{U}(L^{1/\nu}\epsilon)$. We now rescale our X-axis with $L^{1/\nu}\epsilon$ for various ν. It was found that for $\nu = 1$, there was collapse of the Binder Cumulant data.

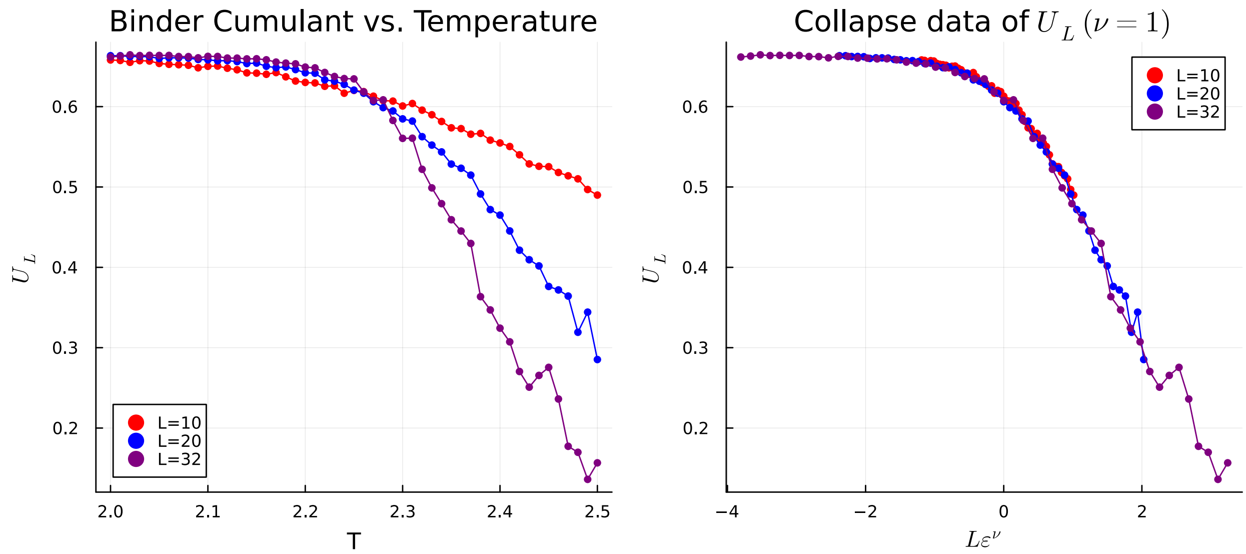


Figure 2.3: Binder cumulant variation with temperature for various lattice sizes at t=1000 MCS (left), Binder Cumulant data collapse (right)

Hence, we verified that the critical exponent $\boxed{\nu = 1}$ **for a 2D Ising model.**

§2.4 Susceptibility per spin

We define the susceptibility per spin as:

$$\boxed{\chi = N\beta\left(\langle m^2\rangle - m^2\right)}$$

We can obtain susceptibility from free energy as:

$$\chi = \frac{\partial m}{\partial h}\bigg|_{h=0} = \frac{\partial^2 f}{\partial h^2}\bigg|_{h=0} = L^{-d+2c}\frac{\partial^2 F}{\partial (L^c h)^2}\bigg|_{h=0} = L^{-d+2c}\tilde{\chi}(L^{1/\nu}\epsilon, 0) = L^{\frac{\gamma}{\nu}}\tilde{\chi}(L^{1/\nu}\epsilon)$$

The susceptibility is related to the derivative of the order parameter m. Since it is a second order phase transition, derivative of the order parameter is discontinuous and hence the susceptiblity diverges at the critical point. However, for finite systems, we will not obtain this divergence. As system size increases, the plot of susceptibility peaks around the critical temperature. As shown above, susceptibility scales as $\chi = L^{\frac{\gamma}{\nu}} f(L^{1/\nu}\epsilon)$. Thus, the data collapse can be obtained if we plot $\frac{\chi}{L^{\frac{\gamma}{\nu}}}$ vs. $L^{1/\nu}\epsilon$.

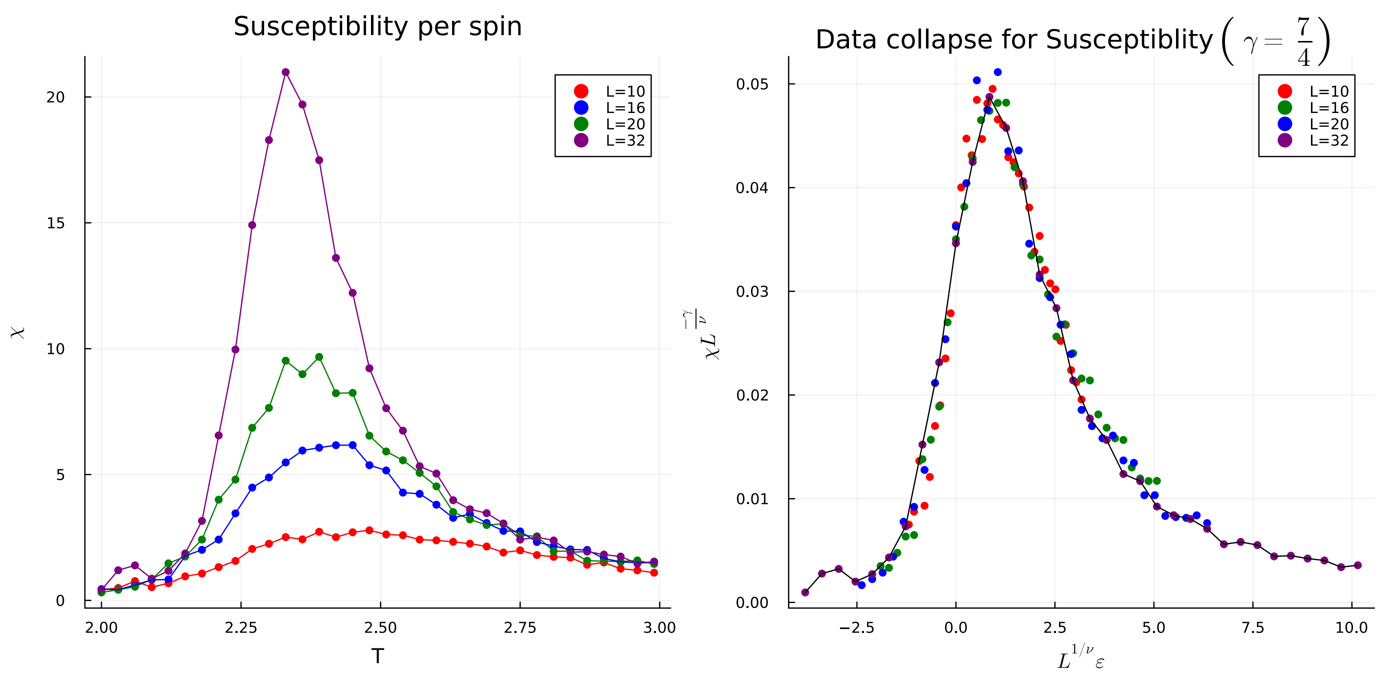


Figure 2.4: Susceptibility per spin variation with temperature for various lattice sizes at t=1000 MCS (left), Susceptibility data collapse (right)

Hence, we verified that the critical exponent $\boxed{\gamma = \frac{7}{4}}$ **for a 2D Ising model.**

§2.5 Persistence Probability

We will now consider the study of persistence in the Ising lattice. The persistence probability $P(t)$ is defined as the probability that a spin has not flipped till time t. We calculate the persistence probability at $T = 0$ since $T = 0$ is the energy-minimising scheme; only the spins at the domain walls will flip.

To numerically obtain the persistence probability, we will start with intial lattice configuration of random spins. For each spin σ_i, we will define a quantity to mark the persistent spins:

$$n_i(t) = \frac{\sigma_i(t)\sigma_i(0) + 1}{2}$$

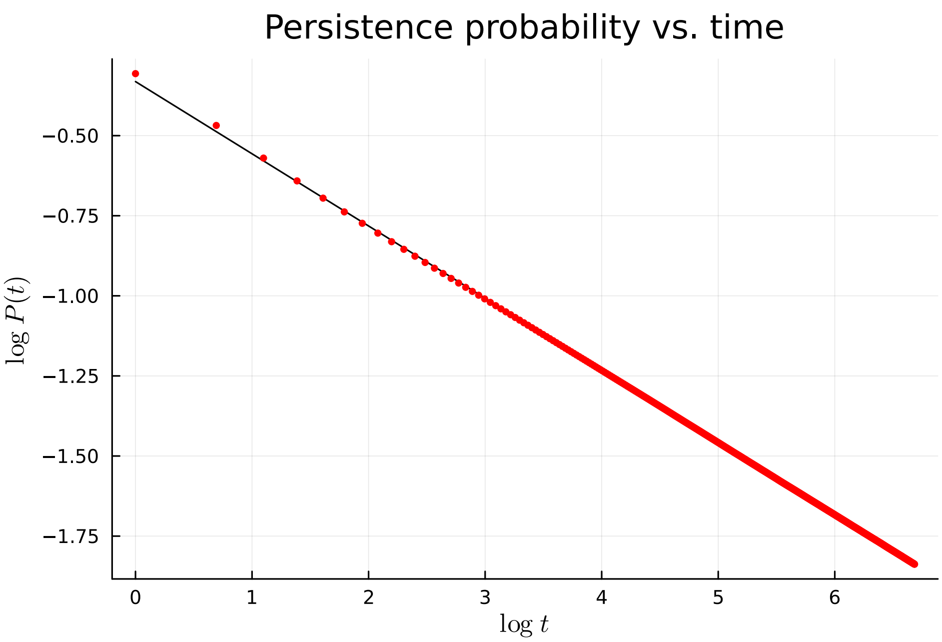
We have $n_i(0) = 1 \ \forall \ i$. When the spin σ_i has flipped, $\sigma_i(t)\sigma_i(0) = -1$, hence, $n_i(t) = 0$. We will fix the value of $n_i(t)$ once it has become 0, since it will not contribute to persistent spins for later times. Then, the persistence probability is

$$P(t) = \frac{\left\langle \sum_i n_i(t) \right\rangle}{N}$$

where the average is over different configurations and N is the total number of spins.
For infinite system size, $P(t) \sim t^{-\theta}$ where θ is the persistence exponent. However, due to finite size scaling,

$$P(t, L) = L^{-z\theta} f\left(\frac{t}{L^z}\right)$$

where z is the dynamic exponent. For Ising Model, $z = 2, \theta \approx 0.22$ from literature values.



We obtained the variation of $P(t)$ with time for lattice of dimension $L = 100$. We have fit the data points with a linear curve and obtained the slope as 0.225 with error of order 10^{-5}, which matches closely with the literature values.

§2.6 Summary

In this chapter, we verified the critical exponents and the scaling laws of various quantitites. In summary:

Quantity	Finite-Size Scaling Form	Exponent
Magnetisation per spin m	$L^{-\frac{\beta}{\nu}}\tilde{m}\left(L^{1/\nu}\epsilon\right)$	$\beta = \frac{1}{8}$
Binder Cumulant U_L	$\tilde{U}\left(L^{1/\nu}\epsilon\right)$	$\nu = 1$
Susceptibility per spin χ	$L^{\frac{\gamma}{\nu}}\tilde{\chi}\left(L^{1/\nu}\epsilon\right)$	$\gamma = \frac{7}{4}$
Persistence Probability $P(t)$	$L^{-z\theta}f\left(\frac{t}{L^z}\right)$	$\theta = 0.225$

3 Random Walker in Spin Space

We will now consider studying the effect of temperature on the dynamics of the Ising Model. Consider a 2D Ising Model on a $L \times L$ lattice. We will associate each spin σ_i in the lattice with a random walker in virtual one-dimension space. After 1 MCS updates, the walker moves either to the left or right, accordingly if the spin σ_i is -1 or $+1$. We will measure time in units of MCS.

We will analyse the distribution of the position x of the walker $S(x,t)$ at different times t, varying with temperature T.

§3.1 At temperature $T > T_c$

We will consider the dynamics at temperature $T = 2.5, 2.6, 3.0, 3.5, 4.0$. For each temperature, we will analyse the distribution for time $t = 1000, 2000, 2500, 3000$.

SInce at high temperature, the spins no longer remain correlated, thus, each walker will perform independent random walks. Thus $x = \sum_i x_i$ where $\{x_i\}$, the positions of the i^{th} walker, are iid random variables. In the large lattice size limit, from the *Central Limit Theorem*, we see that the distribution takes a Gaussian form, with mean around 0 and variance decreasing with temperature[4, 8]. We have:

$$\boxed{S(x,t) \sim \frac{1}{\sqrt{2\pi t}\sigma} e^{-x^2/2\sigma^2 t}}$$

Thus, when we plot $S(x,t)\sqrt{t}$ vs. $\frac{x}{\sqrt{t}}$, we will get the collapse plot of the Gaussian curves for different times at a particular temperature.

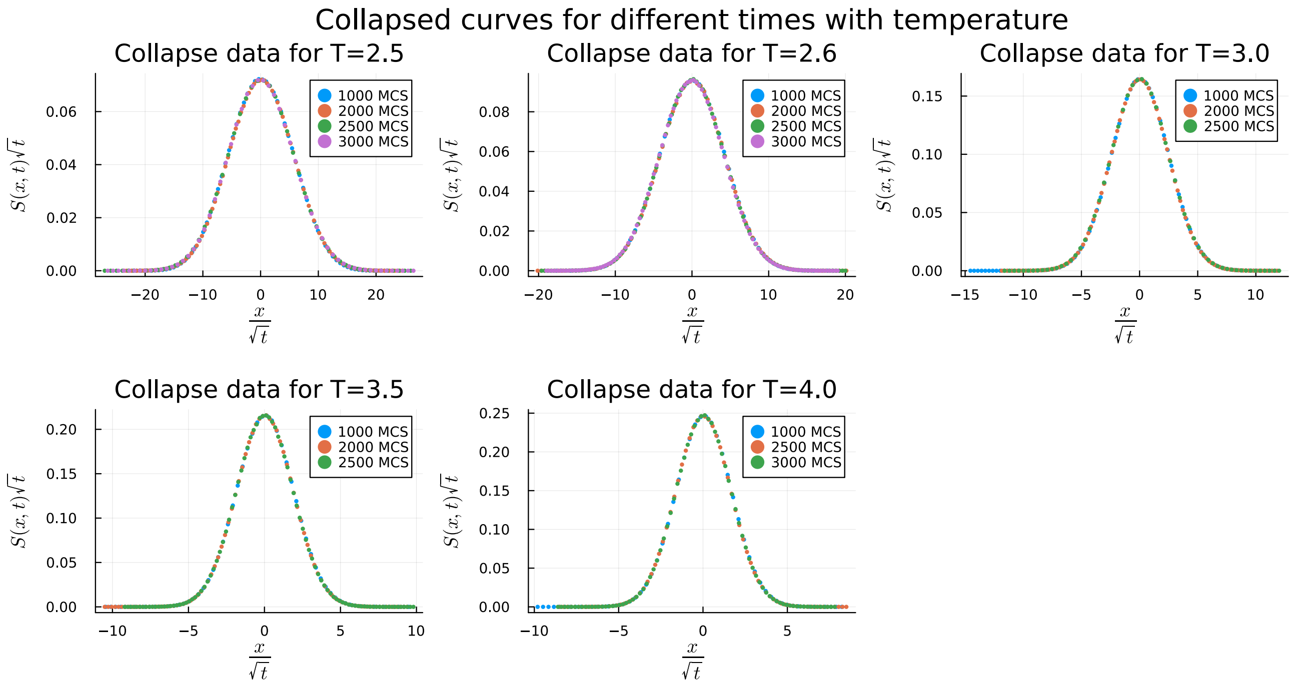


Figure 3.1: Data collapse done for a 100×100 lattice for temperature $T = 2.5, 2.6, 3.0, 3.5, 4.0$ at different times.

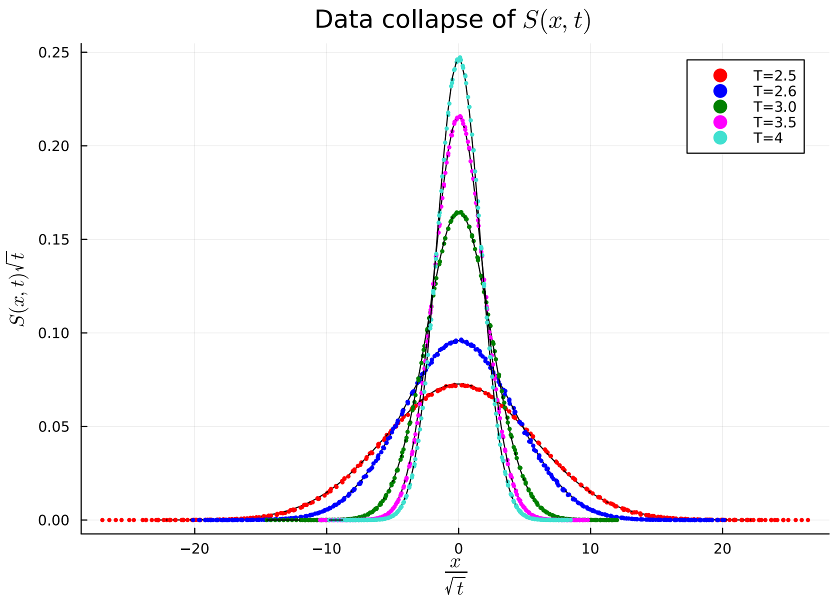


Figure 3.2: Data collapse of all the plots for different times on same plot along with Gaussian fit curve. The width of the Gaussian decreases with increasing temperature.

The average standard deviation of the Gaussian curve at different temperatures were calculated.

Temperature	σ
2.5	5.619
2.6	4.214
3.0	2.454
3.5	1.874
4.0	1.642

The standard deviation was plotted with ϵ. The log-log plot was fit with linear curve.

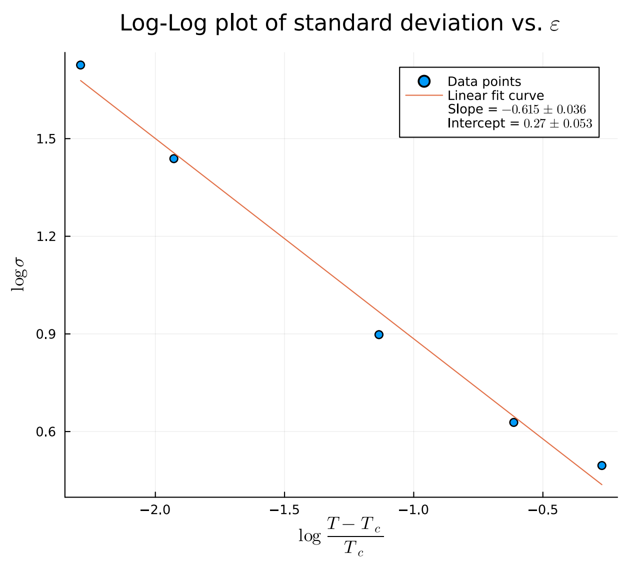


Figure 3.3: Plot of standard deviation with ϵ

The fitting parameters were calculated as:

$$\boxed{\text{Slope} = 0.615 \pm 0.036 \text{ Intercept} = 0.27 \pm 0.053}$$

§3.2 At temperature $T < T_c$

We will analyse the distribution for time $t = 100, 200, 300, 400$ MCS when $T < T_c$. We obtain a double-peaked U-shaped distribution at all times, unlike the Gaussian distribution for $T > T_c$, with the peaks occurring approximately at $S(x = t, t)$.

We define the persistence probability as the probability that a spin does not change sign till time t. For the Ising model, $P(t) \sim t^{-\theta}$ where θ is the persistence exponent. The persistence probability $P(t) \propto S(x = \pm t, t)$.

We analyse the case of $T = 0$ which helps us to estimate the *persistence exponent*. Since $T = 0$ is the energy-minimising scheme, only the spins at the domain wall will flip in consecutive updates, however, spins within the domains will not flip (since the probability of flipping with same neighbour spins in the Glauber case $\dfrac{1}{1 + e^{\Delta E/T}}$ is 0 when $T = 0$).

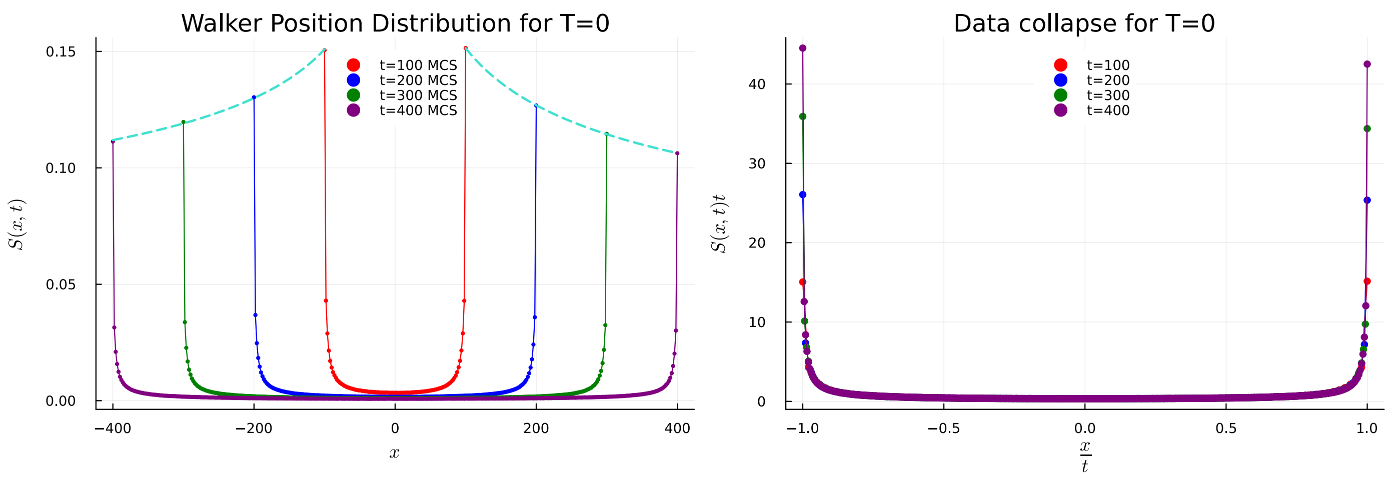


Figure 3.4: Distribution of the position of walker for $T = 0$ at different times with tips fit with $t^{-\theta}$(left) Data collapse for the same (right)

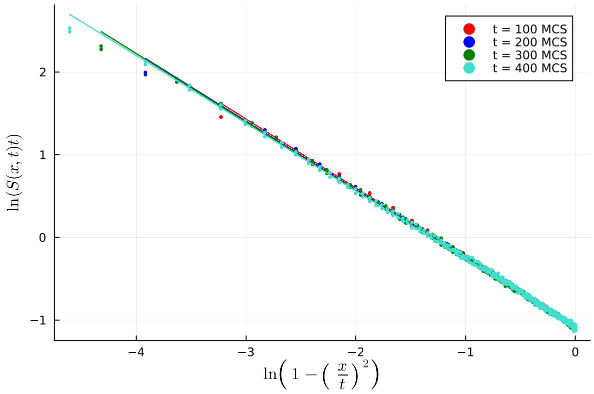
The distribution of walker at different times has been plotted for $T = 0$. In the low-temperature regime, $S(x,t) \approx \frac{1}{t} f(\frac{x}{t})$. Thus, by plotting $S(x,t)t$ vs. $\frac{x}{t}$, we obtained the data collapse.

The persistence exponent can be obtained from the tip of the distribution. The tips will follow the curve $y = x^{-\theta}$. We plotted the curve of $\ln y$ vs $\ln x$ where y denotes the data point of the tips of the curve. The data points were fit with a linear curve. The slopes obtained for the left and right tips are: $m_1 = -0.216 \pm 0.0057$, $m_2 = -0.255 \pm 0.0012$. The average slope obtained:

$$\boxed{\text{Slope} = -0.236 \pm 0.0029}$$

Thus the value of the persistence exponent obtained is $\theta = 0.236 \pm 0.0029$ which is close to the value found in literature $\theta \approx 0.22$.

For $T = 0$, $S(x,t)$ is close to a beta-distribution $\left(1 - \dfrac{x^2}{t^2}\right)^{\theta-1}$ [4]. The log-log plot of the data collapse has been, fit with a linear curve, has been shown below.



The average slope of the linear curves obtained is: -0.827 ± 0.00276. Theoretically, the slope should be $\theta - 1 \approx -0.78$ as per value in the literature.

In the finite low temperature regime, $S(x,t) \approx A\left(1 - B\frac{x^2}{t^2}\right)^{\theta-1}$ where A and B are time-independent parameters depending on the equilibrium magnetisation. We fit the curves according to this form, as shown below.

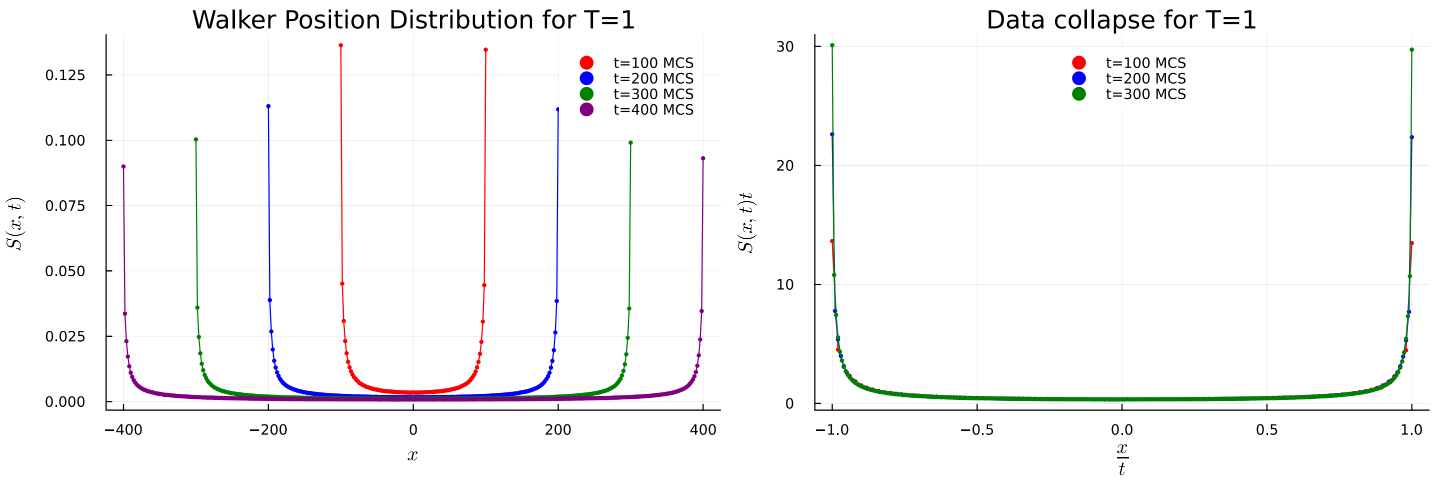


Figure 3.5: Distribution of the position of walker for $T = 1$ at different times and the corresponding data collapse

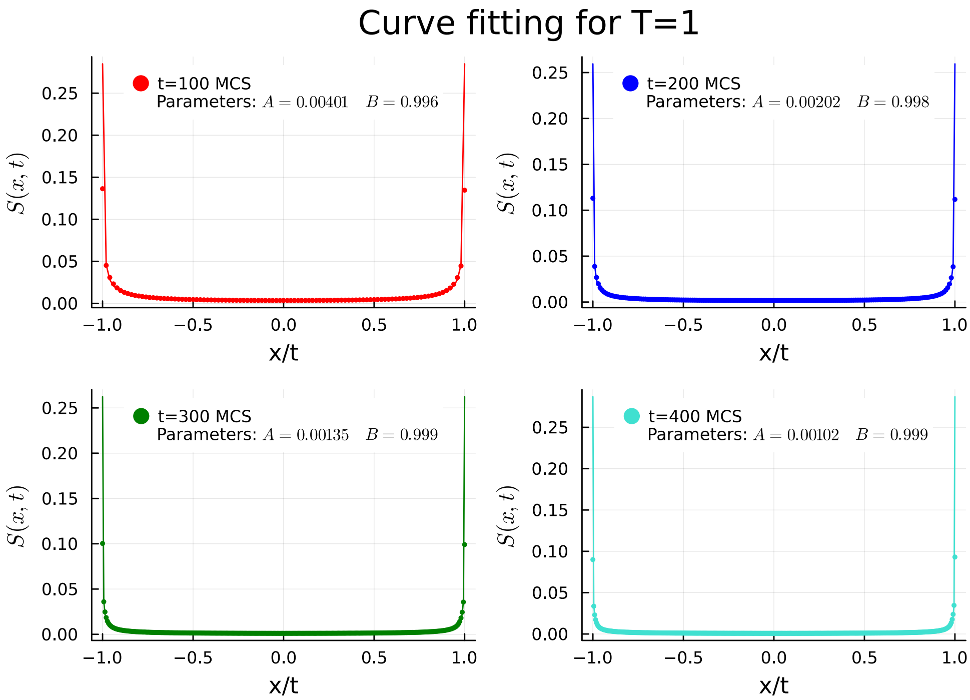
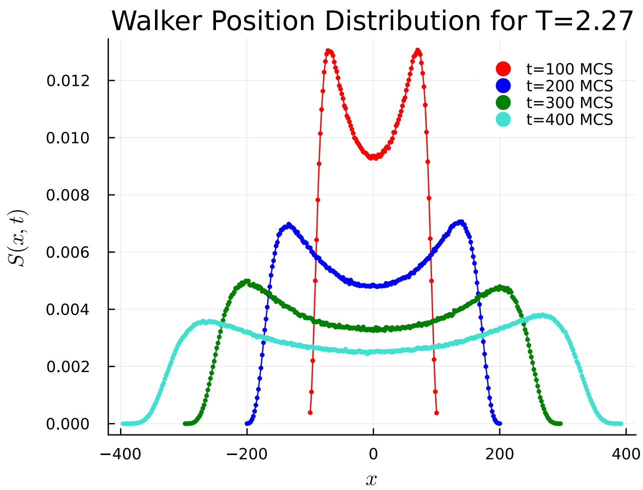


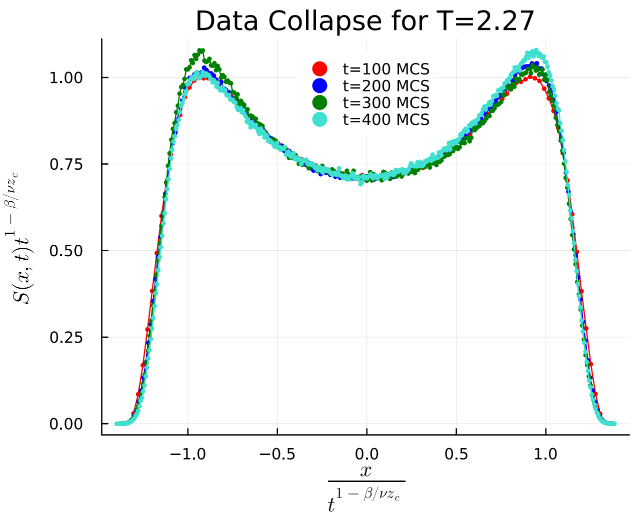
Figure 3.6: Distribution curves fit with the above form for $T = 1$.

The curves are fitted witht the above form and the fitting parameters obtained are mentioned within the plot.

§3.3 At temperature $T \approx T_c$

When temperature is around the critical point $T_c \approx 2.27$, we neither have a sharp U-shaped distribution, nor a Gaussian distribution. We obtain a double-peaked distribution.





In the critical temperature domain, the distribution function $S(x,t) \sim t^{1-\frac{\beta}{\nu z_c}} \phi\left(\frac{x}{t^{1-\frac{\beta}{\nu z_c}}}\right)$ [4], where $z_c \approx 2.17$ is the dynamic critical exponent for 2D Ising Model and ϕ is a universal scaling function. Thus, using this form, we obtained the data collapse.

§3.4 Summary

In this chapter, we analysed the distribution of the position of the random walker at different temperature regimes.

- At high temperatures, $T > T_c$, we found the position distribution to be Gaussian which is expected since the spins become uncorrelated. We obtained the data collapse for different times at various T and analysed the standard deviation of the Gaussian curves so obtained.
- At low temperatures, $T < T_c$, we found that the position distribution follows a U-shaped curve. We analysed the distribution for $T = 0$ and obtained the persistence exponent numerically by fitting the tip of the distributions.
- At critical point, $T \approx T_c$, we found that the position distribution takes a double-peaked bimodal distribution and an approximate data collapse was obtained for the curves.

4 Ising Model in Barabasi-Albert Network

§4.1 Introduction

In this chapter, we will map the Ising Model on the Barabasi-Albert (BA) network which is a particular type of scale-free complex network. We introduce the basic terminologies and definitions needed for such mapping.

4.1.1 Graph

A *graph* is a pair $G = (V, E)$ where $V = \{P_1, P_2, \ldots P_N\}$ is a set of vertices (or nodes) and $E = \{E_1, E_2, \ldots E_N\}$ is the set of edges connecting two elements in V. A graph can be *undirected*, that is, node connections are symmetric or *directed*, node connections are not symmetric.

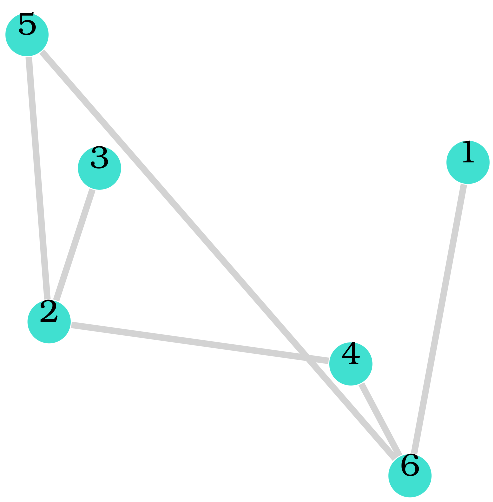


Figure 4.1: Example of a graph with 6 nodes

Adjacency Matrix: A graph is completely denoted by its adjacency matrix which is a $N \times N$ matrix, where N is the number of nodes. It is defined as:

$$A_{ij} = \begin{cases} 1 & \text{if nodes i and j are connected} \\ 0 & \text{otherwise} \end{cases}$$

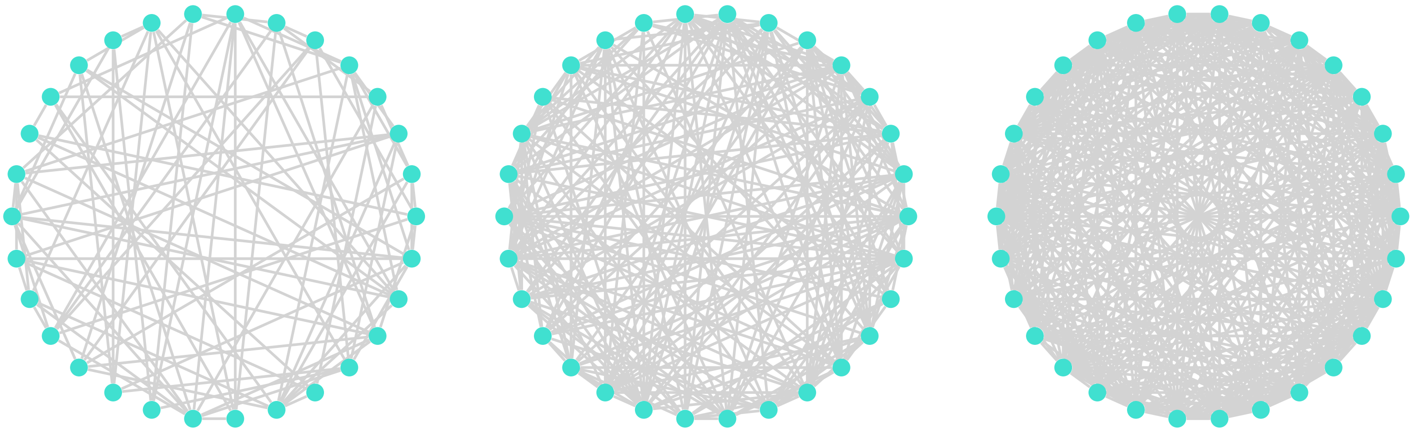
The adjacency matrix corresponding to the above graph is:

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \end{pmatrix}$$

Degree: Degree of a node i is the number of edges connected with that node. Since directed graphs have asymmetric connection, we define outdegree and indegree for such graphs. In the above graph, node 1 has degree 1 (connected to only node 6), node 2 has degree 3 (connected to nodes 3, 4 and 5) and so on.

Erdős-Rényi Model

The Erdős-Rényi Graph is a model for a random graph where the edges are distributed randomly. We start with N isolated nodes and connected each pair of nodes with a probability specified by the parameter p. As we increase p, the number of connected nodes increases and for $p \to 1$, we obtain a complete graph.



(a) $p = 0.2$ (b) $p = 0.5$ (c) $p = 0.8$

Figure 4.2: Realisation of a Random Graph with increasing parameter p, N=30 nodes

Degree of node i of a random graph follows a binomial distribution:

$$P(k_i = k) = \binom{N-1}{k} p^k (1-p)^{N-1-k}$$

In the limit of large N, the distribution converges to the Poisson distribution.

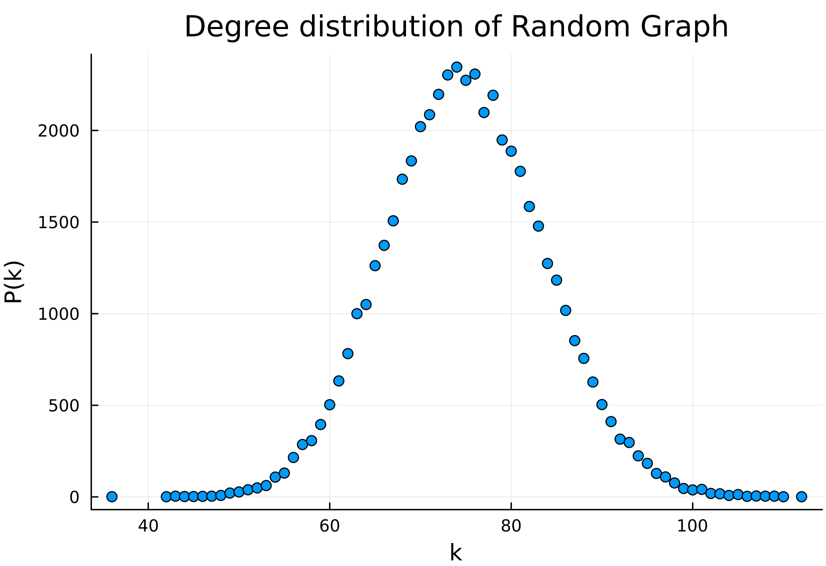


Figure 4.3: Degree distribution of a random grpah with N=50000, p=0.0015

§4.2 Complex Networks

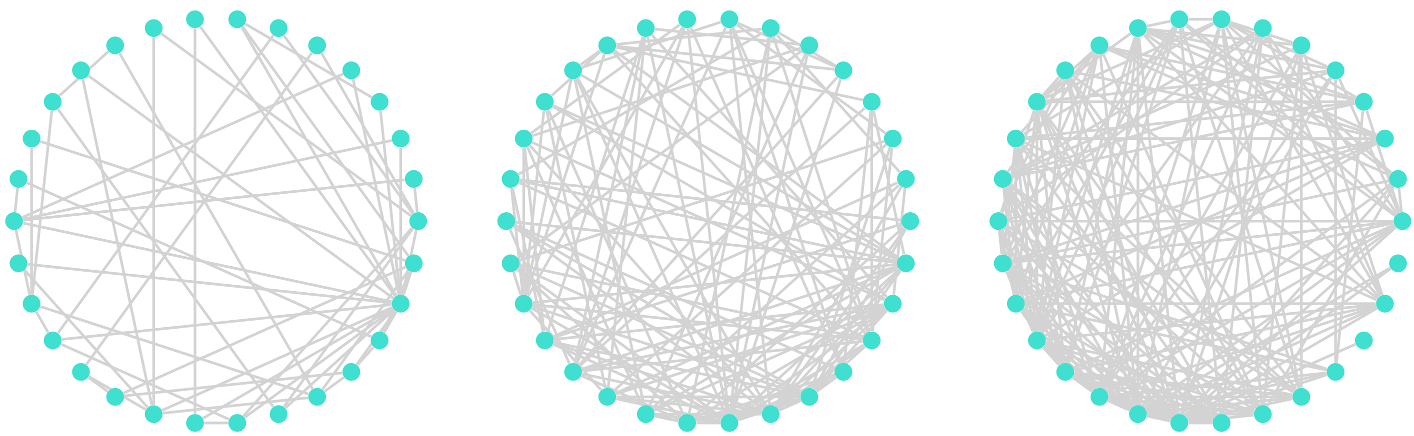
Complex Networks were developed to model real world networks like social network, neural networks in organisms, etc. We will study the *Barabasi-Albert Network*, a type of complex network whose degree distribution follows a *power-law* and is thus called a *scale-free network*.

§4.3 Barabasi-Albert Model

The algorithm to generate a scale-free BA graph is as follows:

1. *Growth*: We start with m_0 number of initial nodes and in every time step, we add a new node with m edges to m pre-existing nodes in the graph.

2. *Preferential Attachment*: We assume that the probability P such that new node will be attached to node i of the graph is given by: $P(k_i) = \frac{k_i}{\sum\limits_j k_j}$



(a) $m = 2$ (b) $m = 5$ (c) $m = 8$

Figure 4.4: Realisation of a BA network with different parameter m, N=10 nodes

The degree distribution of the BA network follows a power law, which takes an asymptomatic form

$$P(k) \sim 2m^{\frac{1}{\beta}} k^{-\gamma}$$

with $\beta = 0.5$ and $\gamma = 1 + 1/\beta = 3$.

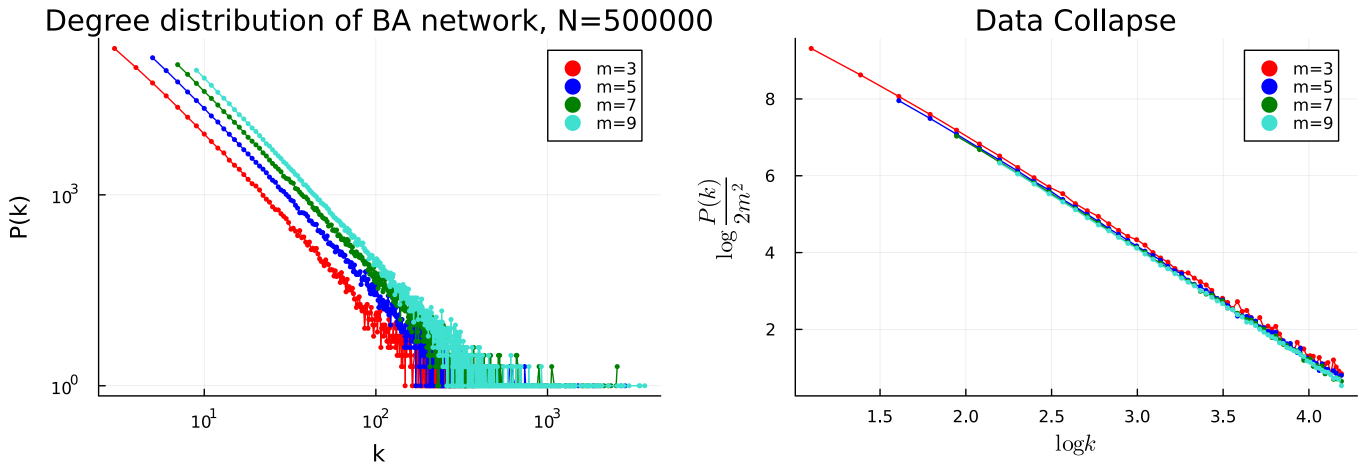


Figure 4.5: Degree distribution and data collapse of distribution for BA network with N=500000 nodes

We plotted the degree distribution for BA network. In log-log plot of the data collapse, we see that the distribution is a straight line. The tail of the distribution is noisy, however, it can be reduced by process of log-binning. The average slope of the linear fit curves for th initlal part of the distribution so obtained is -2.859 which is close to the analytic value of $\gamma = 3$.

§4.4 Ising Model in BA Network

We modify the classical Ising Model to map it onto the BA network. We will consider a BA network with N nodes and parameter m. To each of these N nodes, we will associate the Ising spins $\sigma_i \in \{+1, -1\}$. The Hamiltonian for the system in absence of external field, is defined as:

$$\mathcal{H} = -\frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} \sigma_i \sigma_j$$

where J is the adjacency matrix of the graph.

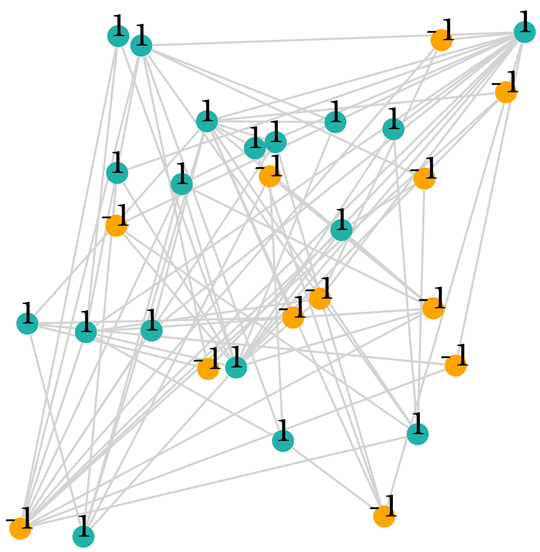


Figure 4.6: One realisation of the Ising Model on the Barabasi-Albert Network with N=30, m=3 and with random spins on each node.

The system is different from the lattice Ising Model as the critical temperature T_c depends on the system size N and parameter m. Thus, finite-size scaling cannot be done for the system. The mean-field solution [3] provides an analytic expression for T_c

$$T_c = \frac{m}{2} \ln N$$

The true critical temperature goes to infinite in the thermodynamic limit $N \to \infty$. This shows that in a scale-free network the ordered phase is the only allowed phase in the thermodynamic limit.

4.4.1 Magnetisation per spin

We analyse the magnetisation per spin in the system, to observe the phase transition. We first observe the non-equilibrium evolution of magnetisation per spin.

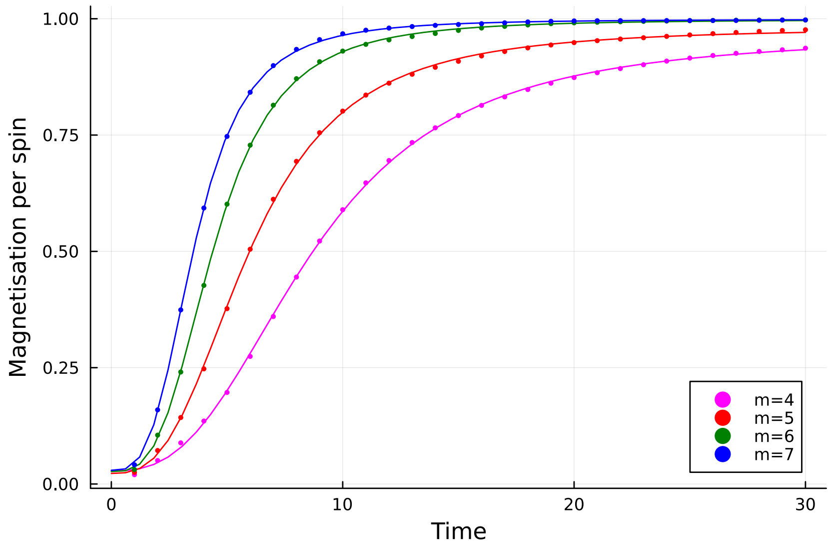


Figure 4.7: Magnetisation per spin vs time for different values of m, $N = 100000$ nodes, along with the fitting curve specified below.

We see that the magnetisation per spin reaches an equilibrium value after a period of time. However, when we plotted the log-log plot, we did not obtain a linear curve, implying that it does not follow a power law growth with time, unlike the case of Ising model on lattice.

When we plotted magnetisation vs. $log(t)$, we observed a functional form similar to the sigmoid function. Thus, from this, we obtained a rough functional form of the time dependence of magnetisation as:

$$\text{magnetisation} = \frac{A}{1 + Bt^c} + D$$

where A,B,C,D are appropriate fitting parameters. We obtained the fitting parameters for different values of m.

m	A	B	C	D
4	0.9365	348.301	-2.71	0.028
5	0.95782	158.089	-2.83	0.022
6	0.9716	114.981	-3.18	0.026
7	0.9692	63.701	-3.24	0.029

Further analysis needs to be done for this.

We now analyse the quilibrium properties of magnetisation. We see that there is indeed a phase transition in the system where with increasing temperature, the system goes into a disordered phase with magnetisation close to zero[6, 1]. We numerically see that for a fixed N with increasing m, T_c increases.

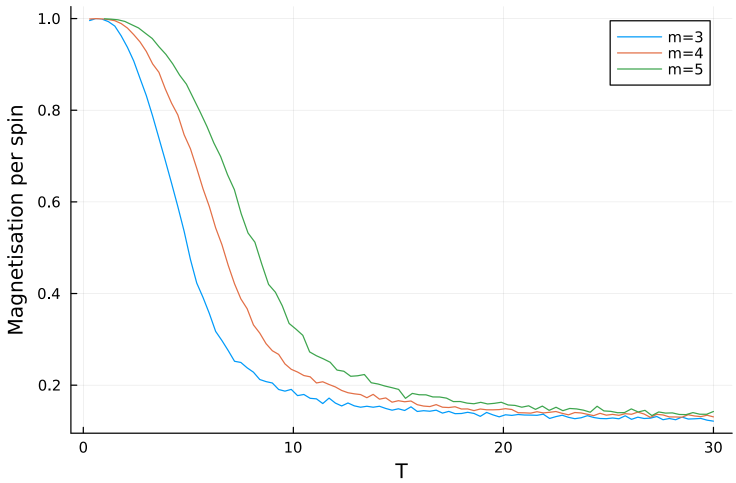


Figure 4.8: Magnetisation per spin vs. temperature for different m, with $N = 1000$

4.4.2 Persistence Probability

We analyse the persistence probability previously defined for the Ising Model on BA network.

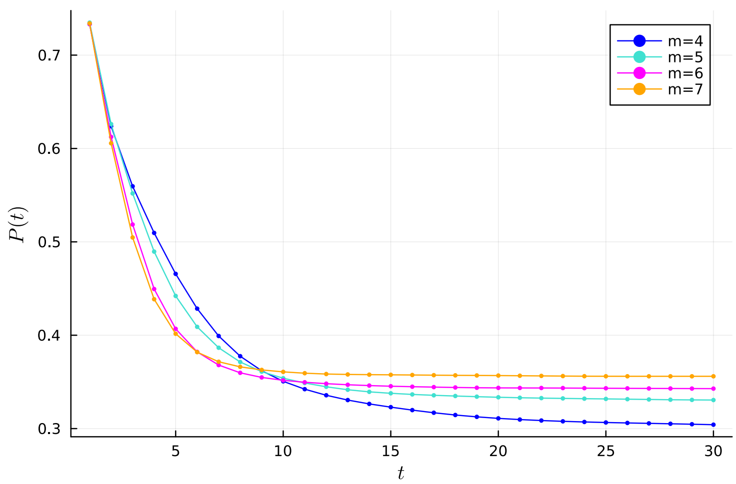


Figure 4.9: Plot of Persistance probability $P(t)$ with time, for $N = 20000$ nodes and different values of m

We obtained the log-log plot of $P(t)$ vs. t but did not obtain a linear curve. Thus, we observe that $P(t)$ does not follow a power-law decay with time, unlike the case of Ising Model in 2D lattice. Further analysis needs to be done.

4.4.3 Random Walker in Spin Space of BA Network Ising Model

We will extend our analysis of the random walker in previous chapter to the BA network. The same Monte-Carlo Simulation has been performed at different times and temperature and the distribution of the position of the random walker is analysed.

Since there is no finite size scaling, we cannot estimate the critical temperature using any observable quantities, thus, we estimate the critical temperature for the system by checking the transition of the distribution of the walker position from a doubel peaked to Gaussian curve. We took $N = 1000$ and did our analysis for $m = 2, 3, 5$. The estimate of critical temperature is as follows:

m	T_c
2	5.3
3	8.3
4	10.8
5	13.9

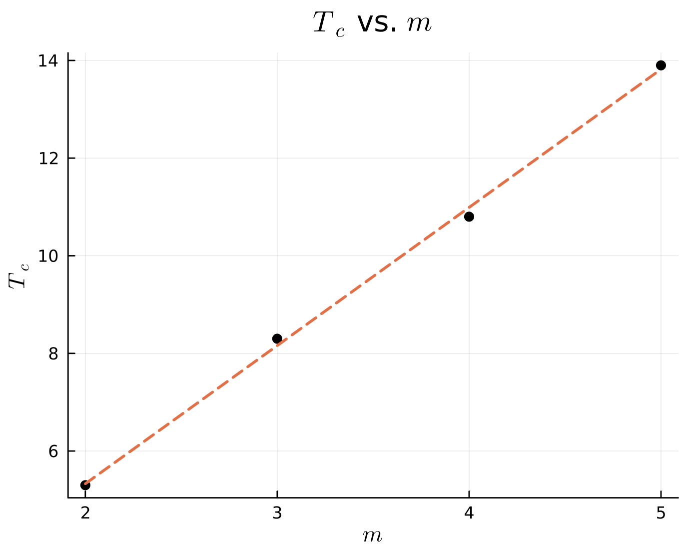


Figure 4.10: Variation of T_c with m for $N = 1000$

We plotted the estimated value of T_c with m and obtained a slope of 2.83 ± 0.07 after fitting the data points with a linear curve. Anlytical expression from the mean field solution gives the slope of T_c vs. m to be $\frac{1}{2} \ln N$ which comes out to be 3.45 for N=1000.

§4.5 $T > T_c$

We obtain a Gaussian curve for the walker position distribution. We collapsed the data using the form similar in the previous chapter $S(x, t)\sqrt{t}$ vs. $x/\sqrt{t}$ and then analysed the width of the collapsed Gaussian curve obtained.

$m=2$			$m=3$			$m=5$		
T	$\frac{T-T_c}{T_c}$	σ	T	$\frac{T-T_c}{T_c}$	σ	T	$\frac{T-T_c}{T_c}$	σ
5.4	0.0189	3.9875	8.4	0.01205	4.4973	14	0.0072	5.6337
5.5	0.0377	3.2259	8.5	0.02410	3.6138	14.1	0.0144	4.7639
5.6	0.0566	2.8214	8.6	0.03614	3.3211	14.4	0.0347	3.4563
5.8	0.0943	2.1263	8.8	0.06024	2.4622	14.5	0.0432	3.0235
6	0.1321	1.8493	9	0.08434	2.1174	14.7	0.0576	2.5911
6.3	0.1887	1.5665	9.5	0.14458	1.6119	15	0.0791	2.1413
6.5	0.2264	1.4750	10	0.20482	1.4099	15.5	0.1151	1.6855
7	0.3208	1.3608	10.5	0.26506	1.3386	16	0.1511	1.5069
7.5	0.4151	1.3101	11	0.32530	1.2933	16.5	0.1871	1.3752
8	0.5094	1.2748	11.5	0.38554	1.2665	17	0.2230	1.3208
8.5	0.6038	1.2581				17.5	0.2590	1.2895

Table 4.1: Width of the collapsed Gaussians obtained at different temperature, for different values of m

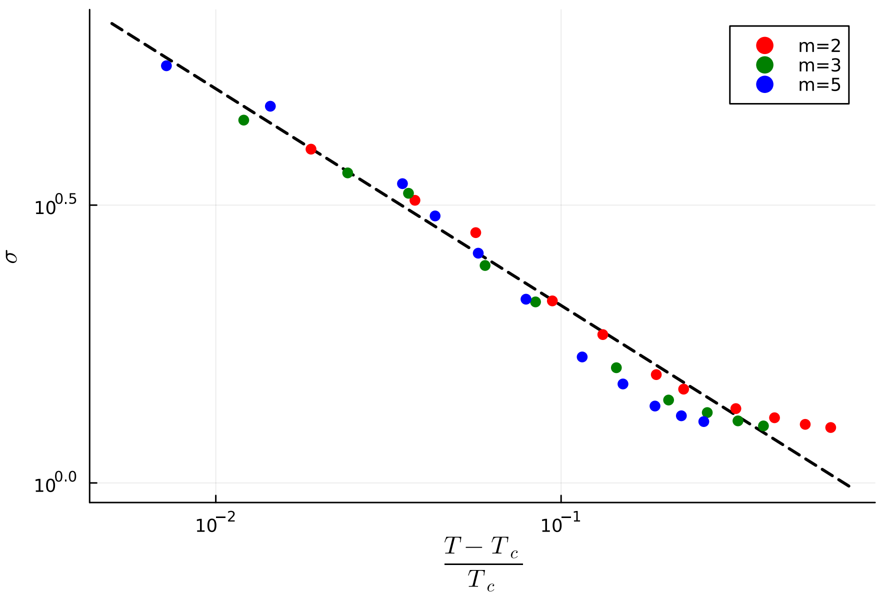


Figure 4.11: σ vs. scaled temperature at $T > T_c$ in log-scale for Ising Model in BA Network with different values of m, N=1000 nodes.

The above plot shows the variation of the Gaussian standard deviation with scaled temperature for different values of m, keeping number of nodes fixed at $N = 1000$. Although not perfectly, we have tried to fit the data with $\left(\frac{T-T_c}{T_c}\right)^{-0.4}$. We obtained an approximate linear fit curve. We might infer that the variation of the Gaussian widths with scaled temperature is independent of the value of m but further analysis needs to be done.

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