Thermal phase transition of two-dimensional classical Ising model

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Abstract

A thorough investigation was done on thermal phase transition of 2D classical Ising model using Monte Carlo simulation, where two algorithms, Metropolis algorithm and Swendsen-Wang algorithm, were implemented. Critical slowing down behaviour of the model near phase transition was studied by comparing the two methods. Finite size scaling effect of the physical observables were shown by performing data collapse of magnetization $|m|$, susceptibility χ and specific heat capacity C. Values of critical temperature $T_c \approx 2.276$ and critical exponent $\eta \approx 0.243$ were extracted via regression analysis with slight deviation from exact values, which implied larger system sizes are needed to further eliminate the finite size effect. Lastly, Binder ratio and its size-independent property at T_c was studied.

Key words: Ising model, Monte Carlo simulation, critical point, finite size scaling

Acknowledgement

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Contents

1 Introduction

Ferromagnetism is a phenomenon that magnetic dipoles of atoms in a material will align in the same direction as the orientation of the magnetic field presented. This phenomenon can be demonstrated by a simple toy model called Ising model. In this model, two discrete values of spin $\sigma = \pm 1$ are used to represent the orientation of atomic spin in one direction, these spins are arranged into a lattice, and the Hamiltonian of the model is governed by

$$H = -\sum_{i,j} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i \tag{1}$$

Where J_{ij} is the interaction between adjacent spins and h is the magnetic field strength. When there is no external field and only nearest neighbouring spins is considered to have non-zero interaction J_{ij}, equation (1) reduced to

$$H = -\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j \tag{2}$$

Where $\langle i, j\rangle$ denotes nearest neighbour interaction. For ferromagnetism, J_{ij} is a positive number. Hence the partition function can be written as

$$Z = \sum_{\sigma} \exp(\frac{1}{k_B T}\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j) \tag{3}$$

Where k_B is the Boltzmann constant and T is temperature. The expectation value of a physical observable can be calculated as

$$\langle A\rangle = \frac{1}{Z}\sum_{\sigma} A(\sigma)\exp(\beta\sum_{\langle i,j\rangle} J_{ij}\sigma_i\sigma_j) \tag{4}$$

The analytic solution of 1D Ising model provided by Ernst Ising does not exhibit phase transition (Ising, 1925). Onsanger has provided an analytic solution of 2D Ising model in

1944, showing that it has a phase transition (Onsager, 1944),

$$\sinh \frac{2J}{k_b T_c} = 1 \tag{5}$$

$$\frac{k_b T_c}{J} = \frac{2}{\ln 1 + 2\sqrt{2}} = 2.269185 \tag{6}$$

Where T_c is the critical temperature. In low temperature limit $T < T_c$, the system is in an ordered phase where all spins in the system align in the same direction. Decoupling of spins occurs when T approaches T_c. So in high temperature limit $T > T_c$, the system is in a disordered phase where orientation of individual spins is random in the system. Physical observables such as net magnetization in this model also exhibits phase transition behaviour with increasing T, therefore they can be used as order parameters of the phase transition.

The further sections of this report are organized as below: In section 2, Monte Carlo method and finite size scaling are introduced to explain how to extract informations from the Ising model. In section 3, results from numerical analysis are presented and compared to exact solutions from previous literature. Section 4 concludes the findings of this report.

2 Method

In this report, let $J_{ij} = -1$ for all neighbouring spin $\sigma_i \sigma_j$, and $k_B = 1$ for simplicity. A square lattice of system size $L \times L = N$ with periodic boundaries is used.

2.1 Monte Carlo simulation

Due to the complex form of partition function in 2D square Ising model and the large number of degrees of freedom in the system, stochastic methods can be used to solve it. Monte Carlo methods utilize random sampling of points of the integrand to construct the integral or the average value of observables. For statistical mechanics where distribution of observables are governed by Boltzmann distribution $e^{H/k_b T}$, importance sampling is used

instead of uniform random sampling. Importance sampling means that sampling of the data will also based on the probability distribution of the variable, so more data will be collected in the peaked region of the distribution, which will lower the statistical fluctuation in the peaked region compared to uniform random sampling. Therefore, importance sampling can obtain functions with high precision when compared to simple sampling given the same number of data points.

To achieve importance sampling, detailed balancing condition is imposed. Firstly, it is assumed that transition of state is independent from its previous transitions, making this series of transition a Markov chain. Then, the distribution of states in the ensemble must remain the same after each transition. For this to hold, ergodicity is assumed where all system states can be attained given enough transitions. Therefore, for a certain state C_i, the number of state transition into that state $N(C_j)P(C_j \to C_i)$ or out of that state $N(C_i)P(C_i \to C_j)$ must be equal in each transition, where C_j are all microstates except C_i, $N(C)$ is the number of a certain state, $P(C_j \to C_i)$ is the probability of state C_j transitioning to C_i and vice versa. Since number of a certain state $N(C)$ are proportional to the probability of the system being in that state $P(C)$, where $P(C) = \frac{1}{Z}e^{-H(C)/k_BT} = \frac{1}{Z}W(C)$ where $W(C)$ is the configuration weight, detailed balancing equation can be written as

$$\frac{P(C_i \to C_j)}{P(C_j \to C_i)} = \frac{W(C_j)}{W(C_i)} \tag{7}$$

By imposing detailed balancing condition, Monte Carlo simulation can be used to compute different observables correctly given sufficient steps. There are many algorithms in Monte Carlo method. In this report, Metropolis algorithm and Swendsen-Wang algorithm were used. The details of these algorithm are discussed below.

2.1.1 Metropolis algorithm

Metropolis algorithm are one of the Monte Carlo algorithms where system evolves with consecutive single spin flips (Metropolis, Rosenbluth, Rosenbluth, Teller, & Teller, 1953). The probability of flipping a spin is given by equation (7), where

$$P^{accept}(C_i \to C_j) = \min\left[e^{-\Delta H/k_B T}, 1\right] \tag{8}$$

$$= \min\left[\exp(\frac{J}{k_B T}(2\sigma_x \sum_{\delta[x]} \sigma_{\delta[x]})), 1\right] \tag{9}$$

Where ΔH is the difference of energy between system, and $\sigma_{\delta[x]}$ are the nearest neighbours of σ_x. This means that if $\Delta H < 0$, i.e., the energy of the new state is lower than the original one, we will accept the new state; if $\Delta H > 0$, we will accept the new state with the probability of the weight ratio $e^{-\Delta H/k_B T}$.

Therefore, the procedures of one Monte Carlo step using Metropolis algorithm are formulated as below, which follow the description of Sandvik (2013):

1. Initialize an arbitrary spin lattice.
2. Select a random spin in the lattice.
3. Flip the spin with probability given in equation (8), with H only considering the nearest neighbours of the spin.
4. Repeat step 2 and 3 for N times.

Metropolis algorithm works well with low standard deviation when T are not near T_c, but when T is in the vicinity of T_c, the sizes of local clusters are large compared to local clusters at high T or low T, so it is harder for consecutive single spin flips to change the shape or size of the clusters. This means that the system between different steps are more correlated to to each other and steps needed to generate statistically independent system are

longer. This is an issue called critical slowing down. Here, a quantity called autocorrelation function can be measured, it is defined as (Sandvik, 2013),

$$A_Q(\tau) = \frac{\langle Q_k Q_{k+\tau} \rangle - \langle Q_k \rangle^2}{\langle Q_k^2 \rangle - \langle Q_k \rangle^2} \tag{10}$$

Where Q can be any physical observables, k is the Monte Carlo steps, and τ is the time lag between system. The decay of autocorrelation function can be characterized by,

$$A_Q(\tau) \to e^{-\tau/\Theta} \tag{11}$$

Where Θ is defined as the autocorrelation time. At T_c, autocorrelation time diverges as a power law,

$$\Theta \sim L^z \tag{12}$$

Where z is called the dynamic exponent. For 2D Ising model using Metropolis algorithm, $z \approx 2.125$ (Swendsen & Wang, 1987).

2.1.2 Swendsen-Wang algorithm

To overcome the problem of critical slowing down, instead of flipping a single spin, a new method could be used to identify local clusters in the system and flip all the spins inside them in one step (Swendsen & Wang, 1987). In this way, the large local clusters at T near T_c can change to statistically independent configuration with just a few Monte Carlo steps, lowering the autocorrelation time. In order to connect spins into a cluster, the probability of connecting two spins σ_i and σ_j are derived as

$$P(\tau_b = 1) = \begin{cases} 1 - e^{-2|J|/T}, & \text{if } \sigma_i(b) = \sigma_j(b), \\ 0, & \text{if } \sigma_i(b) \neq \sigma_j(b). \end{cases} \tag{13}$$

Where b is the bond index and τ_b are the bond between spin $\sigma_i(b)$ and $\sigma_j(b)$. $\tau_b = 1$ means that the bond between the spins is filled, and $\tau_b = 0$ means that there is no bond between the spins. Detailed balance condition are satisfied as $W(C)$ can be written in terms of filled bonds, and it will remain the same after all spins in the system flipped.

The following procedures of a single Monte Carlo step using Swendsen-Wang algorithm described in Sandvik (2013) was implemented:

1. Initialize an arbitrary spin lattice.
2. Cast bonds on parallel spins based on the probability in equation (13).
3. Implement Hoshen–Kopelman algorithm to grow cluster (Hoshen & Kopelman, 1976):
   (a) Select a non-visited spin to be a cluster and label the spin as visited.
   (b) Check if there are filled bonds surrounding the cluster.
   (c) If there is a filled bond and the neighbouring spin have not been visited, connect the neighbouring spin to the cluster and label the spin as visited.
   (d) Repeat (b) and (c) until all non-visited spins with filled bonds surrounding the cluster are exhausted.
   (e) Repeat (a) to (d) until all spins in the system have been visited.
4. flip all clusters with a probability of 1/2.

By using Swendsen-Wang algorithm, the autocorrelation time Θ is lower compared to that of Metropolis algorithm, with $z \approx 0.35$ in equation (12) (Swendsen & Wang, 1987).

2.2 Physical observables

Several physical observables can be extract from the Ising model. The first one is the energy of the system, which can be calculated as the sum of the interactions between neighbouring spins and is given by equation (2).

Orientation of individuals spins also contributed to the net magnetization M of the system. Which can be defined as

$$M = \sum_{i=1}^{N} \sigma_i, \quad m = \frac{M}{N} \tag{14}$$

Where m is normalized magnetization. Because spin reversal symmetry exists in finite systems, all spins can either point upwards or downwards when $T = 0$, the measurement of $\langle m \rangle = 0$ at $T = 0$ when given enough time for the system to evolve. Therefore, $\langle |m| \rangle$ was measured instead of $\langle m \rangle$ to show that the system is in ordered phase when $T < T_c$. For $L \to \infty$, $\langle |m| \rangle$ will behave like a step function, where $\langle |m| \rangle = 1$ when $T < T_c$, and $\langle |m| \rangle = 0$ when $T > T_c$,

The magnetic susceptibility can be defined as the response of magnetization of the system to external field, which can be given by the equation

$$\chi = \frac{1}{N} \frac{1}{T} \left(\langle M^2 \rangle - \langle M \rangle^2 \right) \tag{15}$$

Specific heat capacity of the system is the amount of energy needed to add to the system to raise the temperature per unit mass. It can be calculated as

$$C = \frac{1}{N} \frac{1}{T^2} \left(\langle E^2 \rangle - \langle E \rangle^2 \right) \tag{16}$$

Correlation between spins in the system can be calculated as

$$G(\vec{r}_j - \vec{r}_i) = \langle \sigma_i \sigma_j \rangle \tag{17}$$

Where $\vec{r}$ is the position vector of the spin. For simplicity, only horizontal and vertical distances are considered in this report providing that 2D Ising model is rotational invariant (Bariev, 1976). All spins in system are chosen to be the origin site σ_i to calculate spin-spin correlation with horizontal and vertical distances r up to L.

2.2.1 Finite-size scaling

Correlation length is an important concept in critical phenomena as it shows the length scale where microscopic fluctuation become significant when compared to macroscopic observables. It is defined as

$$\xi \sim t^{-\nu} \tag{18}$$

Where t is the reduced temperature,

$$t = \frac{|T - T_c|}{T_c} \tag{19}$$

And ν is one of the critical exponents. For continuous phase transition in an infinite lattice, ξ diverges at critical point. The effect of long-ranged correlation is too strong near T_c that it cannot be deemed as a perturbation, thus renormalization group theory is developed to solve it (Cardy, 1996).

In renormalization group theory, a property of phase transition is used where macroscopic observables are mostly independent from microscopic effect, so these observables can be catergorized into differentuniversality classes based on their diverging properties (Cardy, 1996). Universality classes are useful as system belonging in the same classes will have the same critical exponents, therefore simpler toy model can be used to extract exponent from more complicated system, one example is to map n-dimensional quantum Ising model into (n+1)-dimensional classical Ising model in a transverse field (Hesselmann & Wessel, 2016).

For spin-spin correlation, when T is not near T_c and the ξ is small, mean field approximation can be applied to ignored the interactions and it has a form called Ornstein-Zernike

equation (Ornstein, 1914),

$$G(\vec{r}) \sim \frac{\mathrm{e}^{-r/\xi}}{r^{(d-2)/2}} \tag{20}$$

where d is the dimension of the system.

This relation are only suitable when $r \gg \xi$ according to Ginzburg criterion (Als-Nielsen & Birgeneau, 1977). Therefore when it is at T_c where $\xi \ll r$, it has a different form (Kadanoff, 1966),

$$G(\vec{r}) \sim \frac{1}{r^{d-2+\eta}} \tag{21}$$

where $\eta = 1/4$ in 2D Ising model (Wu, McCoy, Tracy, & Barouch, 1976),

For magnetization, it decays as the following equation (Kadanoff, 1966),

$$\langle m \rangle \begin{cases} \sim (T_c - T)^{\beta}, & \text{when } T < T_c \\ = 0, & \text{when } T > T_c \end{cases} \tag{22}$$

The power law of susceptibility and specific heat are defined respectively as below (Kadanoff, 1966),

$$\chi \sim t^{-\gamma} \tag{23}$$

$$C \sim t^{-\alpha} \tag{24}$$

In group renormalization theory, by using the property of scale invariance, free energy and also spin-spin correlation function of a system that only has short range interaction can be reiterated by coarse graining method called block spin transformation until they are just functions of d and two constants called renormalization group eigenvalues y_t and y_h (Cardy, 1996). Since all 3 observables above can be derived from free energy, the critical exponents β, γ, α from observables and exponents ν, η from correlation function can all be expressed in the form of d, y_t, and y_h. Therefore, all critical exponents are related to each other, giving

rise to the scaling relations as below (Kadanoff, 1966),

$$\begin{aligned} \gamma &= \nu(2-\eta) \\ \nu d &= 2-\alpha \\ \gamma &= 2-\alpha-2\beta \end{aligned} \tag{25}$$

The exact solutions of critical exponents in 2D square Ising model are (Kadanoff, 1966):

$$\alpha = 0 \tag{26}$$

$$\beta = 1/8 \tag{27}$$

$$\gamma = 7/4 \tag{28}$$

$$\nu = 1 \tag{29}$$

In finite system, ξ is not able to diverge as the maximum value of ξ is limited by system size L. Hence, instead of diverging, free energy would have a finite peak at critical point. Therefore, scaling hypothesis predict that the peak free energy and physical observables be described by an analytic function which scales with system size. For example, magnetization is hypothesised the have the following scaling form (Sandvik, 2013).

$$|m|(T_c - T, L) = L^{\sigma} f\left(\xi/L\right) \tag{30}$$

From equation (18),

$$t \sim \xi^{-1/\nu} \tag{31}$$

Therefore, equation (30) turns to,

$$|m|(T_c - T, L) = L^{\sigma} f\left((T_c - T)L^{1/\nu}\right) \tag{32}$$

Comparing with equation (22), σ must be $-\beta/\nu$ in order for equation (30) to reduce to $(T_c - T)^{\beta}$ when $L \to \infty$, therefore the equation becomes

$$|m|(T_c - T, L) = L^{-\beta/\nu} f\left((T_c - T)L^{1/\nu}\right) \tag{33}$$

This shows that in the scaling regime $(T_c - T)L^{1/\nu} \ll 1$, the scaling function becomes noticeable, and the magnetization will have a smooth decay instead of having a singularity at critical point. Apart from this, 3 observations could be made in finite system (Cardy, 1996):

1. The decay is shifted by $L^{-1/\nu}$ from the critical point. Since periodic boundary is used to suppress fluctuation at boundary, the effective T_c would be higher and the decay will shift to the right. With higher L, the shift will be smaller.

2. The height of the decay is scaled by $L-\beta/\nu$. This means that the function decay to a lower value with increasing L.

3. The width of the decay is scaled by $L^{-1/\nu}$. This means that the function decay at a faster rate with increase L.

Similar observation could be made on susceptibility and specific heat capacity. The results in section 3 will be used to verify these claims.

The scaling function of magnetization can then be written as,

$$f_m\left((T_c - T)L^{1/\nu}\right) = |m((T_c - T), , L)|L^{\beta/\nu} \tag{34}$$

Similarly, scaling function of susceptibility and specific heat can be written as (Sandvik, 2013),

$$f_\chi\left(tL^{1/\nu}\right) = \chi(t, L)L^{-\gamma/\nu} \tag{35}$$

$$f_C\left(tL^{1/\nu}\right) = C(t, L)/\ln(L) \tag{36}$$

For equation (36), $\ln(L)$ is used instead of $L^{-\alpha/\nu}$ because $\alpha = 0$ in 2D Ising model. $\ln(L)$ is used as an approximation.

By plotting the scaling function of different system size against its argument, the finite size effects mentioned above are eliminated, causing the scaling function to collapse onto each other. Since the scaling function contains T_c and various critical exponents. Only the correct combination of T_c and critical exponents will cause data to collapse. Thus, the correct value of T_c and critical exponents can be extracted from data collapse method.

In this report, firstly physical observables was plotted against T to show that they exhibits phase transition and to verify the claims of finite size effect. Then, an attempt was made to extract T_c by performing logistic regression on the $|m|$ against T. After that, finite size scaling is performed to verify the exaction solutions of T_c, β, γ, and ν. If C shows approximate collapse with $\ln(L)$, $\alpha = 0$ can be verified too.

2.3 Binder ratio

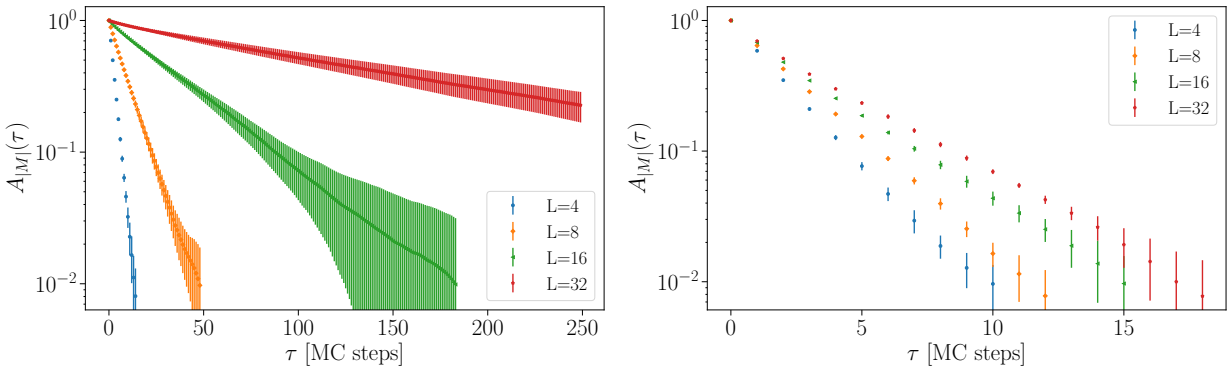
If two observables have the same scaling function, their ratio will be dimensionless and thus it will act as a scaling function. The ratio of different system sizes L will simply cross each other at the critical point when plotted against T. This ratio is called Binder ratio, and below is one of the examples of Binder ratio using magnetization of the system (Binder, 1981),

$$Q = \frac{\langle m^2 \rangle}{\langle |m| \rangle^2} \tag{37}$$

Binder ratio is useful as T_c can be extracted from it without previous knowledge of any critical exponents in the system.

Same as magnetization, this Binder ratio should behave like a scaling function,

$$Q \sim f_B\left((T_c - T)L^{1/\nu}\right) \tag{38}$$



(a) Semi-log plot of $A_{|M|}(\tau)$ using Metropolis algorithm

(b) Semi-log plot of $A_{|M|}(\tau)$ using Swendsen-Wang algorithm

Figure 1: A comparison of autocorrelation function $A_{|M|}(\tau)$ at $T = 2.269$ between (a) Metropolis and (b) Swendsen-Wang algorithm. With 1000000 Monte Carlo steps. Large error bars touching x-axis indicates that $A_{|M|}(\tau) \to 0$.

3 Result and Discussion

For the results, Monte Carlo simulations were ran on 2D Ising model with system size $L = 4$, 8, 16, and 32 respectively, with temperature ranging from 1.5 to 3.5 in 21 equidistant temperature steps. For each temperature steps, 1000 Monte Carlo steps were performed to ensure the system reaches equilibrium state, and 100000 Monte Carlo steps were ran for measurement unless specified otherwise. The 100000 Monte Carlos steps were grouped into 100 bins with 1000 Monte Carlos steps each, and the mean value of each individual bin is calculated. The expected value and standard deviation of physical observables were then obtained from the mean of means of all bins and standard deviation of means of all bins respectively. The program is written in Python 3.8.12.

3.1 Autocorrelation

From Figure 1a, it can be seen that the when L increased, $A_{|M|}(\tau)$ decayed exponentially at a slower rate using Metropolis algorithm. $A_{|M|}(\tau)$ of system size $L = 32$ did not converge to 0 even after $\tau = 250$. On the other hand, Figure 1b shows that $A_{|M|}(\tau)$ of all system size L decayed quicker using Swendsen-Wang algorithm when compared to those using Metropolis

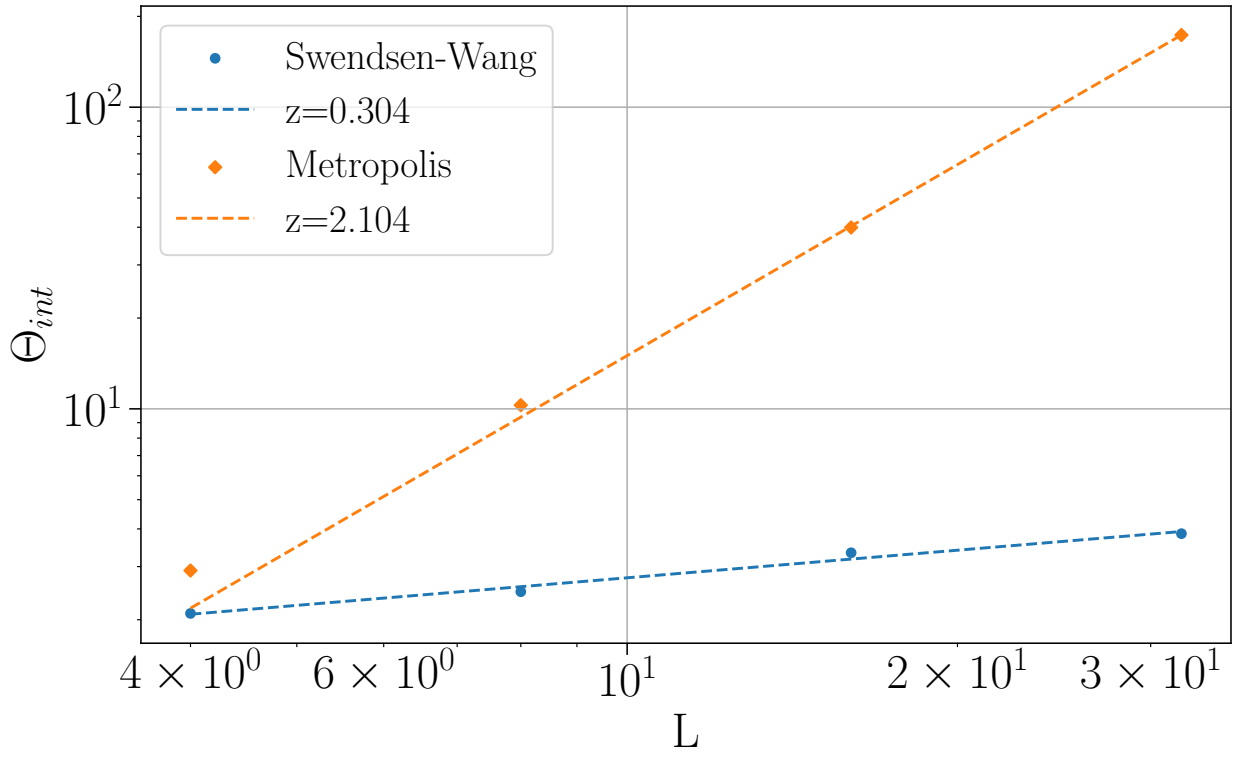
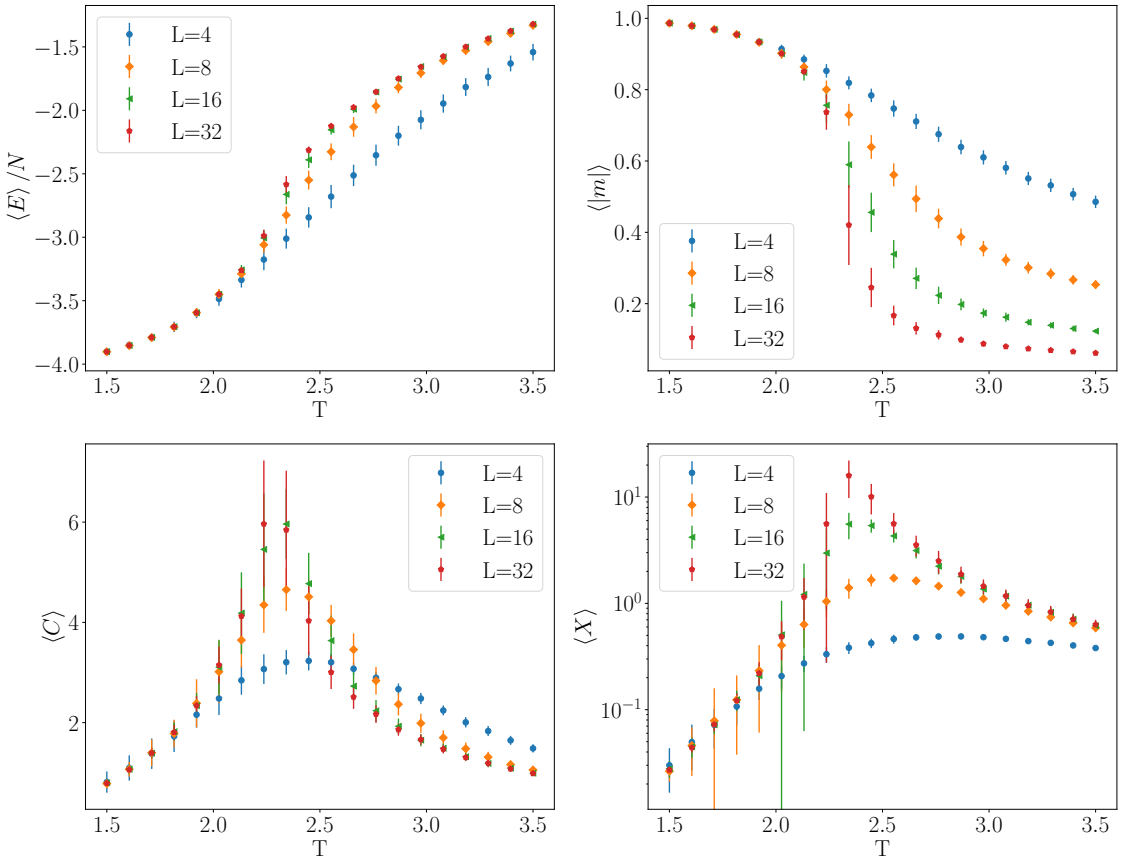


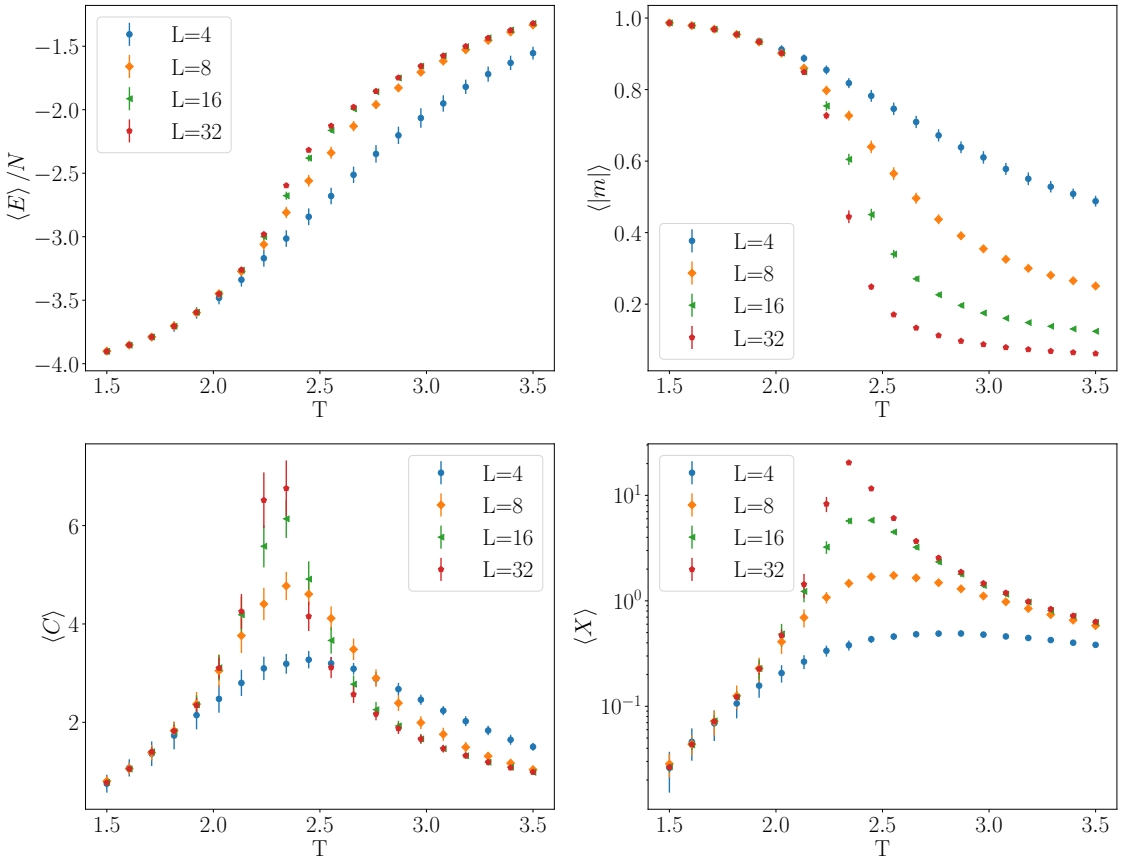
Figure 2: Autocorrelation time Θ between the two algorithms

algorithm, where $A_{|M|}(\tau)$ of system size $L = 32$ approached 0 after $\tau = 16$ using Swendsen-Wang algorithm.

From Figure 2, data of $L = 4$ were omitted during fitting as the system size is too small. After fitting, $z \approx 0.304$ was obtained for Swendsen-Wang algorithm, while $z \approx 2.104$ was obtained for Metropolis algorithm. The former deviates from literature value of $z \approx 0.35$ by 14%, while the latter is in reasonable accord with the literature values $z \approx 2.125$ for Metropolis algorithm (Swendsen & Wang, 1987). To obtain a more precise value, more data points with larger system size is needed to have a better fit. Nevertheless, the large difference in the dynamic exponent obtained shows that Swendsen-Wang algorithm performs better than Metropolis algorithm at the vicinity of T_c.



(a) $\langle E\rangle/N$, $\langle|m|\rangle$, $\langle C\rangle$, and $\langle\chi\rangle$ against T plots using Metropolis algorithm



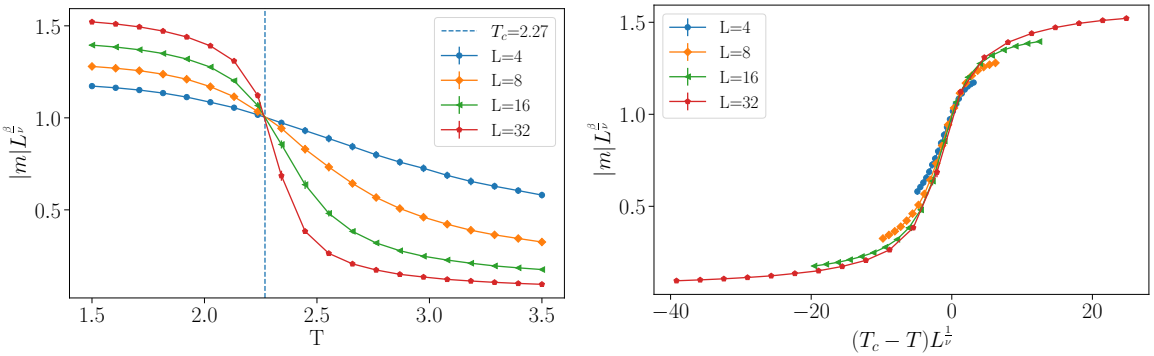
(b) $\langle E\rangle/N$, $\langle|m|\rangle$, $\langle C\rangle$, and $\langle\chi\rangle$ against T plots using Swendsen-Wang algorithm

Figure 3: Physical observables with (a) Metropolis algorithm and (b) Swendsen-Wang algorithm for lattice size $L = 4, 8, 16, 32$.

3.2 Physical observables

All physical observables showed phase transition behaviour using both Metropolis algorithm and Swendsen-Wang algorithm as shown in Figure 3a and 3b. It can be seen that the fluctuations of observables became larger near the critical point using Metropolis algorithm when compared to Swendsen-Wang algorithm, which demonstrate the issue of critical slowing down in Metropolis algorithm. All observables exhibited finite size effects which are in line with the three predictions mentioned in section 2, which are shifting decay/peak to the left with increasing L, increasing height of decay/peak with increasing L, and decreasing width of decay/peak with increasing L.

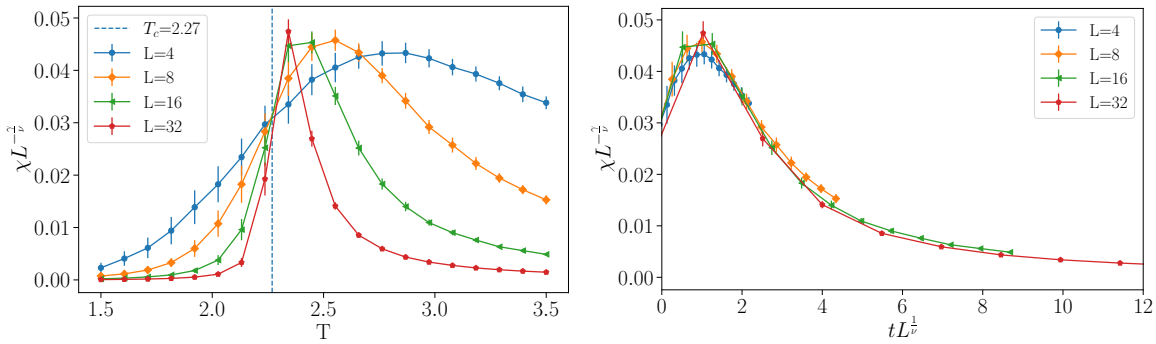
For magnetization, it can be seen that the function were behaving more like a step function as L increase, with ordered phase $T < T_c$ having magnetization $m = 1$ while disordered phase $T > T_c$ having magnetization $m = 0$. The logistic regression of $|m|$ against T returns value of $T_c \approx 2.276$, which is slightly higher than the exact solution of $T_c \approx 2.269$ by 0.31%. This shows that there are still remaining finite-size effects at $L = 32$, and larger system sizes are needed to obtain a more precise value of T_c.



(a) f_m against T plot

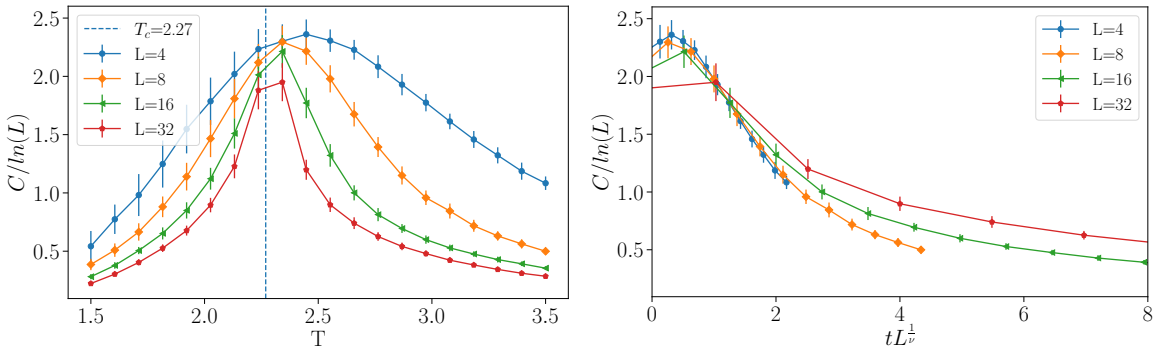
(b) Data collapse of $|m|$

Figure 4: Finite-size scaling plot of the absolute value of magnetization for lattice size $L = 4, 8, 16, 32$. $\beta = 1/8$ and $\nu = 1$.



(a) f_χ against T plot (b) Data collapse of χ

Figure 5: Finite-size scaling plot of the magnetic susceptibility for lattice size $L = 4, 8, 16, 32$. $\gamma = 7/4$ and $\nu = 1$.



(a) f_C against T plot (b) Data collapse of C

Figure 6: Finite-size scaling plot of the specific heat capacity for lattice size $L = 4, 8, 16, 32$. $\alpha = 0$ and $\nu = 1$.

3.3 Finite-size scaling

Following a standard procedure in determining T_c and critical exponents, firstly the scaling functions of the observables were plotted against T as shown in Figure 4a, 5a, 6a. By varying the values of ratios between critical exponents β/ν for $|m|$ and γ/ν for χ, all scaling function crossed at a single point with the correct values of exponent ratio, and the single point is also the value of T_c. The exponent ratios β/ν, γ/ν and T_c was then used to plot scaling function against its argument. Scaling functions successfully collapsed onto each other with the correct value of exponent $1/\nu$ in the argument, and hence β and γ can be

determined.

With the exact values of T_c, β, γ, and ν, data have collapsed successfully in Figure 4b, 5b, and 6b, which supported the scaling hypotheses in equations (34), (35), (36), and also the exact solutions in equations (6), (27), (28), (29). Specific heat capacity only has an approximate data collapsed with $1/\ln L$, which supports the claims of equation (26).

3.4 Spin-Spin Correlation

Figure 7 shows different behaviour of $G(r)$ at different T, G(r) decayed exponentially to the background noise is reached which is the magnetization $|m|$ of the system. Therefore, G(r) only decayed a little as $|m| \approx 1$ at $T = 3.5$, and it decayed to 0.5 and 0 when $T = 2.24$ and $T = 3.5$ respectively. It can be seen that the function is symmetric as periodic boundary is applied, where G(r) will rebound to its original position after $r = L/2$.

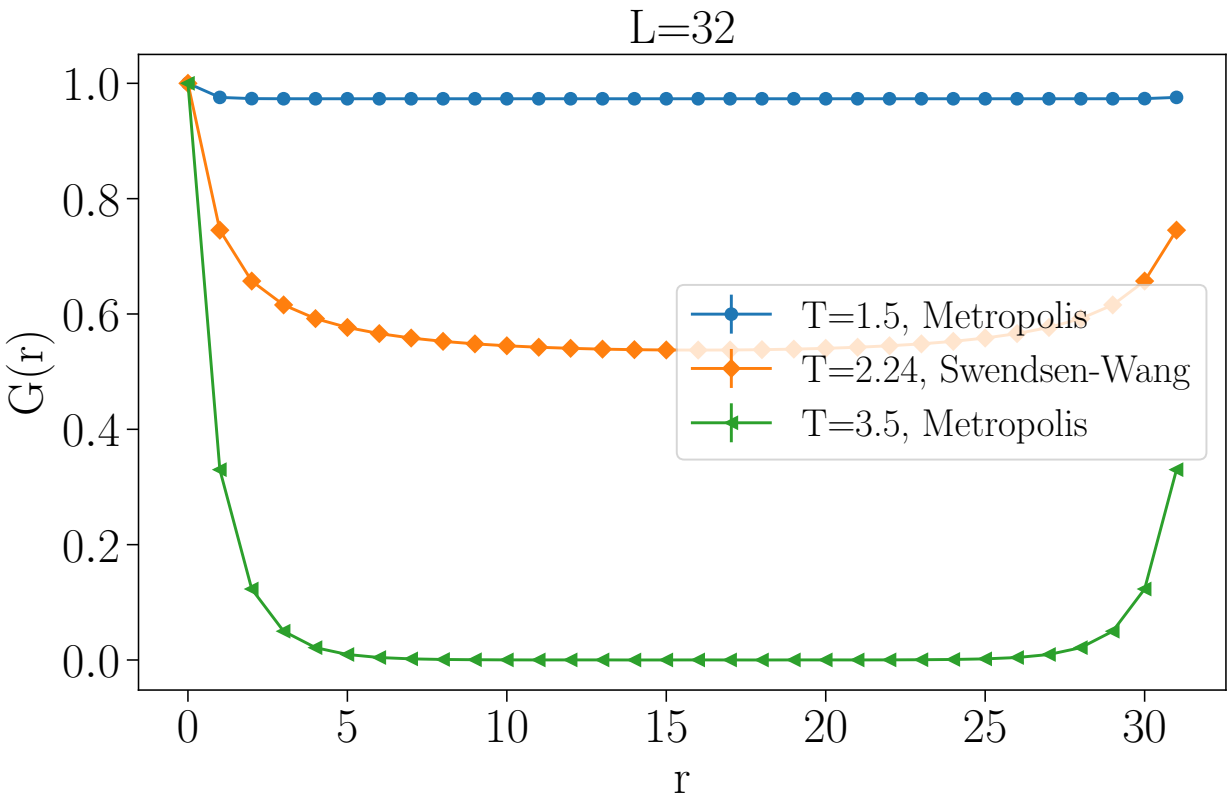
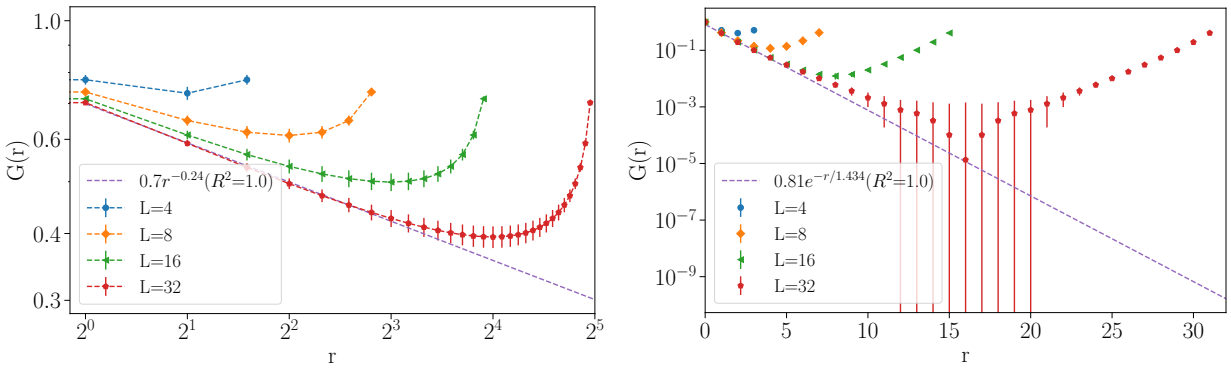


Figure 7: Spin-spin correlation function $G(r)$ at temperature $T = 1.5, 2.2, 3.5$



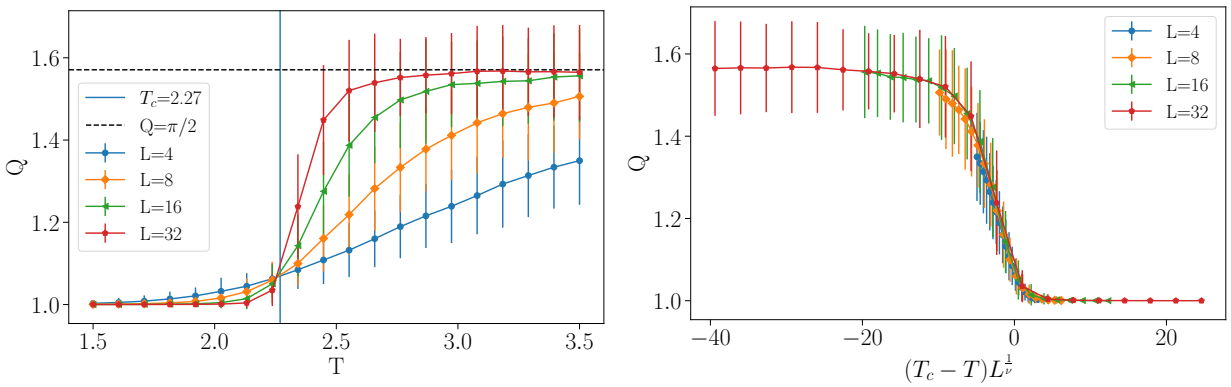
(a) Log-log plot of G(r) at T=2.285

(b) Semi-log plot of G(r) at T=3

Figure 8: Spin-spin correlation function $G(r)$ for lattice size $L = 4, 8, 16, 32$ at temperature (a) $T = 2.285$ and (b) $T = 3$. Large error bars touching the x-axis indicates that $G(r) \to 0$. $d = 2$ and $\nu = 1$.

Data of system size $L = 32$ were used to fit the decay of $G(r)$, where the data of r=0 was omitted to avoid error and the last 23 data were also omitted due to periodic boundary condition. $G(r)$ of different system size L decayed asymptotically as equation (21) which can be seen in Figure 8a, with $\eta \approx 0.243$ which deviates from analytic value $\eta = 0.25$ by roughly 2.8%. Moreover, the result of η was obtained at $T = 2.285$, which deviates from analytic solution of $T_c \approx 2.269$ by 0.70%. This could be due to the finite size effect of the system shifting the effective T_c to a higher value. Fine-tuning of effective T_c with higher precision is needed to obtain a more accurate value of η.

When $T = 3$, $G(r)$ of different system sizes L decayed asymptotically as Ornstein-Zernicke form in equation (20), with a correlation length of $\xi \approx 1.439$ as illustrated in Figure 8b, this is in line with the fact that ξ is small when T is away from T_c.



(a) Q against T plot

(b) Data collapse of Q

Figure 9: Binder ratio for lattice size $L = 4, 8, 16, 32$. $T_c \approx 2.269$ and $\nu = 1$.

3.5 Binder ratio

Binder ratio was computed by performing element-wise division of $\langle m^2 \rangle$ by $\langle |m|^2 \rangle$, and the standard deviation of the ratio is computed by error propagation using standard deviation of the two observables. From Figure 9a, the Binder ratio crossed each other near the exact solution of T_c, demonstrating the ability of Binder ratio in extracting T_c from finite size systems. Apart from that, the result converges to $\pi/2$ at high temperatures, which is in agreement with the prediction in Sandvik (2013). Figure 9b shows that Binder ratio of different system sizes successfully collapsed onto each other, verifying the scaling hypothesis in equation (38). However, the error becomes larger with increasing T as shown in Figure 9, so better method of computing Q is needed, such as calculating standard deviation by repeated measure of Q. A more precise value of T_c can be extracted by measuring Q at a narrower temperature range around T_c, and the size dependence of T_c can be demonstrated by seeing the systematic drift of crossing points between Q of different system sizes L.

4 Conclusion

In conclusion, Monte Carlo methods consisting of Metropolis algorithm and Swendsen-Wang algorithm were implemented to analyze the thermal transition of 2D classical Ising model, and finite size scaling was used to studied the critical phenomena. All physical observables exhibit critical behaviour during phase transition, and numerical results of T_c and η obtained have slight deviations from exact solutions, which the errors can be accounted by finite size effects. $|m|$, χ, and C collapsed successfully with the exact values of T_c, β, γ, and ν, which supports the scaling hypothesis of the 2D square Ising model. Last but not least, Binder ratio was implemented to demonstrate its usage in extracting T_c. Further simulations with larger system sizes L are needed to to obtain a more accurate value of T_c and ν , and bootstrap method could be implemented in the future to reduce running time of the simulations. Further investigation could be done on 2D quantum Ising model by mapping it to 3D classical Ising model in a transverse field.

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Appendix A Code for Metropolis algorithm

```
@jit
def Metropolis(Config,L,T):
    for a in range(L):
        for b in range(L):
                i = np.random.randint(0, L)
                j = np.random.randint(0, L)
                S1 = Config[i,j]
                S2 = Config[(i+1)%L, j] + Config[i,(j+1)%L]
                                + Config[(i-1)%L,j] + Config[i,(j-1)%L]
                dE = 2*S1*S2
                # if P_accept(C_i -> C_j) > 1, i.e. W(C_j)>W(C_i)
                if dE < 0:
                    S1 *= -1
                # if P_accept(C_i -> C_j) < 1 & r < P_accept(C_i -> C_j)
                elif np.random.rand() < np.exp(-dE/T):
                    S1 *= -1
                Config[i, j] = S1

    return Config
```

Appendix B Code for Swendsen-Wang algorithm

```
    @jit
def SwendsenWang(Config,L,T):
    bprob = 1 - np.exp(-2/T)
    #generate bond configuration
    bond = np.full((2,L,L), False)
    for i in range(L):
        for j in range(L):
            if Config[i,j] == Config[(i+1)%L,j]:
                if np.random.rand() < bprob:
                    bond[0,i,j] = True
            if Config[i,j] == Config[i,(j+1)%L]:
                if np.random.rand() < bprob:
                    bond[1,i,j] = True
    #cluster search procedure
    notvisited = np.full((L,L), True)
    for i in range(L):
        for j in range(L):
            if notvisited[i,j]:
                cseed = Config[i,j]
                if np.random.rand() < 0.5: #corrrect to 0.5 later
                    flipclus = True
                    Config[i,j] *= -1
                else:
                    flipclus = False
                notvisited[i,j] = False
```

```
stack = np.empty((L*L,2), dtype=np.int32)
stack[0] = np.array([i,j])
nstack = 1

while nstack > 0:
    a,b = stack[nstack-1]
    s0 = Config[a,b]
    #print(f"s0=[{a},{b}]")
    nstack -= 1

    #down
    if bond[0,a,b] and notvisited[(a+1)%L,b]:
        notvisited[(a+1)%L,b] = False
        if flipclus:
            Config[(a+1)%L,b] *= -1
        nstack += 1
        stack[nstack-1] = [(a+1)%L,b]

    #right
    if bond[1,a,b] and notvisited[a,(b+1)%L]:
        notvisited[a,(b+1)%L] = False
        if flipclus:
            Config[a,(b+1)%L] *= -1
        nstack +=1
        stack[nstack-1] = [a,(b+1)%L]
```

```
                #up
                if bond[0,(a-1)%L,b] and notvisited[(a-1)%L,b]:
                    notvisited[(a-1)%L,b] = False
                    if flipclus:
                        Config[(a-1)%L,b] *= -1
                    nstack +=1
                    stack[nstack-1] = [(a-1)%L,b]

                #left
                if bond[1,a,(b-1)%L] and notvisited[a,(b-1)%L]:
                    notvisited[a,(b-1)%L] = False
                    if flipclus:
                        Config[a,(b-1)%L] *= -1
                    nstack +=1
                    stack[nstack-1] = [a,(b-1)%L]

    return Config
```