Study on Phase Transitions of Classical and Quantum Ising Model with Monte Carlo Simulation

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Acknowledgement

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Contents

Introduction

The Ising model was proposed by Wilhelm Lenz (1920) and it was given to his student Ernst Ising (1925). It is one of the fundamental mathematical models of ferromagnetism in statistical mechanics.[1] Ising solved the one-dimensional Ising model and proved that there is not phase transition in one-dimensional case, while other scientists like Lars Onsager then investigated and found out that there is an analytical solution for thermal phase transitions of two-dimensional classical Ising model.[1] After that, with a transverse field being added to a classical Ising model, the quantum Ising model was proposed and it can experience both quantum phase transition and thermal phase transition.

In this research, we have used three different Monte Carlo simulations methods, which are Metropolis algorithms, Wolff algorithm and Swendsen-Wang algorithm to simulate different physical observables of the two-dimensional square Ising model in the vicinity of thermal phase transitions temperature. Then, the thermal phase transition temperature of the model is identified by using Binder ratio and finite size scaling properties of Ising model, followed by the study of autocorrelaton time of the three different Monte Carlo simulations methods. After that, we would move on to quantum Ising model and study the quantum phase transition by using the same Monte Carlo simulations methods used before, and study the thermal phase transition temperature of the model in the vicinity of the quantum critical points.

Classical Ising model

Definition of physical observables

The main interest in the context of Ising model is **magnetization**[1]. The full magnetization M of the model is defined as $M = \sum_{i=1}^{N} \sigma_i$ and size-normalized quantity is defined as $m = \frac{M}{N}$, where N is the size of the system[1].

We are also interested in defining **magnetic susceptibility**, which is

$$\chi = \frac{d\langle m \rangle}{dh}$$

It can interpreted as the linear response of the model to the a uniform magnetic field or the rate of change of $\langle m \rangle$ over the change of h, which is the variables describing the strength of magnetic field. By using expression of partition function and definition of $\langle m \rangle$ with simple differentiation,

$$\langle m \rangle = \frac{1}{Z} \sum_S m e^{-(\frac{E_0 - hM}{T})} \text{ and } Z = \sum_S e^{-(\frac{E_0 - hM}{T})}$$

We obtain $\chi = \frac{1}{N}\frac{1}{T} (\langle M^2 \rangle - \langle M \rangle^2)$. Theoretically, the susceptibility would divergences at the phase transition point when h = 0.

Besides, as the expression of energy is

$$E = -J \sum_S \sigma_i \sigma_j - h \sum_S \sigma_i \text{ and J =1 (i.e. set this for simplicity)}$$

For the case of classical Ising model, h=0 and the specific heat of the Ising model is defined as $C = \frac{1}{N}\frac{dE}{dT}$. By similar procedures to the derivation of susceptibility, we can find that $C = \frac{1}{N}\frac{1}{T}(\langle E^2\rangle - \langle E\rangle^2)$.

Detailed Balance[1]

For the configurations of Ising model that follows a certain probability distribution P, consider 2 different configurations C_i and C_j, they would follow the **master equation**,

$$\sum_{j\neq i}[N_0(C_j)P(C_j \rightarrow C_i) - N_0(C_i)P(C_i \rightarrow C_j)] = 0 \quad (1)$$

i.e. The configuration C_i and C_j would attain equilibrium, which means the number of configurations changing from C_i to C_j would the same as number of configurations changing from C_j to C_i.

With $N_0(C_i) \propto P(C_i)$, (i.e. the number of configurations is proportional to its probability), we can re-write the master equation to be

$$\sum_{j\neq i}[P(C_j)P(C_j \rightarrow C_i) - P(C_i)P(C_i \rightarrow C_j)] = 0 \quad (2)$$

There are many solutions that satisfy (2). We can consider each term in the summation to be equal 0 and we would obtain,

$$P(C_j)P(C_j \rightarrow C_i) - P(C_i)P(C_i \rightarrow C_j) = 0$$

$$\frac{P(C_i \rightarrow C_j)}{P(C_j \rightarrow C_i)} = \frac{P(C_j)}{P(C_i)} \quad (3)$$

As the configuration follows Boltzmann distribution, $P(C_i) = \frac{1}{Z}e^{-\frac{E(C_i)}{T}}$. Also, $P(C_i \rightarrow C_j) = P^{attempt}(C_i \rightarrow C_j)P^{accept}(C_i \rightarrow C_j)$ and $P^{attempt}(C_i \rightarrow C_j) = constant$. Putting these two back to the equation (3), we can deduce

$$\frac{P^{accept}(C_i \rightarrow C_j)}{P^{accept}(C_j \rightarrow C_i)} = \frac{W(C_j)}{W(C_i)} \quad (4)$$

One of the solution that can satisfy it is **Metropolis acceptance probability**,

$$P^{accept}(C_i \rightarrow C_j) = \min\left[\frac{W(C_j)}{W(C_i)}, 1\right] = \min\left[e^{-\frac{1}{T}(E_{C_j} - E_{C_i})}, 1\right]$$

There are two situations,

1) If $\frac{W(C_j)}{W(C_i)} < 1$, we will accept the new configurations C_j if $\frac{W(C_j)}{W(C_i)}$ is greater than a random number selected in the interval (0,1].

2) If $\frac{W(C_j)}{W(C_i)} > 1$, we will always accept new configurations C_j.

Whatever the situation is, two sides of the equation are always the same in this case.

Monte Carlo methods for numerical simulation of Ising model transition

Metropolis Algorithm[1]

With the energy $E = -J \sum_S \sigma_i \sigma_j - h \sum_S \sigma_i$, $P^{accept}(C_i \to C_j) =$ min [$e^{-\frac{1}{T}(E_{C_j} - E_{C_i})}$, 1] and h =0 for classical Ising model case, we can deduce that,

$$P^{accept}(C_i \to C_j) = \text{ min } [\exp\left(\frac{2J}{T}\ \sigma_i \sum \sigma_j\ \right), 1]$$

σ_i refers to the spin (either spins up or down) at the selected site, while $\sum \sigma_j$ refers to the 4 spins surrounding σ_i in 2D square Ising model. Plugging the above equation back to (4), we can see that 2 sides are equal.

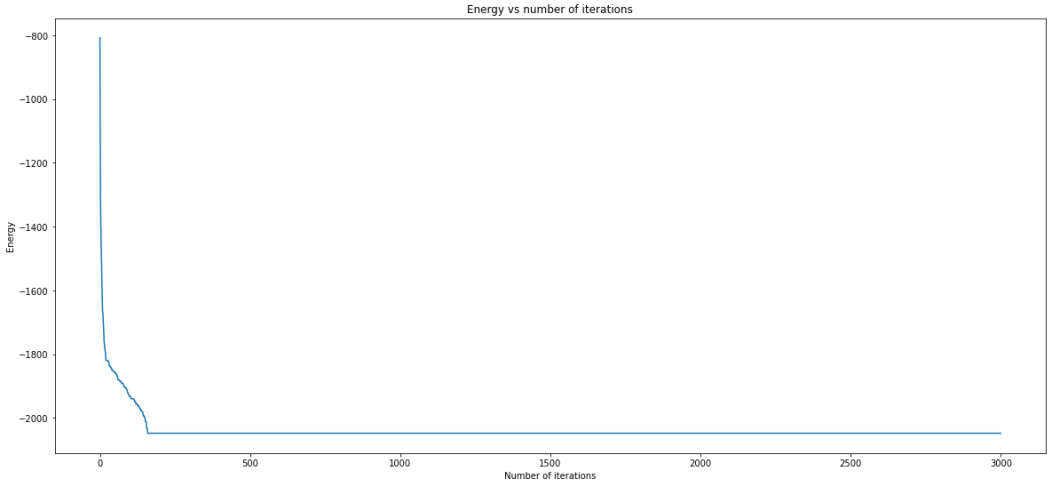
Programme Implementation

There are mainly 4 parts in the programme implementation,

1) Thermalization

- At the start of updating, the configuration would change constantly and it might not follow the Boltzmann distribution. Therefore, we will give the configuration time to flip (i.e. Monte Carlo Steps) will not take the configurations generated at the start of simulation.

- Below is the plot of the energy of square lattice with side 32 over the iterations,



We can see that the energy of the system has not reached equilibrium until iteration around 250.

2) Updating the configuration by Metropolis algorithm

   - Randomly selected a site in the Ising model
   - If the energy after flipping is lower, the flipping is accepted. Besides, if the energy after flipping is higher but the probability $e^{-\Delta E/T}$ is larger than a random number in the range [0,1], the flipping is also accepted. Otherwise, the flipping is not accepted.
   - Repeat the above steps for N (i.e. the size of Ising model) times.

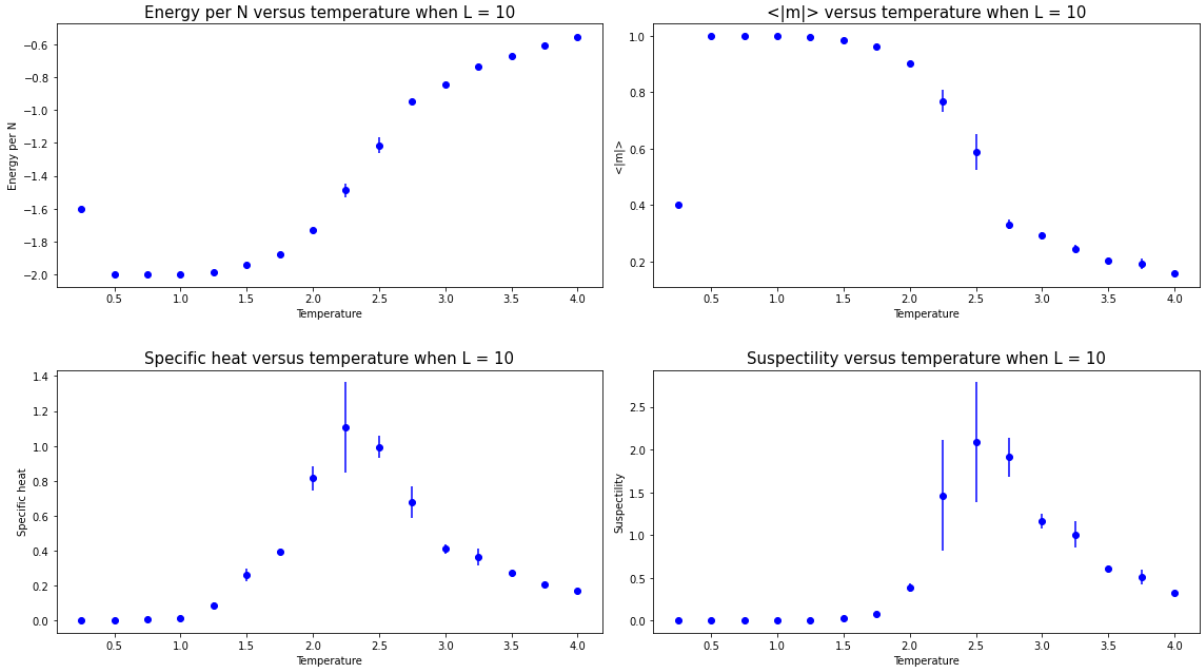
3) Binning and collecting data

   - Since all the configurations are generated from updating the previous one, the configurations near to each other in Markov Chain are not statistically independent enough and it is not statistically worthwhile to measure the physical observable after each update. Therefore, we would bin the data and take average of the data after certain iterations. (We would discuss more in the autocorrelation part)

4) Plotting the 4 physical observables over the temperature

Result

With the size of lattice equal to 10, iteration time = 1000 and binning for every 100 iterations, we get the values of physical observables over the temperature [0.25, 4],



We can see that the energy per site and magnetization changes its state at around T = 2.269, while the specific heat and susceptibility diverges at around the same temperature. T = 2.269 is the transition temperature. For a more precise way to obtain transition temperature, we would discuss it in the finite size scaling part.

Swendsen Wang algorithm

Swendsen Wang algorithm is another algorithm that can satisfy detailed balance condition (4). Consider two Ising model configurations C_i and Ising model configurations C_j, the transition from C_i to C_j must pass through a particular bond configuration.[2] So LHS of (4) becomes,

$$\frac{P(C_i \to C_j)}{P(C_j \to C_i)} = \frac{P(C_j|Bond\ configuration)P(Bond\ configuration|C_i)}{P(C_i|Bond\ configuration)P(Bond\ configuration|C_j)}$$

As the probability for a bond configuration to go to any Ising configuration consistent with it is uniform[3], therefore the only difference would be the missing bond between neighbouring spin and the probability is $(1-p) = 1-(1-\exp(-2\beta J)) = \exp(-2\beta J)$. The above equation would become

$$\frac{P(C_j|Bond\ configuration)P(Bond\ configuration|C_i)}{P(C_i|Bond\ configuration)P(Bond\ configuration|C_j)} = \frac{\exp\left(-2\beta \sum_{\langle l,m\rangle} \delta_{\sigma_l,\sigma_m} J_{lm}\right)}{\exp\left(-2\beta \sum_{\langle l,m\rangle} \delta_{\sigma'_l,\sigma'_m} J_{lm}\right)} = e^{-\beta \Delta E} = RHS$$

As a result, we can see that Swendsen Wang algorithm satisfy the detailed balance condition and it can be used to simulate the phase transition of Ising model.[3]

Programme Implementation

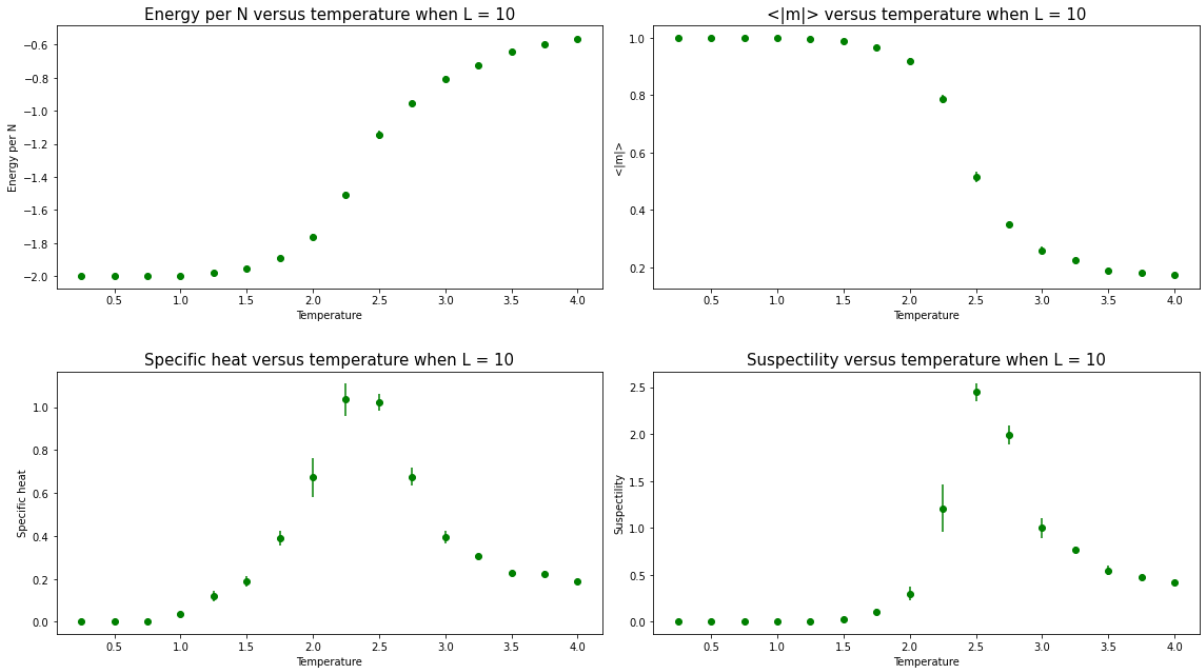
There are mainly 4 parts in the programme implementation,

1) Thermalization
2) Updating the configuration by using Swendsen Wang algorithm
    a. Going through each site of the Ising model.
    b. If a particular site has the same spin as the nearest neighbours, there will be bond between the 2 sites if the probability $1-\exp(-2\beta J)$ is greater than a randomly selected number in the intervals (0,1]. The site with bonds would come together and form the cluster.
    c. The clusters generated in part b) would be flipped if a randomly selected number in the intervals (0,1] is greater than 0.5.
3) Binning and collecting data

4) Plotting the 4 physical observables over the temperature

Result

With the size of lattice equal to 10, iteration time = 1000 and binning for every 100 iterations, we get the values of physical observables over the temperature [0.25, 4],



Wolff algorithm

Wolff algorithm is also algorithm that can satisfy detailed balance condition (4) and it can be proved by using similar ways in the previous part. It takes a shorter time for computing than Swendsen Wang algorithm and it is proven numerically that it has a shorter autocorrelation length than Swendsen Wang algorithm[4].

Programme Implementation

There are mainly 4 parts in the programme implementation,

1) Thermalization
2) Updating the configuration by using Wolff algorithm
    a. Randomly choose a site in Ising model to start.
    b. Explore the nearest neighbour of the randomly chosen site. If the neighbouring site
    (i) have the same spin as the randomly chosen site
    (ii) have not been reached before
    (iii) the bonding probability $p = 1 - \exp(-2\beta J)$ is greater than a randomly selected number in the interval (0,1], where $\beta = \frac{1}{Temperature}$

then the neighbouring site would be added to the cluster. Otherwise, it will be marked as being explored. This would repeat for every site in the boundaries of the cluster.

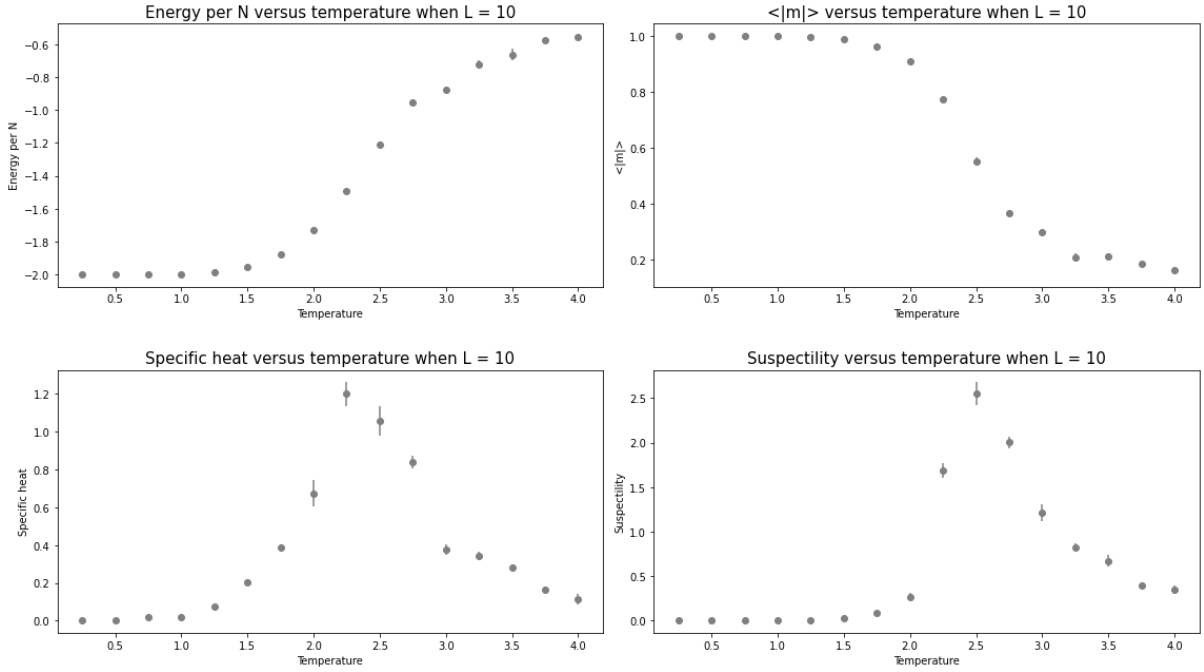
c. Flip all the spin in the cluster.

3) Binning and collecting data

4) Plotting the 4 physical observables over the temperature

Result

With the size of lattice equal to 10, iteration time = 1000 and binning for every 100 iterations, we get the values of physical observables over the temperature [0.25, 4],



Finite Size Scaling and Binder Cumulant

Binder ratio and Binder Cumulant

Binder ratio and Binder Cumulant are the two dimensionless quantities that does not depend on the size of the system, and they are useful for extracting transition temperature T_c without knowing the values of critical exponents.

Definition of Binder Ratio and Binder Cumulant

Binder ratio are either defined as

$$B_r = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2} \text{ or } B_r = \frac{\langle m^2 \rangle}{\langle |m| \rangle^2}$$

We will be using the first definition $B_r = \frac{\langle m^4 \rangle}{\langle m^2 \rangle^2}$ in the following part.[5] Besides, by defining another quantity Binder Cumulant,

$$U = \frac{3}{2}(1 - \frac{1}{3}B_r)$$

we can observe that Binder Cumulant of the system would **approaches 0 when $T > T_c$** and **approaches 1 when $T < T_c$** for increasing L^5 (i.e. Larger the system size, these properties would be more obvious). Also, the Binder Cumulant of different system size would cross at $T = T_c \approx 2.269$.

Result

Fig 1. Binder Cumulant versus temperature

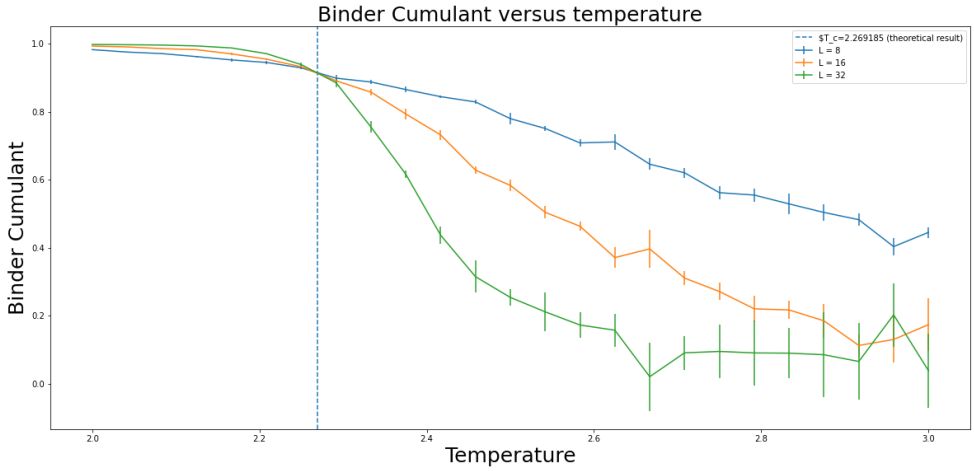
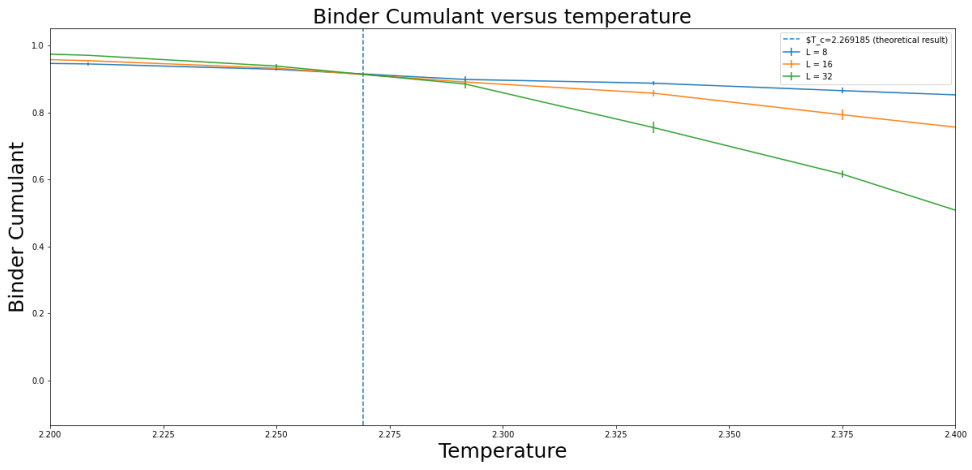


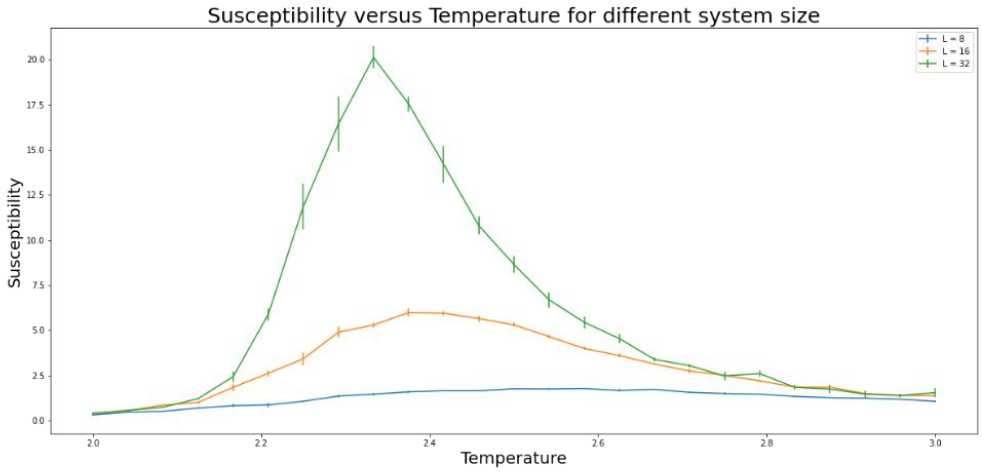
Fig 2. Binder Cumulant versus temperature (zoom in version)



We can see from the graph above that different system size would cross at the transition temperature, which can help us to locate the transition temperature without knowing the critical exponents.

Finite Size Scaling

Before introducing finite size scaling, we can look of the following graph,



We can see that there are 2 features,

1) Larger the system size, larger the value of susceptibility χ near the transition temperature T_c
2) Larger the system size, smaller the width of the critical region (i.e. The region under the curve)

The following two relations[5] were proposed to describe the 2 features above,

$$\chi_{max}(L) \sim L^{\gamma/\nu} \text{ (5) and } |t_{max}(L)| \sim L^{-1/\nu} \text{ (6) where } t = \frac{(T-T_c)}{T_c}$$

They are initially proposed based on the phenomenological considerations but were later found out that they could be derived using the renormalization group theory.[5]

Similar relation can also be applied to specific heat changes over temperature.

Hypothesis of finite size scaling

We can combine the relation (5) and (6) and form the form the following relationship between the susceptibility and temperature,

$$\chi(T, L) = L^{\frac{\gamma}{\nu}} F_{\chi}[\,(T - T_c\,)\, L^{\frac{1}{\nu}}]\,,$$

where F_x is some function that takes in T − T_c and $L^{1/\nu}$.

By rewriting the above equation,

$$\chi(T, L)L^{-\frac{\gamma}{\nu}} = F_{\chi}\left[(T - T_c\,)\, L^{\frac{1}{\nu}}\right] \quad (7)$$

Then we can simulate again and obtain susceptibility values versus temperature as in the **Monte Carlo methods for numerical simulation of Ising model**. Then, if the relation is correct, by

multiplying $L^{-\frac{\gamma}{\nu}}$ on the susceptibility and doing some modification on the temperature values, we can see the data collapse. (i.e. The susceptibility would fall in one line.)

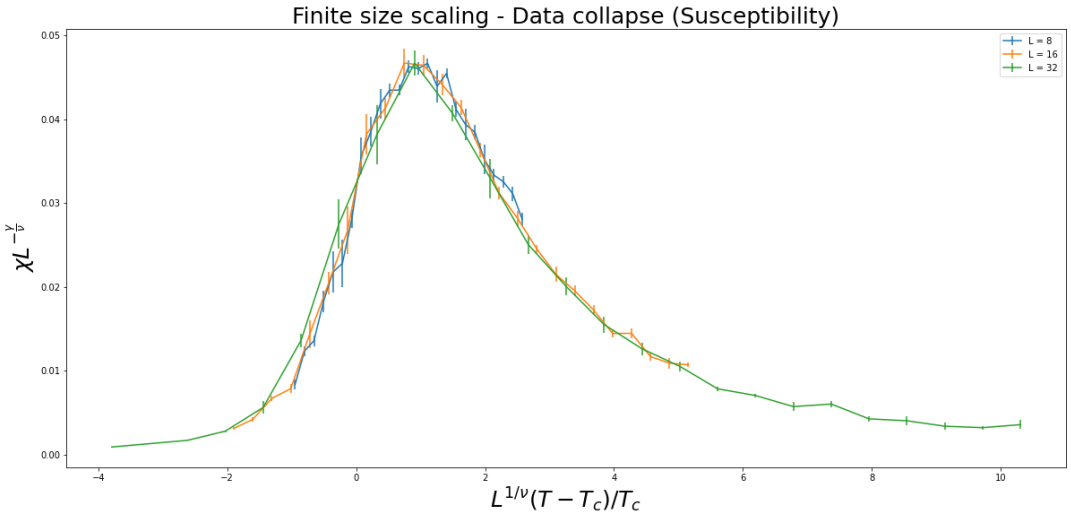
Besides, there is also scaling relation for magnetization,

$$m(T,L) = L^{-\frac{\beta}{\nu}} F_m\left[(T-T_c)L^{\frac{1}{\nu}}\right] \quad (8)$$

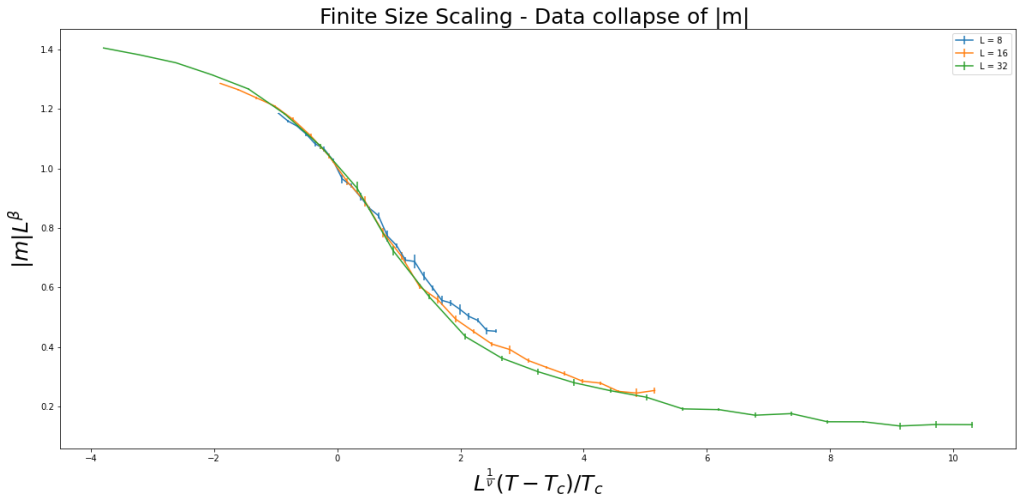
Also, if the relation is correct, we can see the data collapse.

Result

1) $\chi(T,L)L^{-\frac{\gamma}{\nu}} = F_\chi[(T-T_c)\,L^{\frac{1}{\nu}}]$



2) $m(T,L) = L^{-\frac{\beta}{\nu}} F_m[(T-T_c)L^{1/\nu}]$



By plugging in T_c and Ising critical exponents ν, γ, β (obtained from Onsager's solution), we can see that the data collapse of both magnetization and susceptibility and therefore, we can conclude that (7) and (8) is correct.

Crossing point analysis[6]

For a pair of system (L,2L), the crossing point of their Binder cumulant values versus temperatures would follow,

$$T^c(L) = T_c + aL^{-(\frac{1}{\nu}+\omega)} \quad (9)$$

where a is a constant and T_c is the transition. It means that **if we can fit this function to the data we obtained, we can find the transition temperature by locating the intercepting point**.

Explanation of equation (9)

Consider $\delta = T - T_c$ and the standard finite size scaling form $O(\delta, L) = L^{-\frac{\kappa}{\nu}} F_O[\delta L^{\frac{1}{\nu}}, \lambda L^{-\omega}]$, at the critical point, we can use Taylor expansion and get,

$$O(\delta, L) = L^{-\frac{\kappa}{\nu}} \left(a_0 + a_1 \delta L^{\frac{1}{\nu}} + b_1 L^{-\omega} + \cdots\right).$$

Then, consider 2 system sizes, $L_1 = L$ and $L_2 = rL$ where $r > 1$, there intercepting point could be obtained by setting,

$$O(\delta^*, rL) - O(\delta^*, L) = 0$$

$$\delta^*(L) = \frac{a_0}{a_1} \frac{\left(1 - r^{-\frac{\kappa}{\nu}}\right)}{r^{(1-\kappa)/(\nu-1)}} L^{-\frac{1}{\nu}} + \frac{b_1}{a_1} \frac{\left(1 - r^{-\left(\frac{\kappa}{\nu}+\omega\right)}\right)}{r^{(1-\kappa)/(\nu-1)}} L^{-\left(\frac{1}{\nu}+\omega\right)}$$

If the quantity O is dimensionless (e.g. Binder Cumulant), then $\kappa = 0$ and the first term is cancelled out,

$$\delta^*(L) = a * L^{-\left(\frac{1}{\nu}+\omega\right)}$$

$$T^c(L) = T_c + aL^{-(\frac{1}{\nu}+\omega)}$$

Therefore, we obtain equation (9).

Result

Fig 3. Binder Cumulant versus temperature

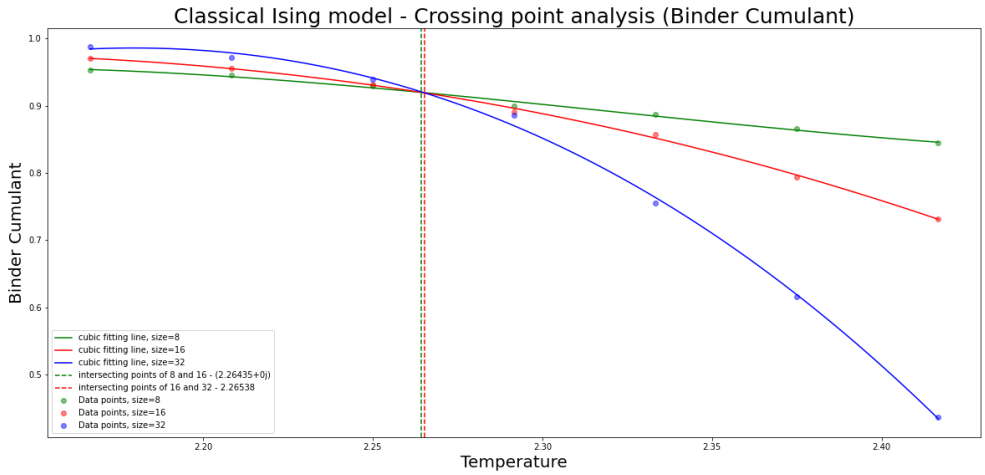
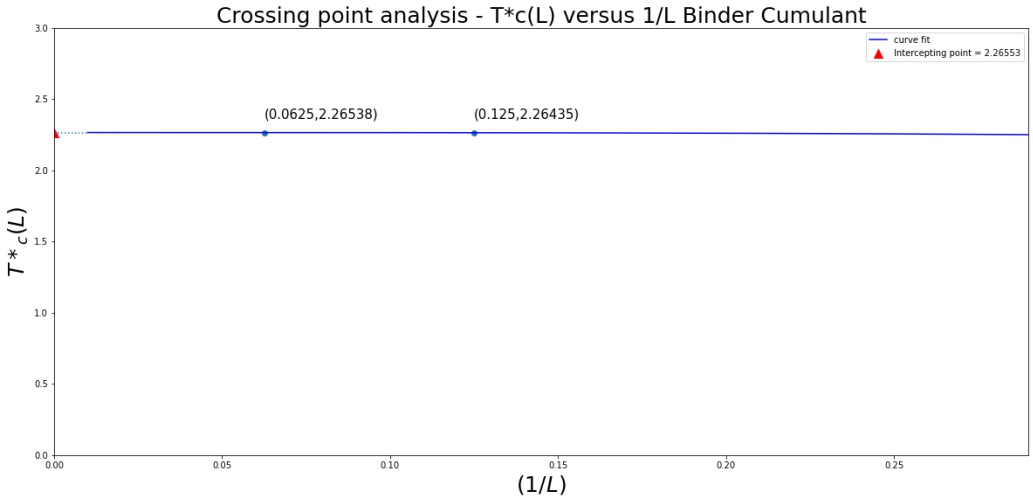


Fig 4. Plot the graph according to equation (9)



We obtain the crossing temperature from Fig 3 and plot it in figure 4. We can see that the intercept of figure 4 is 2.26553, which is close to the theoretical values 2.26918.

Without computational resource limitations, we can do larger size pair like (64,128), (128,256) etc. to locate the intercept more precisely.

Autocorrelation

We generate a new configuration by updating the previous one with different updating algorithms, which we have mentioned in part *Monte Carlo methods for numerical simulation of Ising model transition.* However, the new and previous configurations might still be correlated after updating. Therefore, we need a measure that tells us after how many steps of updating, the two configurations are not correlated, or at least the correlation between the 2 configurations are small enough. As a result, we need to introduce the concepts of autocorrelation.[7]

Theoretical background and definition of autocorrelation function

The correlation function between 2 quantities A and B is,

$$A_{AB}(\tau) = \frac{\langle A(\tau_0)B(\tau)\rangle - \langle A\rangle\langle B\rangle}{\langle AB\rangle - \langle A\rangle\langle B\rangle}$$

If A = B, then the function is called autocorrelation function (or called linear correlation function), which is equivalent to correlation between the same quantities after τ steps of updating.

If $A = B = \sigma$, (the spin of configuration), we can write the autocorrelation function as,

$$A_{|M|}(\tau) = \frac{\langle \sigma(\tau_0)\sigma(\tau)\rangle - \langle \sigma(\tau_0)\rangle^2}{\langle \sigma^2(\tau_0)\rangle - \langle \sigma(\tau_0)\rangle^2}$$

where τ and τ_0 referring to the 2 different positions in the Markov Chain of updating (i.e. Putting all the spin configurations in a line). We would the fix the value of τ_0 and varies the value of τ , with a view to seeing the changes in the values of autocorrelation function.

Programme implementation

Here are the steps in the programme, for a particular size of system,

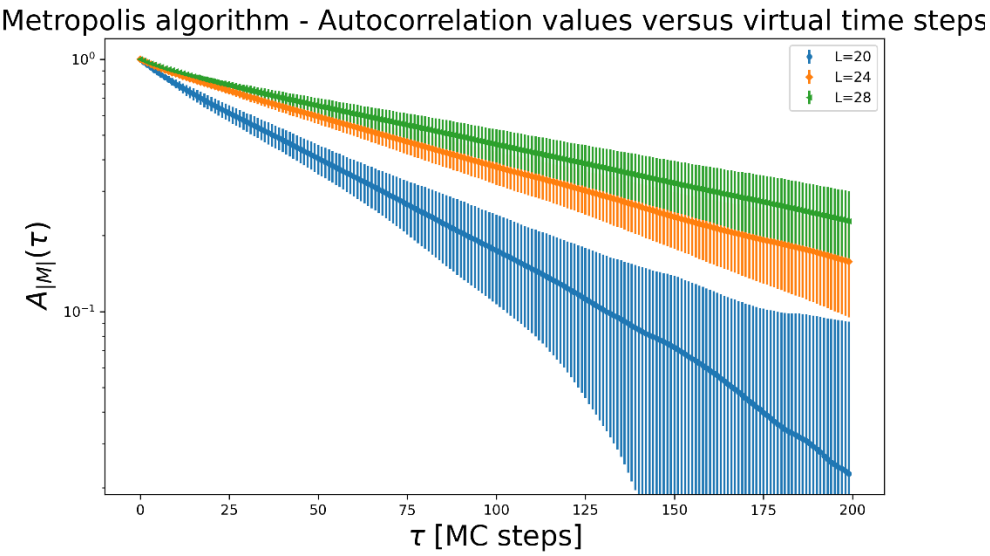
1) Thermalization
2) Generate a configuration and updating it for k times. Record the absolute m value for each time.
3) Calculate values of autocorrelation (Loop through configuration generated)
    - Set τ_0 equal to 250, which means that we would study correlation between the current configuration and 1st, 2nd, … 250th configuration after the current configuration
    - divide the $k - \tau_0$ into 10 groups. Take the mean of the autocorrelation values in this group.
    - If the correlation calculated after certain steps is smaller than 0.01, then we stop doing the autocorrelation calculation.

Result

Autocorrelation values of Metropolis algorithm

Using k $=$ 300000, $\tau_0 = 200$, we investigate the classical Ising model with size $L = 20,24,28$ with Metropolis algorithm.

Fig 1. Plot of $\log(A_{|M|}(\tau))$ versus τ for Metropolis algorithms



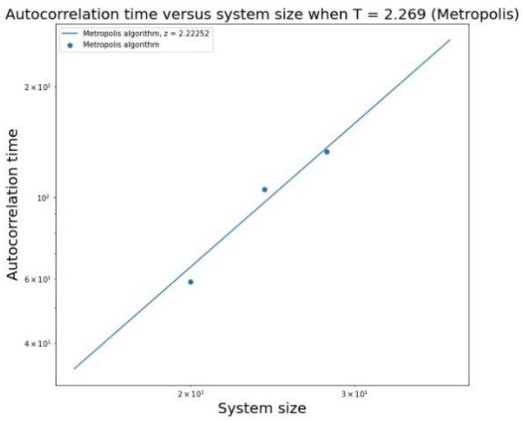
Deduced by using renormalization group theory, the autocorrelation and z has the following relation,

$$A_{|M|} = e^{-\frac{1}{z}}$$

The negative inverse of the slope of each line in Fig 1. is defined as z, the linear dynamical critical exponent. Smaller the z, less steps are used to generate statistically independent configurations.

We can plot $\log(Autocorrelation\ time)$ against $\log(system\ size)$ and extract the slope, which is the linear dynamical critical exponent of the algorithm.

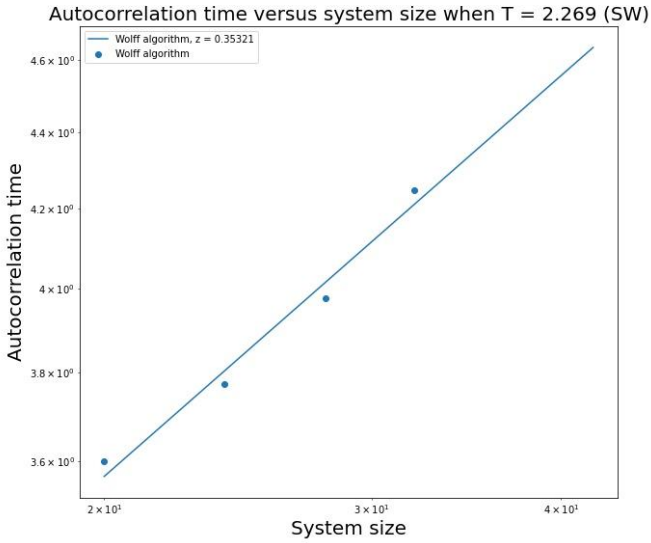
Fig 2. Plot of $\log(Autocorrelation\ time)$ versus $\log(system\ size)$ for Metropolis algorithms



The slope (i.e. dynamical critical exponents) is ≈ 2.22252 ,which is quite close to the literature value ≈ 2.215, with 0.34% error.

Autocorrelation values of Swendsen-Wang and Wolff algorithm

Similarly, Using $k = 300000$, $\tau_0 = 200$, we investigate the classical Ising model with size $L = 20,24,28,32$ with Swendsen-Wang algorithm and Wolff algorithm.



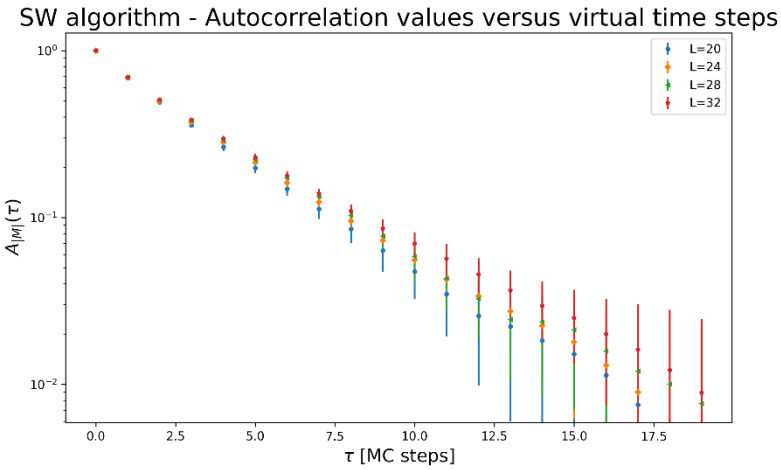


Fig 3. Plot of $\log(\Phi_m)$ versus τ for Swendsen-Wang algorithms

The slope ≈ 0.35321 for Swendsen Wang simulation, which is also quite close to the literature value $\approx 0.35^3$ with 0.917% error.

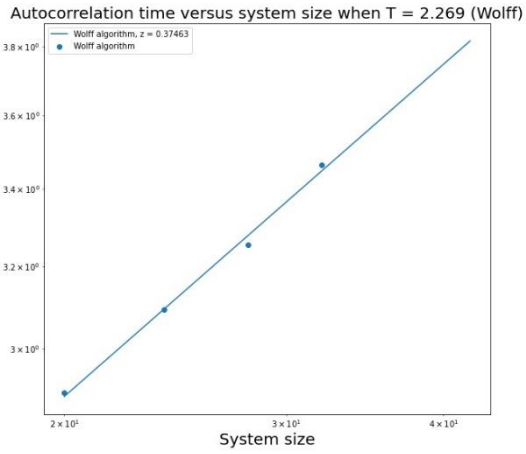
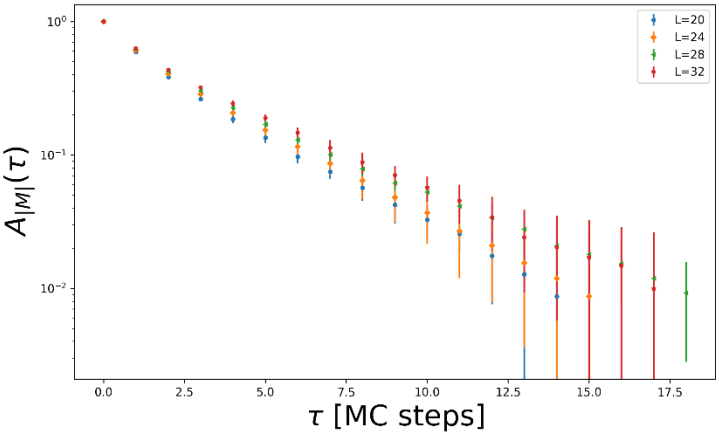


Fig 4
for S

Fig 5. Plot of $\log(Autocorrelation\ time)$ versus $\log(system\ size)$ for Wolff algorithm



$ize)$

Fig 6. Plot of $\log(\Phi_m)$ versus $\log(system\ size)$ for Wolff algorithm

The slope ≈ 0.37463 for Wolff algorithm simulation, which deviates from the the literature value ≈ 0.25[4] with 49%. However, if we can study it without computational recourse limitations, a more precise value of z of Wolff algorithm can obtained by simulating large system sizes.

Transverse Field Ising Model

Mapping to Classical system

Transverse field Ising model is the classical Ising model with a transverse field imposed on it. By studying the partition function of transverse field Ising Model, it is found that a 2-dimensional transverse field Ising model can be mapped to a 3-dimensional classical Ising model, with different bond strength between different layers along imaginary time axis. We would focus on the 1-dimensional transverse field Ising model, then prove that it can be mapped to a 2-dimensional classical Ising model. The mapping of 2-dimensional transverse field Ising model can also be done in the same way.

The Hamiltonian of the transverse field Ising model is

$$H = H_0 + H_1 = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - h \sum_i \sigma_i^x$$

The partition function is

$$Z = tr(e^{-\beta H})$$

And by setting $\beta = L\,\Delta\tau$, we can rewrite the partition function as,

$$Z = tr(e^{-L\Delta\tau H}) = tr(e^{-\Delta\tau H} e^{-\Delta\tau H} \dots e^{-\Delta\tau H}),$$

which the product inside the trace can be considered as a **succession of imaginary time evolution**. (i.e., The concept is like the evolution of wave function in quantum mechanics)

Then, we insert a complete set of σ_i^z eigenstates between the exponentials,

$$Z = \sum_{\{S_{i,l}=\pm 1\}} \langle S_1^Z | e^{-\Delta\tau H} | S_L^Z \rangle \langle S_L^Z | e^{-\Delta\tau H} | S_{L-1}^Z \rangle \dots \langle S_2^Z | e^{-\Delta\tau H} | S_1^Z \rangle \quad (10)$$

Which the product of matrix element representing the system changes from “imaginary time slice l” to “imaginary time slice l+1”

Now, we consider each element in equation (10),

$$\langle S_{l+1}^Z | e^{-\Delta\tau H} | S_l^Z \rangle = \langle S_{l+1}^Z | e^{-\Delta\tau H_1 - \Delta\tau H_0} | S_l^Z \rangle$$

By using Trotter-Suzuki approximation,

$$\langle S_{l+1}^Z | e^{-\Delta\tau H_1 - \Delta\tau H_0} | S_l^Z \rangle \approx \langle S_{l+1}^Z | e^{-\Delta\tau H_1} e^{-\Delta\tau H_0} + O(\epsilon) | S_l^Z \rangle \text{ if } \epsilon \ll 1$$

where,

$$\epsilon \ll 1$$

$$[\Delta\tau H_0, \Delta\tau H_1] \ll 1$$

$$(\Delta\tau)^2 Jh \ll 1$$

$$\boldsymbol{L \gg \beta\sqrt{Jh}}$$

After that, we can rewrite each elements in equation (10) as

$$\left\langle S_{l+1}^{Z} \middle| e^{-\Delta\tau H_1 - \Delta\tau H_0} \middle| S_l^Z \right\rangle \approx \exp\left(\Delta\tau J \sum_{i=1}^{N} S_{i,l}^{Z} \, S_{i+1,l}^{Z} \right) \left\langle S_{l+1}^{Z} \middle| e^{-\Delta\tau H_1} \middle| S_l^Z \right\rangle$$

As the matrix elements can be evaluated in the following form,

$\left\langle S_{l+1}^{Z} \middle| e^{-\Delta\tau H_1} \middle| S_l^Z \right\rangle = \Lambda \, e^{\gamma}$, where Λ and γ are the constants that we want to find.

By using the formula $e^{\Delta\tau h\sigma_x} = Icosh(\Delta\tau h) + \sigma_x \sinh(\Delta\tau h)$ and evaluating 2 cases, $S_Z = S_z'$ and $S_Z = -S_z'$, we can get

$$\langle S|e^{-\Delta\tau h\sigma_x}|S\rangle = \cosh(\Delta\tau h) = \Lambda e^{\gamma} \quad (11)$$

$$\langle -S|e^{-\Delta\tau h\sigma_x}|S\rangle = \sinh(\Delta\tau h) = \Lambda e^{-\gamma} \quad (12)$$

Multiplying (11) with (12) and dividing (12) with (11), we can get,

$$\gamma = -\frac{1}{2}\ln(\tanh(\Delta\tau h)) \;\; \& \; \Lambda^2 = \sinh(\Delta\tau h)\cosh(\Delta\tau h)$$

Plugging back the result to every term in equation (10), we can see the partition function of a transverse field Ising model is like,

$$Z = \Lambda^{NL} \sum_{\{S_{i,l} = \pm 1\}} \exp\left(\Delta\tau J \sum_{i}^{N} \sum_{l}^{L} S_{i,l} \, S_{i+1,l} + \gamma \sum_{i}^{N} \sum_{l}^{L} S_{i,l} \, S_{i,l+1} \right)$$

It is basically the same partition function of a 2-dimensional classical Ising model, but with only a different strength constant between the layers along imaginary time axis. The mapping of 2-dimensional transverse field Ising model to a 3-dimensional classical Ising model can also be done by the same way.

Programme implementation

As Trotter-Suzuki approximation is used, we need to preserve the relation $L \gg \beta\sqrt{Jh}$. Therefore, we would set $\Delta\tau = 0.1$, and calculate L (the length of imaginary axis) by using $L = \frac{\beta}{\Delta\tau}$.

The steps involved are similar to simulating the phase transition of classical Ising model, while instead of varying temperature, we vary h, the strength of transverse field in order to observe the quantum phase transition.

1) Generate equilibrium lattice
2) Updating the transverse field Ising model with Swendsen Wang Algorithm at a certain h
    a. Binning and collecting the mean of $\langle |m| \rangle$ for every 100 updates

b. Repeat step 2 with another h values

3) Repeat steps 1-2 with different system size

4) Plot the graph $\langle|m|\rangle * L^{\beta}$ versus h and locate the transition h by using crossing part analysis (i.e. the same as in the part of Finite size scaling and Binder ratio)

Result

We set k = 25000, size = [8,12,18] (i.e. they are geometric sequence with r =1.5), we first plot $\langle|m|\rangle * L^{\beta}$ versus h for T = 2, 1, 0.5 and applied the crossing point analysis to find the phase transition point.

Below are the graph $\langle|m|\rangle * L^{\beta}$ versus h at T = 2 and the crossing point analysis

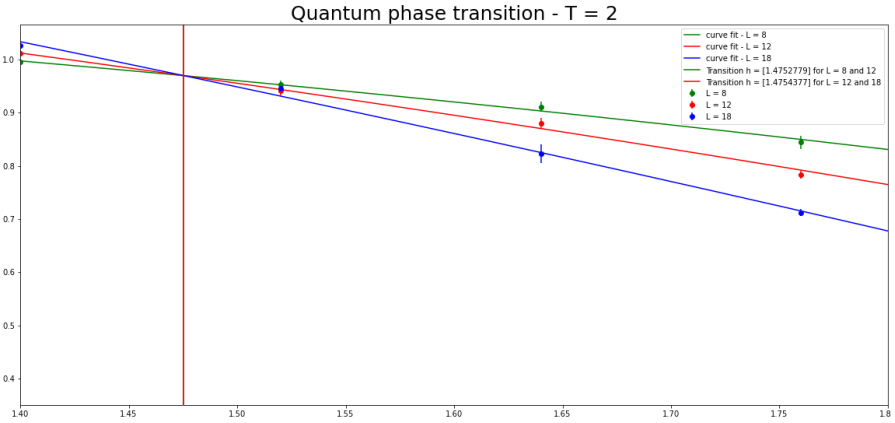


Fig 7. Plot of $\langle|m|\rangle * L^{\beta}$ versus h at T = 2

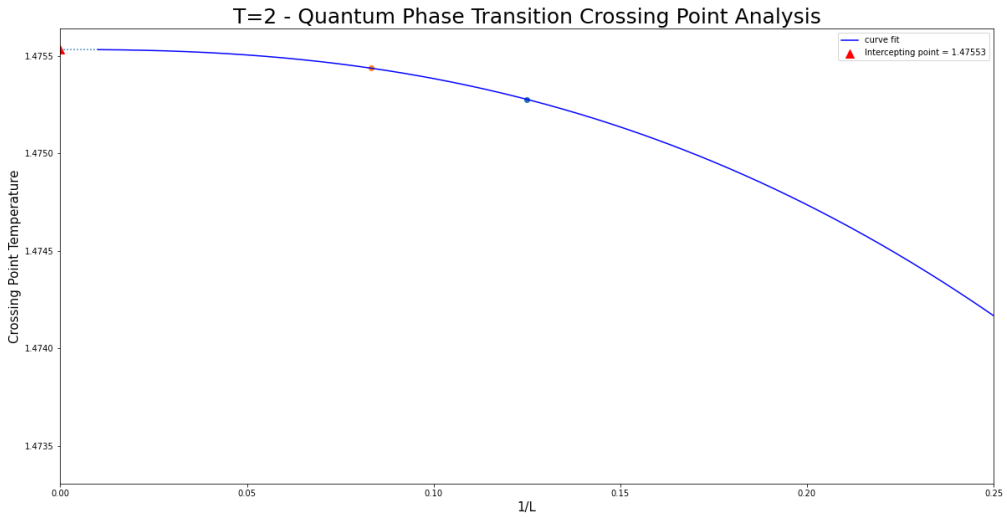


Fig 8. Crossing point analysis at T = 2

Then, as we get the relation

$T_c \propto |h - h_c|^{z\nu}$, where $z = 1$ and $\nu = \nu_{3D} = 0.62998$.[2] from Onsager's Solution

We can plot the T_c versus $(h - h_c)/h_c$ in log scale and extract the slope from the graph.

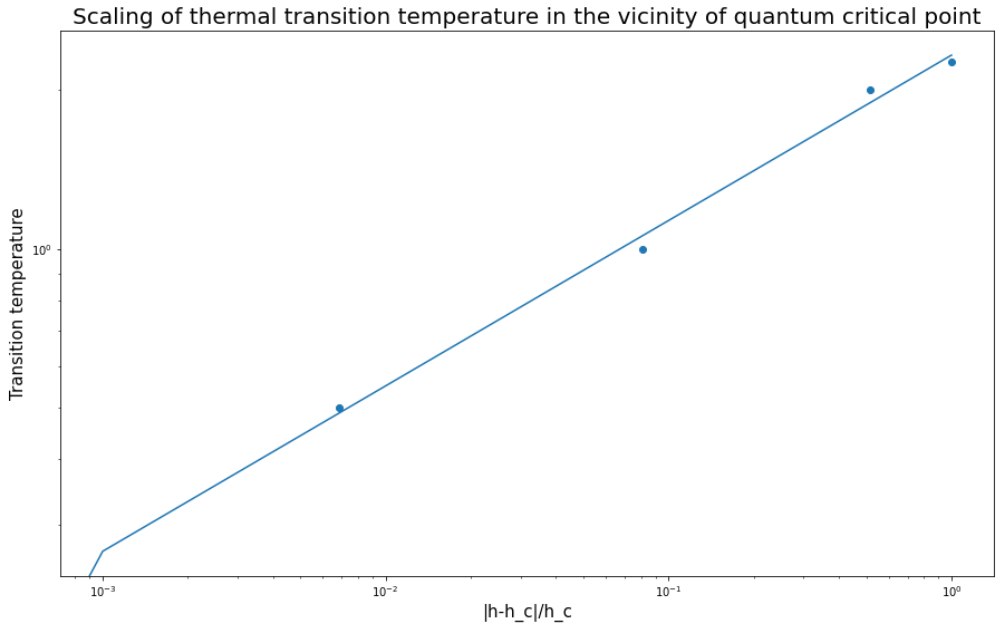
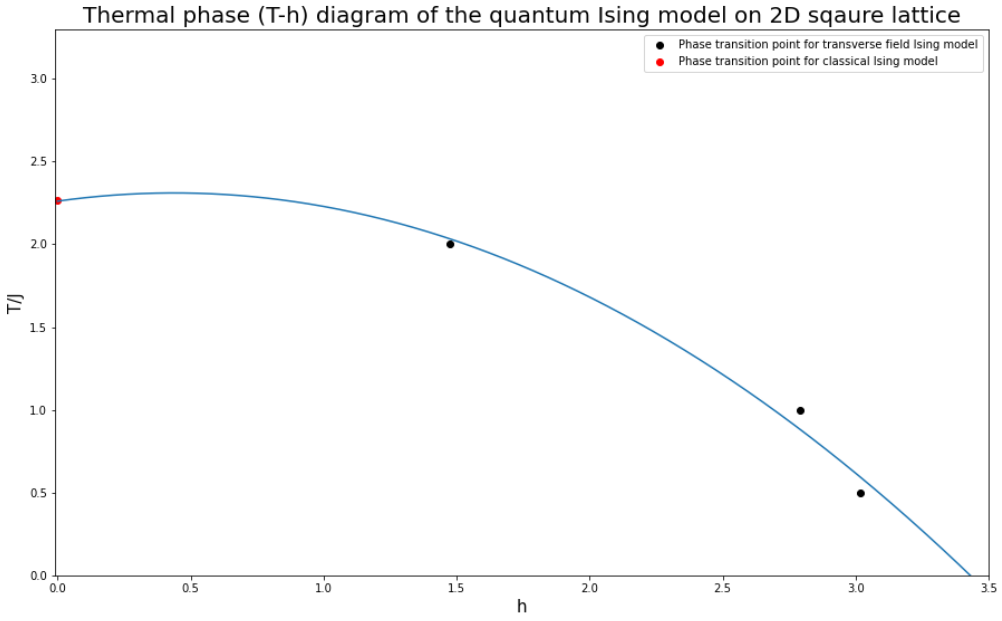


Fig 9. T_c versus $(h - h_c)/h_c$ in log scale

We fit the line to the points and find that the slope is $vz \approx 0.31336146$ which deviates quite lot from the theoretical value $vz = 0.62998$[2].

From the plot below,



We can see that the points near T = 0 deviates more significantly from the fitting line, which reflects that the standard deviation of the values are larger and the mean values we take might not close to the literature value. We can solve this problem by increasing the iteration times to larger numbers, if we do not have the computational resources limitations.

Conclusion

Three Monte Carlo simulation algorithms, which are Metropolis algorithm, Wolff algorithm and Swendsen-Wang algorithm are implemented to investigate the phase transition of 2-dimensional classical Ising model, where finite size scaling and Binder ratio are implemented with crossing point temperature analysis to obtain the values of thermal transition temperature. All the physical observables exhibit the predicted behaviour and the value of critical temperature obtained for the 2D classical Ising model is close to the literature value, though simulation of larger system size can also be implemented to get a more precise value of transition temperature. Besides, the simulated data all exhibits data collapse, which proves numerically that the finite size scaling relations are accurate enough to describe the model. For the transverse field Ising model, Swendsen-Wang algorithm is implemented and values of transition temperature at different transverse field strength are obtained. However, the T-h phase line deviates significantly near T = 0, where more accurate values can be obtained by simulating the quantum phase transition at temperature near T = 0 if better computational resources are used.

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