PHYS4999 Final Year Project

Quantum Monte Carlo Simulation of Entanglement Entropy in the Transverse Field Ising Model

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Abstract

This project explores the intricate relationship between the one-dimensional (1 dimensional) Transverse Field Ising Model (TFIM) and the two-dimensional (2 dimensional) Classical Ising Model through a theoretical mapping, focusing on the analysis of quantum phase transitions and entanglement properties. The 1 dimensional TFIM, characterized by a quantum magnetic field perpendicular to the spin alignment, exhibits rich quantum mechanical behaviors and phase transitions that are pivotal for understanding quantum computation and condensed matter physics. By employing a well-established theoretical framework, this study maps the 1 dimensional TFIM onto an equivalent 2 dimensional Classical Ising Model, thereby bridging the gap between quantum and classical statistical mechanics.

To quantitatively analyze the entanglement, we measure the Rényi Entanglement Entropy, a key indicator of quantum correlation and entanglement in the system. The measurement is conducted using the Monte Carlo Markov Chain (MCMC) method, renowned for its effectiveness in studying statistical distributions and thermodynamic properties in complex systems. The MCMC simulations provide insights into the entanglement entropy across different phases and system sizes, revealing how entanglement entropy behaves near critical points.

The project aims to make use of the computational method to reproduce the renowned result and match the theoretical prediction.

Contents

Acknowledgements

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Preface

1 Outline

1. Introduction to the Classical Ising Model:
   Begin by outlining the structure and fundamental properties of the classical Ising model. By knowing the form of entropy and the concept of phase transition in the Ising model.

2. Overview of Markov Chain Monte Carlo Methods:
   The two Markov chain Monte Carlo (MCMC) method (Metropolis and Wolff Algorithm) will be used for the simulation through out the report. The basic introduction and derivation will be given in this section for the two updating method.

3. Exploration of the Quantum Ising Model:
   Exploration on the 1-D transverse field Ising model of phase transition. Demonstrate on how to map the model to 2-D classical Ising model.

4. Measure Renyi Entropy by MCMC stimulation:
   Base on the structure of 1-D transverse field Ising model, the new periodic boundary condition is applied. And, make use of the MCMC mehtod to measure the entropy. The computational result will further analyze with Comformal field theory (CFT) prediction.

Main Content

2 2-D classical Ising model

Ising model is a idealised model, which consist of the lattice and fill with the particle only contain two state, the spin up,$|\uparrow\rangle$ and spin down, $|\downarrow\rangle$. We are interested in the configuration of the spin in the lattice and the phase transition point in the given physical condition.

The Hamiltonian is [1],

$$H = -J\sum_{\langle i,j\rangle} s_i s_j - h\sum_i s_i \tag{2.1}$$

In the Ising model, each spin s_i and s_j equal to ± 1 in x and y direction respectively. The coupling constant donoted as $-J$, characterizes the strength of interaction between neighboring spins; it is negative in the Ising model. The quantity h is the strength for external magnetic field. For the classical case, it is common to set h = 0 for the Hamiltonian to focus on the interactions due solely to the spins, without the influence of an external field.

2.1 Second order phase transition

For the first order phase transition, it is related to latent heat, which absorb heat without raIsing the temperature. We will not discuss the first order phase transition as it is not observable in the Ising model.

For the second order phase transition, the system change from the ferromagnetic order paramagnetic order. In the context of Ising model, the ferromagnetic order is the conition for all spin is aligned in the same direction and the temperature is lower than the critical temperature T_c. While, for the paramagnetic order, which is higher than T_c, the spin is oriented in a random manner.

2.1.1 Behavior at critical temperature

The critical behavior at T_c leads to the disorder orientation of the spin, since since the thermal fluctuation is strong enough at T_c to distort the structure of the lattice. The value of T_c can be approximated by the follow derivation:
The general expression of Entropy is given by [1],

$$S = k_B ln(\#) \tag{2.2}$$

Which # is the number of configuration, $\# = 2^N$ for the Ising model Then,

$$S = Nln(2) \tag{2.3}$$

Apply the free energy expression, since $T = T_c$, $F = 0$, we then have,

$$TS = E \tag{2.4}$$

$$-TNln(2) = -2N \tag{2.5}$$

$$T = \frac{2}{ln(2)} \tag{2.6}$$

The approximated value for $\frac{2}{ln(2)}$ is 2.885, but the corrected estimated value raised by Onsager (1944) is given by [1],

$$T_c = \frac{2}{ln(1+\sqrt{2})} \tag{2.7}$$

Which the value is 2.269, though, it is still a theoretical approximation on how to obtain the temperature at T_c.

3 Metropolis Algorithm

The Metropolis Algorithm is a key Markov Chain Monte Carlo (MCMC) method that performs important sampling on specified models. It is highly effective for updating models using random samples. To illustrate the concept of the algorithm, we primarily focus on the example of the two-dimensional classical Ising model. Relevant results will be presented to demonstrate the application and efficacy of the Metropolis Algorithm.

3.1 Markov chain

Assume that we have two configuration $\{X\}$ and $\{Y\}$, which can be correlated together by the finite number of steps to update. We can generalize the process into two probability – acceptance probability and transition probability. The product of them define the probability of Markov chain [7],

$$M(X \to Y) = a(X \to Y)t(X \to Y) \tag{3.1}$$

Here, $M(X \to Y)$ is the probability of Markov chain, where $a(X \to Y)$ is the acceptance probability and $t(X \to Y)$ is the transition probability.

The significance for the transition probability is that, we need to know how the configuration $\{X\}$ can update one step further to the configuration $\{X + 1\}$. Therefore, for the n^{th} order of Markov chain, it carries the transition probability whether the configuration $\{X\}$ will be updated to configuration $\{X + n\}$.

3.2 Master Equation

Consider the rate of change for configuration $\{Y\}$ at time step t, The evolution of this configuration can be described by the master equation, which accounts for two primary components. The configuration $\{X\}$ flow or reach into the configuration $\{Y\}$. And $\{Y\}$ is flowed out to $\{X\}$, which form the master equation [7].

$$\frac{dP(Y,t)}{dt} = \sum_{X \neq Y} [M(X \to Y)P(X,t) - M(Y \to X)P(Y,t)] \tag{3.2}$$

- $P(Y,t)$ is the probability of being in configuration $\{Y\}$ at time t.
- $M(X \to Y)$ is the Markov chain probability from configuration $\{X\}$ to $\{Y\}$, contributing to the inflow into $\{Y\}$.
- $M(Y \to X)$ represents the transition probability from $\{Y\}$ to $\{X\}$, accounting for the outflow from $\{Y\}$.

For the stationary distribution or "equilibrium' in the term of physics. The configuration

$\{Y\}$ is not dependent on t, therefore,

$$\frac{dP(Y,t)}{dt} = 0 \tag{3.3}$$

Then, for the sufficient condition, we have [7],

$$M(X \to Y)P(X) = M(X \to Y)P(Y) \tag{3.4}$$

For the Metropolis Algorithm in 2-D classical Ising model, the acceptance probability is given by [7],

$$A(X \to Y) = min[1, exp(-\frac{\Delta E}{T})] \tag{3.5}$$

1. $\Delta E = E(Y) - E(X)$ implies the energy difference between the configuration $\{X\}$ and $\{Y\}$
2. The min function shows that $exp(-\frac{\Delta E}{T})$ will not exceed 1, which means that it will always accept if the energy decrease $A(X \to Y) = 1$ and for $A(Y \to X) = exp(\frac{\Delta E}{T})$, which is the inverse case. While for the increase of energy, it only accept with the probability $exp(-\frac{\Delta E}{T})$ (within the range of probability $[0, 1]$).

It also worth to mention that, to satisfy the detail balance condition, we have [7],

$$A(Y \to X)P(Y) = A(X \to Y)P(X) \tag{3.6}$$

$$\Rightarrow exp(\frac{\Delta E}{T})P(Y) = P(X) \tag{3.7}$$

$$\Rightarrow \frac{P(Y)}{P(X)} = exp(-\frac{\Delta E}{T}) \tag{3.8}$$

We verify this formula in the detail balance condition,

$$M(X \to Y)P(X) = M(X \to Y)P(Y) \tag{3.9}$$

$$\Rightarrow \frac{P(Y)}{P(X)} = \frac{M(X \to Y)}{M(Y \to X)} \tag{3.10}$$

$$\Rightarrow \frac{T(X \to Y)}{T(X \to Y)} = 1 \tag{3.11}$$

3.3 Example for Metropolis Algorithm

The application for the MCMC update of metropolis Algorithm will be shown by calculating the magnetization versus temperature for 2-D classical Ising model.

One update:

1. randomly choose a (x,y) position in the lattice
2. compute the $\Delta E = 2Js_i \sum_{\langle i,j \rangle} s_i s_j$
3. flip the spin for $\Delta E < 0$ or probability $exp(-\frac{\Delta E}{T})$ is larger than a random number $\in [0, 1)$

The magnetization is given [7],

$$M = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \tag{3.12}$$

For the graph in $L = 8, 12, 16, 24$, We perform 10000 Metropolis update to flip the spin of

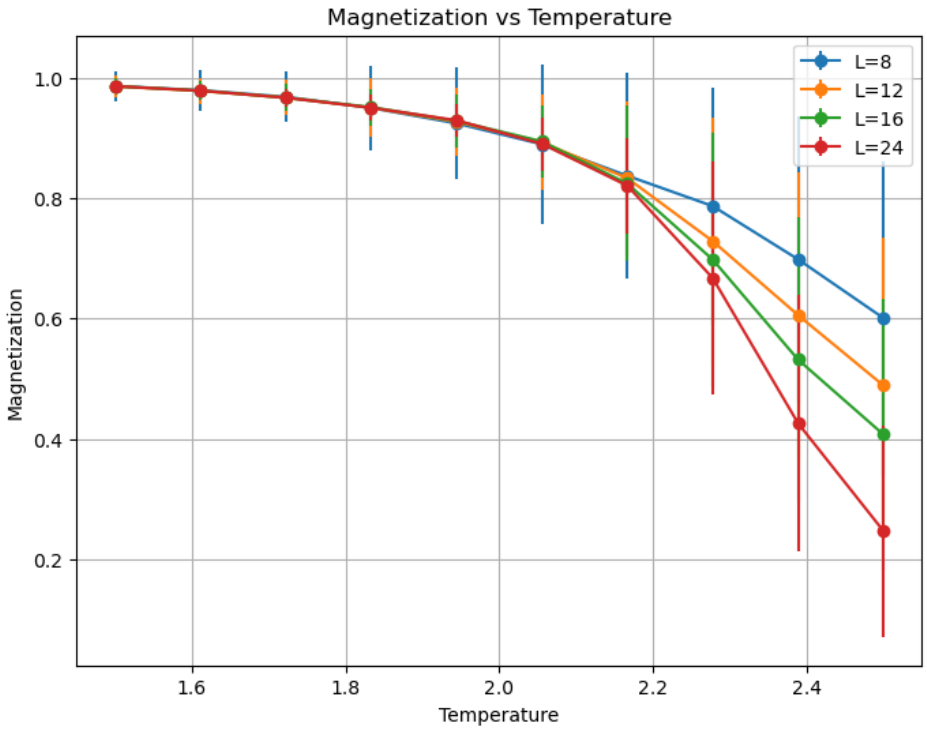


Figure 1: Metropolis update:10000 steps

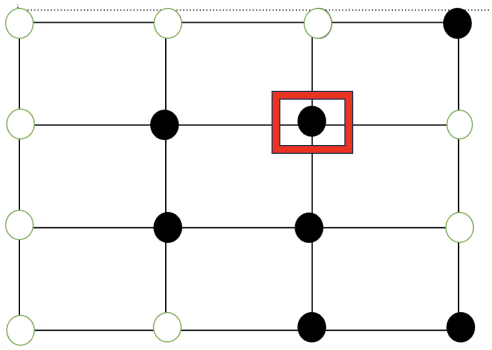
the lattice, we observe that there is some fluctuation for the curve. Though, we still can see the trend for the larger system size tends to the phase transition point $T_c = 2.269$. The fluctuation may due to the insufficient step for the Metropolis update or take the step for the equilibrium before running the Metropolis update.

4 Wolff Algorithm

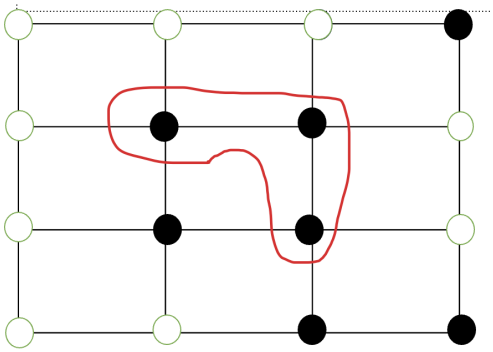
The Wolff algorithm represents a robust Monte Carlo Markov Chain (MCMC) method designed to update the Ising model using a breadth-first search (BFS) strategy. The advantage comparing to Metropolis Algorithm is the efficiency of flipping the spin. For the Metropolis Algorithm, it flip single spin by determining the required probability, while for Wolff Algorithm, it will grow the cluster by condition probability. After the search for the whole lattice, it will flip the whole cluster for one MC update.

Down below are the detail procedures for Wolff Algorithm:

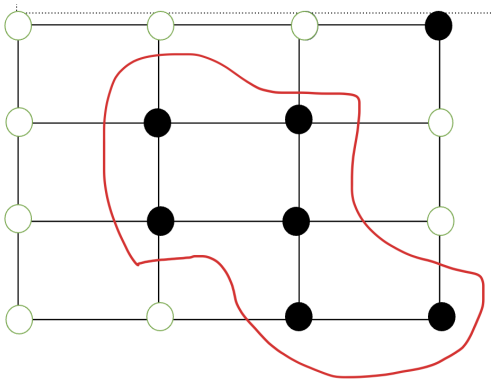
1. Choose a random site in the lattice, which black color, denoted as spin down, and white color denoted as spin up. We will also create the cluster list and the frontier list [2].



2. as the chosen spin (activated spin) is spin down $|\downarrow\rangle$, add the neighbouring spin if it is in the same state with a probability $1 - exp(-2J/T)$ for classical case. For all spin is accepted by the probability, the spin will be added to the cluster and frontier list, but the frontier list will dequeue the activated spin [2].



3. Then, we proceed to consider each spin within the frontier list, repeating the procedure outlined in step 2. This process is iterated until the frontier list is empty, meaning that all relevant spins have been considered. This completes one growth of cluster. Which constitutes one Monte Carlo (MC) update in the Wolff algorithm [2].



4.1 Real example

Consider the 2-D classical Ising model, magnetization versus temperature plot:

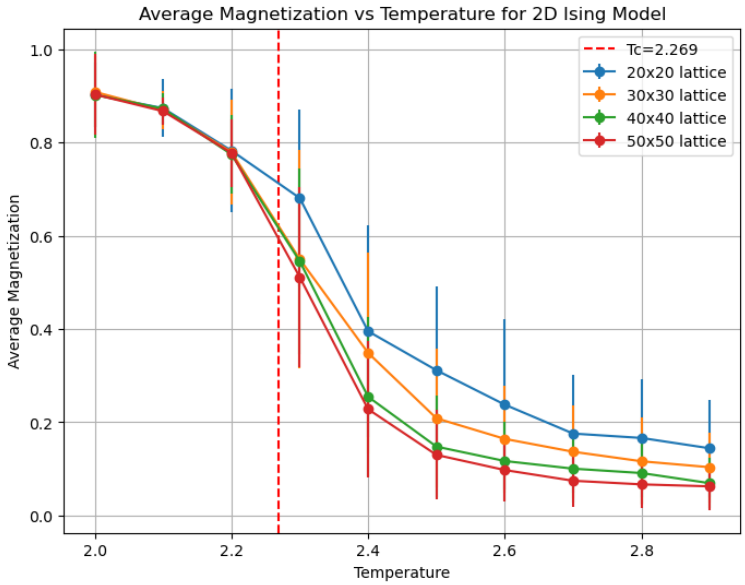


Figure 2: Wolff update:10000 steps, equilibrium:5000 steps

From the graph, we observe that for 50x50 lattice, the slope is steepest in the point T = 2.269, comparing to the low system size. It conclude that, for a larger system size, he computational prediction will approach the theoretical prediction. The advantage of Wolff algorithm is proved here. Since the the Wolff algorithm has a higher efficiency (shorter run time), which allow us to update a larger system size and observe the variation of the slope.

5 Transverse field Ising model

5.1 1-D Transverse field Ising model

The Hamiltonian of 1-D transverse field quantum Ising model is given by [3]:

$$H = -J\sum_{i=1}^{N}\sigma_{i+1}^{z}\sigma_{i}^{z} - h\sum_{i=1}^{N}\sigma_{i}^{x} \tag{5.1}$$

We define σ^z and σ^x by the computational basis, which $|0\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ and $|1\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. Then, $\sigma^x = |0\rangle\langle 1| + |1\rangle\langle 0|$, $\sigma^z = |0\rangle\langle 0| - |1\rangle\langle 1|$

5.2 Mapping to 2-D classical Ising model

We are interested in mapping a 1-D quantum Ising model to 2-D classical Ising model.
The partition function is [3]:

$$Z = Tre^{\beta H} = Tr[e^{-\Delta\tau H-\Delta\tau H-\Delta\tau H...-\Delta\tau H-\Delta\tau H}] \tag{5.2}$$

Where L is the product of $\Delta\tau\Delta\tau...\Delta\tau$.
We define $\beta = L\Delta\tau$ [3] Then, the product inside the trace is a succession of imaginary time operator. Which means that we have a new 3-D axis that in terms of the unit of $\triangle\tau$. For the approximations for the trace, each exponential pair can insert a complete set of σ^z's eigenvector, which is analogous to insert a identity inside the series.

The eigenvector of σ^z are $|0\rangle$ and $-|1\rangle$, which:

$$\sigma^z|0\rangle = |0\rangle \tag{5.3}$$

$$\sigma^z|1\rangle = -|1\rangle \tag{5.4}$$

$$\sum_{S^z\pm 1}^{N}|S_i^z\rangle\langle S_i^z| = 1 \tag{5.5}$$

1 is the identity operator.
We can evaluate on $\sum_{S^z\pm 1}^{N}|S_i^z\rangle\langle S_i^z| = 1$, it indicate that there are two possible state in a two dimension Hilbert space.

Now, we want to extend it to the system of N spins, for the entire system we need to consider every possible configuration of all N spins. Each configuration can be described by a specific choice of up or down for each spin, which we denote as $\left\{S_i^z\right\}$. Then, the total identity 1 is the tensor product of single spin identity. In the context here, the symbol of

tensor product: $\otimes$ is equal to $\prod$. Then the equation becomes [3]:

$$\prod(\sum_{S_i^z \pm 1}^{N} |S_i^z\rangle\langle S_i^z|) = 1 \tag{5.6}$$

$$\Rightarrow \sum_{\{S_{i,j}^z\}}^{N} |S_i^z\rangle\langle S_i^z| = 1 \tag{5.7}$$

We rewrite the partition function:

$$Tre^{-\beta H} = \sum_{\{S^z\}} \langle S^z|e^{-\beta H}|S^z\rangle \tag{5.8}$$

Then, after inserting the identity operator in between, the partition function becomes [3]:

$$Z = \sum_{\{S_{i,j}^z\}} \langle S_1^z|e^{-\Delta\tau H}|S_J^z\rangle\langle S_J^z|e^{-\Delta\tau H}|S_{J-1}^z\rangle\langle S_{J-1}^z|e^{-\Delta\tau H}|S_{J-2}^z\rangle \ ... \ \langle S_3^z|e^{-\Delta\tau H}|S_2^z\rangle\langle S_2^z|e^{-\Delta\tau H}|S_1^z\rangle \tag{5.9}$$

Since Z is in trace, we have the same state of bra-ket pair at the beginning and the end of the summation. It also suggested that it is the periodic boundary condition in time, such that the state is cyclic back to the first state.

For the series of $e^{-\Delta\tau H}$ is an evolution operator in imaginary time axis, in the time step of $\Delta\tau$.

5.2.1 Trotter–Suzuki approximation

Consider the terms of each time step:
let $H = H_0 + H_1$,
Apply the Trotter-Suzuki approximation, then we have [3],

$$\langle S_{J+1}^z|e^{-\Delta\tau H}|S_J^z\rangle \approx \langle S_1^z|e^{-\Delta\tau H_0}e^{-\Delta\tau H_1}|S_J^z\rangle \tag{5.10}$$

Then, we can apply the Baker-Campbell-Hausdorff (BCH) formula, which BCH formula state that:

$$e^A e^B = e^C \tag{5.11}$$

which,

$$C = A + B + \frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] - \frac{1}{12}[B,[A,B]] + \cdots \tag{5.12}$$

where $[A, B] = AB - BA$

Then we have,

$$e^{-\delta\tau H_1} e^{-\Delta\tau H_0} \approx e^{-\delta\tau(H_1+H_0)+\frac{1}{2}[-\Delta\tau H_1, -\Delta\tau H_0]+\ldots} \tag{5.13}$$

$$\approx e^{-\Delta\tau(H_1+H_0)+\frac{1}{2}(\Delta\tau)[H_1, H_0]+\ldots} \tag{5.14}$$

From the commutator terms, the leading term of Trotter error is $(\Delta\tau)^2$, combining the coupling constant J and the strength of the external magnetic field h. The trotter error is approximated in the order of $O((\Delta\tau)^2 Jh)$.

To evaluate the error, once require that the error is small, such that the Trotter-Suzuki approximation can match the actual result, then [3]:

$$(\Delta\tau)^2 Jh \ll 1 \tag{5.15}$$

$$(\beta/L)^2 Jh \ll 1 \tag{5.16}$$

$$L \gg \beta\sqrt{Jh} \tag{5.17}$$

The result implies that the time scale parameter $\Delta\tau$ can be controlled by the scale of β/L, and the Trotter-Suzuki approximation allow us to evaluate on the exponential of two discrete Hamiltonian into product of two exponential.

We revisit the partition function again, by inserting the complete set of S^z and set h = 0 for the Hamiltonian, which is the limiting case(classical),

$$Z = Tre^{-\beta H} \tag{5.18}$$

$$= Tre^{\beta J \sum_{i=1}^{N} \sigma_{i+1}^z \sigma_i^z} \tag{5.19}$$

$$\tag{5.20}$$

As $\sigma^z|0\rangle = S^z|0\rangle$,$\sigma^z|1\rangle = -S^z|1\rangle$ and $\sum_{\sigma^z=\pm1}|\sigma^z\rangle\langle\sigma^z| = I = 1$ for single particle in 2-dimension Hilbert space (one particle with 2 spin).

Now, we extend it to the N-particle with N-spin configuration, then, the partition function becomes [3]:

$$Z = (\prod_{i=1}^{N} \sum_{S_i^z})(\prod_{i=1}^{N} \langle S_i^z|) e^{\beta J \sum_{i=1}^{N} \sigma_{i+1}^z \sigma_i^z} (\prod_{i=1}^{N} |S_i^z\rangle) \tag{5.21}$$

$$= (\prod_{i=1}^{N} \sum_{S_i^z})(\prod_{i=1}^{N} \langle S_i^z|) e^{\beta J \sum_{i=1}^{N} S_{i+1}^z S_i^z} (\prod_{i=1}^{N} |S_i^z\rangle) \tag{5.22}$$

$$= \sum_{\{S^z\}} e^{\beta J \sum_{i=1}^{N} S_{i+1}^z S_i^z} \tag{5.23}$$

Notice that the transform from σ^z to S^z on the ground that S^z is the eigenvalue of σ^z. For the $\prod_{i=1}^{N} \sum_{S_i^z}$, the $\prod_{i=1}^{N}$ is the tensor product for the spin while the $\sum_{S_i^z}$ is the summation for the N particle, therefore, we can conclude that we can doing the summation of all the configuration of N particle $\sum_{\{S^z\}}$.

Base on the new Hamiltonian, inserting back into the Trotter-Suzuki approximation [3],

$$\langle S_{j+1}^z | e^{-\Delta\tau H_1} e^{-\Delta\tau H_0} | S_j^z \rangle = \langle S_{j+1}^z | e^{-\Delta\tau h \sum_{i=1}^{N} \sigma_i^x} e^{\Delta\tau \sum_{i=1}^{N} S_{i+1}^z S_i^z} | S_j^z \rangle \tag{5.24}$$

$$= e^{\Delta\tau \sum_{i=1}^{N} S_{i+1}^z S_i^z} \langle S_{j+1}^z | e^{-\Delta\tau h \sum_{i=1}^{N} \sigma_i^x} | S_j^z \rangle \tag{5.25}$$

For each matrix element, $\langle S_{j+1}^z | e^{-\Delta\tau h \sigma_i^x} | S_j^z \rangle$. Which, $e^{-\Delta\tau h \sigma_i^x} = I cosh(\Delta\tau h) + \sigma^x sinh(\Delta\tau h)$.

Take the requirement that [3],

$$\langle S_{j+1}^z | e^{-\Delta\tau h \sigma_i^x} | S_j^z \rangle = \Lambda e^{\gamma S_z' S_z} \tag{5.26}$$

We are interested in the constant Λ and γ, to determine, we divide it into two case, same spin: $S_z' = S^z$ and different spin: $-S_z' = S^z$ [3].

The general from is:

$$\langle S_z' | e^{-\Delta\tau h \sigma_i^x} | S_z \rangle = \langle S_z' | cosh(\Delta\tau h) | S_z \rangle + \langle S_z' | \sigma_x sinh(\Delta\tau h) | S_z \rangle = \Lambda e^{\gamma S_z' S_z} \tag{5.27}$$

For same spin $S_z' = S_z$,

$$\langle S_z | e^{-\Delta\tau h \sigma_i^x} | S_z \rangle = \langle S_z | \cosh(\Delta\tau h) | S_z \rangle + \langle S_z | \sigma_x \sinh(\Delta\tau h) | S_z \rangle \tag{5.28}$$

$$\langle S_z | e^{-\Delta\tau h \sigma_i^x} | S_z \rangle = \langle S_z | \cosh(\Delta\tau h) | S_z \rangle + \langle S_z | \sinh(\Delta\tau h) | -S_z' \rangle \tag{5.29}$$

$$= \cosh(\Delta\tau h) = \Lambda e^{\gamma} \tag{5.30}$$

For different spin $S_z = -S_z'$

$$\langle -S_z' | e^{-\Delta\tau h \sigma_i^x} | S_z \rangle = \langle -S_z' | \cosh(\Delta\tau h) | S_z \rangle + \langle -S_z' | \sigma_x \sin(\Delta\tau h) | S_z \rangle \tag{5.31}$$

$$\langle S_z | e^{-\Delta\tau h \sigma_i^x} | S_z \rangle = \langle S_z | \cosh(\Delta\tau h) | S_z \rangle + \langle S_z | \sin(\Delta\tau h) | -S_z' \rangle \tag{5.32}$$

$$= \sinh(\Delta\tau h) = \Lambda e^{-\gamma} \tag{5.33}$$

Combining the eq.(1.30) and eq.(1.33),

$$tanh(\Delta\tau h) = e^{-2\gamma} \tag{5.34}$$

$$\gamma = \frac{1}{2} ln(tanh(\Delta\tau h)) \tag{5.35}$$

While,

$$\Lambda = sinh(\Delta\tau h) cosh(\Delta\tau h) \tag{5.36}$$

After solving the constant, we back to the approximation terms eq.(1.24) and it becomes [3],

$$\langle S^z_{j+1}|e^{-\Delta\tau H_1} e^{-\Delta\tau H_0}|S^z_j\rangle = e^{\Delta\tau J \sum_{i=1}^{N} S^z_{i+1} S^z_i} \langle S^z_{j+1}|e^{-\Delta\tau h \sum_{i=1}^{N} \sigma^x_i}|S^z_j\rangle \tag{5.37}$$

$$= \Lambda^N e^{\Delta\tau J \sum_{i=1}^{N} S^z_{i+1} S^z_i + \gamma \sum_{i=1}^{N} S^z_{i+1} S^z_i} \tag{5.38}$$

Here, the sum inside the exponential involves all N spins, which means the operator applies a similar transformation to each spin independently. If the spins are non-interacting or the interactions are handled separately, the contributions from each spin are multiplicative (due to the properties of exponentials and the independence of the operators for different i). Thus, the overall factor becomes λ, multiplying the individual contributions.

For the partition function, it becomes [3],

$$Z = \Lambda^{LN} \sum_{\{S_{i,j=\pm 1}\}} e^{\Delta\tau J \sum_{i=1}^{N} \sum_{j=1}^{L} S^z_{i+1,j} S^z_{i,j+1} + \gamma \sum_{i=1}^{N} \sum_{j=1}^{L} S^z_{i+1,j} S^z_{i,j+1}} \tag{5.39}$$

$$H_0 = -J \sum_{i=1}^{N} \sum_{j=1}^{L} S^z_{i+1,j} S^z_{i,j+1} \tag{5.40}$$

$$H_1 = -\gamma \sum_{i=1}^{N} \sum_{j=1}^{L} S^z_{i+1,j} S^z_{i,j+1} \tag{5.41}$$

The term H_0 facilitates interactions between spins that are neighbors in space but exist within the same imaginary time slice. This part of the Hamiltonian models traditional spatial interactions typical in Ising models, where spins influence their immediate spatial neighbors.
Conversely, H_1 introduces interactions between spins that occupy the same physical location but are situated in neighboring (consecutive) slices of imaginary time. This aspect of the

Hamiltonian captures temporal correlations in the behavior of spins, essentially linking the state of a spin at one time with its state at the next time step.

5.2.2 Mapping constant term

Compare to the partition function of the classical Ising model,

$$E = -J \sum_{\langle i,j \rangle} s_i s_j \tag{5.42}$$

$$Z = \sum_{\langle s_i \rangle} e^{\beta_{Cl} J \sum_{\langle i,j \rangle} s_i s_j} \tag{5.43}$$

$$= \sum_{\langle s_i \rangle} e^{\beta_{Cl} (J_x \sum_{\langle i \rangle}^{N_x} + J_y \sum_{\langle j \rangle}^{N_y}) s_i s_j} \tag{5.44}$$

The notation $\langle i, j \rangle$ specifies that the sum includes only the nearest neighbors of each spin in the horizontal (left-right) and vertical (up-down) directions on the lattice. The coupling constant J quantifies the strength of interaction between these adjacent spins, and it is uniform across both the x-axis and y-axis ($J_x = J_y$). Which show that it is a 2-dimension Ising model.

Then, we compare the 1-D transverse field Ising model, with the 2-D classical Ising model, it surprIsingly that they can match together by the following condition:

$$\beta_{Cl} J_x = \Delta\tau J \tag{5.45}$$

$$\beta_{Cl} J_y = \gamma \tag{5.46}$$

While, $N = N_x$ and $L = N_y$, we can map the 1-D transverse field Ising model to a 2-D classical Ising model, since their partition function are the same by adopting the conditions. The significance for the mapping is that, we can view a imaginary time axis map to a classical axis, this allow us to further study the quantum phase transition and compare to the classical model. And make use of the model to measure the Rényi entropy of the entanglement in the Ising model.

5.3 Magnetization measurement for 1-D transverse field Ising model

The phase transition for transverse field Ising model is differ from the 2-D classical Ising model, In the transverse field version, the critical phase transition occurs at an absolute zero temperature T_0.

In addition to temperature, we may observe the phase transition through the variation of external magnetic field (h). Here is graph for the system size: 16x36, 16x48, 16x60, 16x72, magnetization versus h.

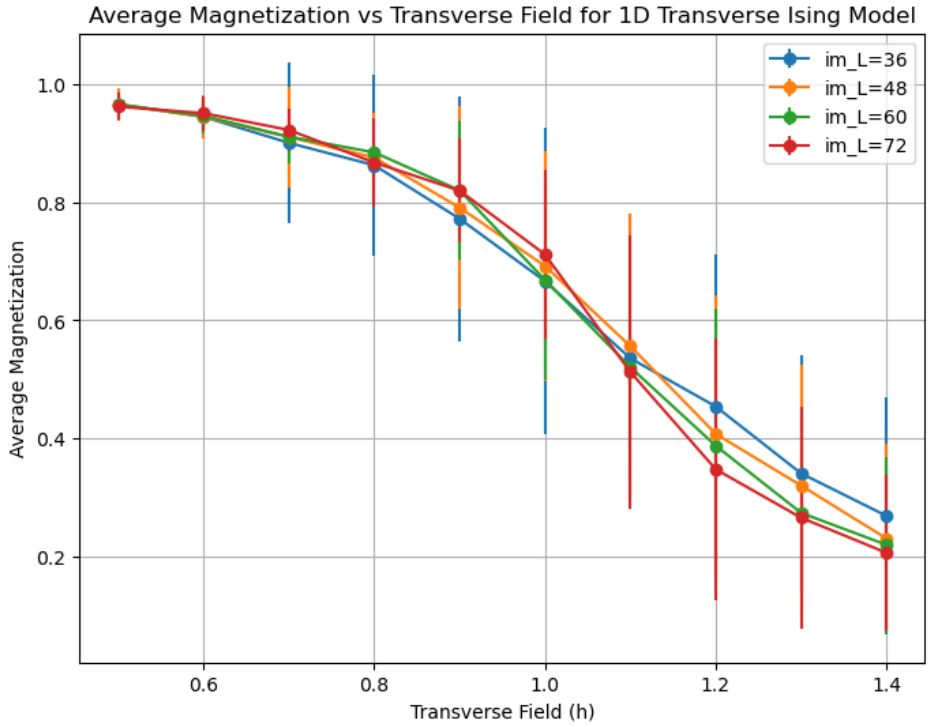


Figure 3: Wolff update:10000 steps

From the above graph, we observe that for the system size ($60x60$) gain a larger slope when it is close to $h_c = 1$. Moreover, we may observe the crossing point near the phase transition, which is not exactly hitting $h_c = 1$, it may due to the lack of iteration of the update and the small system size.

5.4 2-D transverse field Ising model

The Hamiltonian on 2-D transverse field Ising model is given by:

$$H = \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + h \sum_i \sigma_i^z \tag{5.47}$$

We can apply similar approximation approach to map the 2-D transverse field Ising model to 3-D classical Ising model. The case in here is to test the phase transition point for the 2-D transverse field Ising model match the theoretical result. The phase transition point for temperature T =1 is $h_c \approx 2.68$.

We may follow the matching result from 1-D transverse field to 2-d classical. Which, $J_{xy} = 1$ and $J_z = \gamma/\beta_{cl},$. Then, the partition function is:

$$Z = \sum_{\langle s_i \rangle} e^{\beta_{Cl}(J_{xy} \sum_{\langle i,j \rangle}^{N_{xy}} + J_y \sum_{\langle z \rangle}^{N_z}) s_{i,j} s_z} \tag{5.48}$$

Which $N_{x,y} = L^2$, $N_z = imL = \frac{\beta}{\Delta\tau}$, The plotting result is shown as follow:

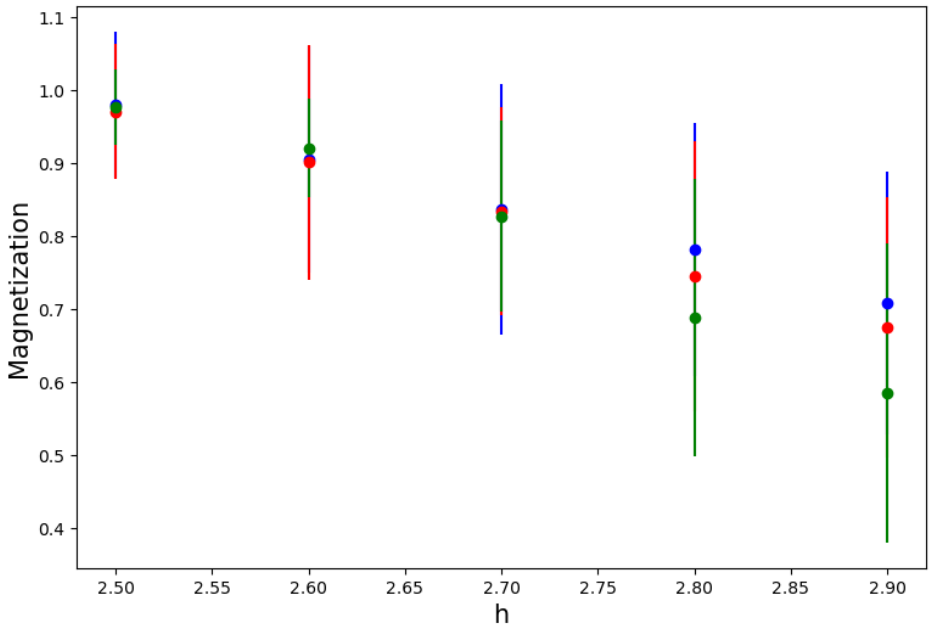


Figure 4: Metropolis update:20000 steps, L = 6,8,12, delta tau = 0.1, beta = 1/T

From the graph, we observe that the phase transition point on the magnetization-field (M-h) plot is marked by the intersection of three lines at system sizes L = 6,8,12. And it is expected that for a larger system size, the slope reaches its highest position before the phase transition

point and subsequently declines to its lowest position after crossing this point, which is same as the result for 1-D transverse Ising model. This trend could be influenced by limitations such as the insufficient size of the measurement and an inadequate number of iterations in the Metropolis update algorithm.

6 Measurement of Rényi entropy of the entanglement

6.1 Introduction

The Rényi entanglement entropy is given by [5]:

$$S_{A,q}^{E} = \frac{1}{1-q} ln \rho_{A}^{q} \tag{6.1}$$

The ρ is the reduced density matrix. The entanglement entropy describe a sub-system A is embedded inside a larger system, while q indicate the dimension of the system, we presume to take q = 2, for the transverse field Ising model.

To measure the entropy, we estimate two partition functions Z_A and Z_o, where Z_A is the glued replicas in the time-imaginary axis on subsystem A, and Z_o is the independent replicas. The meaning of replicas implies that there are multiple copies of the ensembles that can be glued together or apply the periodic boundary condition to it and measure the entanglement entropy. The first estimator being proposed to measure the entropy is not effective, it is given that [4]:

$$\left\langle S_{q}^{E} \right\rangle = \frac{1}{1-q} \ln \left\langle \frac{N_A}{N_o} \right\rangle \tag{6.2}$$

This limits the case for N_A being too small and N_o being too large.
It can be calculated by restricting the incremental increase of the subsystem A, and measure the entropy repeatably. The basic description is down here: The ratio initially,

$$R_n(A') = \frac{Z_n(A')^{n}}{Z_1(A')} \tag{6.3}$$

$Z_n(A')$ is the glued partition function, $Z_1(A')^n$ is the n independent partition function.

Compute the step wise ratio:

$$R_n(A \to A') = \frac{R_n(A')}{R_n(A)} \tag{6.4}$$

Update the new entanglement entropy,

$$S_{A'}^{(n)} = S_{A}^{(n)} + \frac{1}{1-n} \log R_n(A \to A') \tag{6.5}$$

Let us break it part-by-part and discuss the detail of the measurement.

6.2 Preparation of ensembles

Perform an extended ensemble simulation which split by independent ensemble and glued ensemble of replicas. And the update the system by Markov chain Monte Carlo method (use metropolis Algorithm and Wolff Algorithm in this context) and count the step in each of the ensemble. To reach equilibrium at finite time t, the probability is given by the Master equation [4]:

$$\frac{dP_A(t)}{dt} = P_\emptyset(t)p_{\emptyset\to A} - P_A(t)p_{A\to\emptyset} \tag{6.6}$$

The Master equation is defined as:

$$\frac{dP_i(t)}{dt} = \sum_j [W_{ij}P_j(t) - W_{ji}P_i(t)] \tag{6.7}$$

In this context, the probability counted in the independent ensemble $P_\emptyset(t)$ is $P_j(t)$ and $p_{\emptyset\to A}$ is W_{ij} which is the transition rate from independent ensemble to glued ensemble.And this is the inverse process for $P_A(t)$ and $p_{A\to\emptyset}$.

In an equilibrated Markov chain configuration, we have,

$$\frac{dP_A(t)}{dt} = 0 \tag{6.8}$$

$$\Rightarrow P_A(t)p_{A\to\emptyset} = P_\emptyset(t)p_{\emptyset\to A} \tag{6.9}$$

$$\Rightarrow \frac{P_A}{P_\emptyset} = \frac{p_{\emptyset\to A}}{p_{A\to\emptyset}} \tag{6.10}$$

As,

$$\frac{N_A}{N_\emptyset} = \frac{N_A}{N_\emptyset + N_A}\frac{N_A + N_\emptyset}{N_A} = \frac{P_A}{P_\emptyset} \tag{6.11}$$

The entanglement Rényi entropy is [4],

$$S_q^E = \frac{1}{1-q} ln(\frac{p_{\emptyset\to A}}{p_{A\to\emptyset}}) \tag{6.12}$$

6.3 Interpretation of transition probability

The detail of probability $p_{\emptyset\to A}$ is that, since it describe the condition moving from the independent ensemble $\{\emptyset\}$ to glued ensemble $\{A\}$. Its process is equivalent to finding all identical state in the A region for each replicas, which i belongs 2 replicas for 2-d case. For the graphical solution, it is more easily to observe that, for all collected state, (red to red state) and (green to green state) in $\{\emptyset\}$ ensemble, we are counting the chance for the each pair

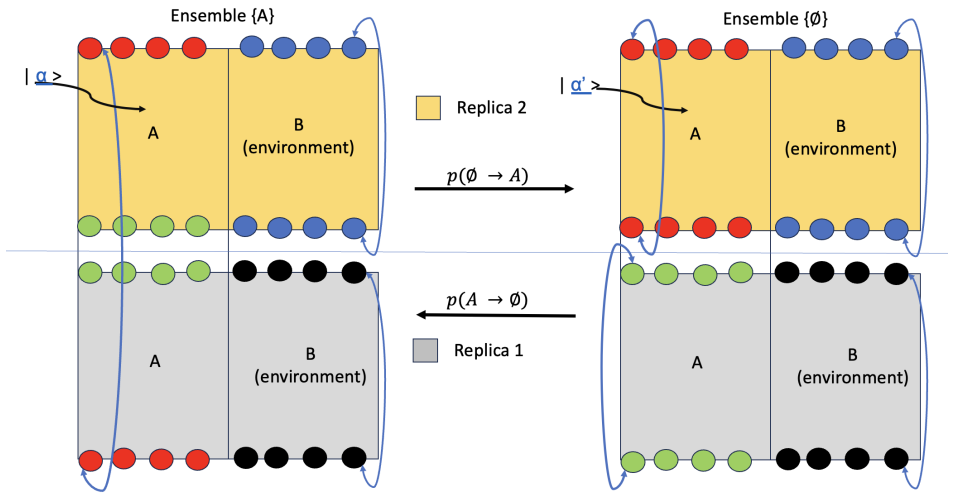


Figure 5: The graph is taking the refernce [4]

of independent state $|\alpha'\rangle$ pretended to be same as the glued state $|\alpha\rangle$ in the $\{A\}$ ensemble. We denote the chance for counting $|\alpha'\rangle = |\alpha\rangle$ is the probability $P_{identical_A}$ as $p_{\emptyset\to A}$ in here. The part of the entropy becomes:

$$S_1 = \frac{1}{1-q} ln P_{identical_A} \tag{6.13}$$

The detail of probability $p_{A\to\emptyset}$ is that, it is the opposite condition from the above, for each glued state in the $\{A\}$ ensemble, we are counting the chance that for each glued state $|\alpha\rangle$ to become a pair of independent state $|\alpha'\rangle$ in the $\{\emptyset\}$ ensemble. The part of entropy is denoted as [4]:

$$S_2 = -\frac{1}{1-q} ln p_{A\to\emptyset} \tag{6.14}$$

Therefore,

$$S_1 + S_2 = \frac{1}{1-q} ln p_{\emptyset\to A} - \frac{1}{1-q} ln p_{A\to\emptyset} \tag{6.15}$$

$$= \frac{1}{1-q} ln(\frac{p_{\emptyset\to A}}{p_{A\to\emptyset}}) \tag{6.16}$$

6.4 Result

Base on the above set up, we investigate the entropy characteristics of a quantum system at near-zero temperatures. Specifically, we focus on how entropy scales with the size of subsystems within a larger system at a very low but finite temperature. Our method is to

scale the time scale parameter $\beta = \frac{1}{T}$ to a factor of 10 with respect to the length of the system.

The graph below will demonstrate the result for the prediction at a low finite temperature.

First, for the size: 24x240, the graph is shown as follow:

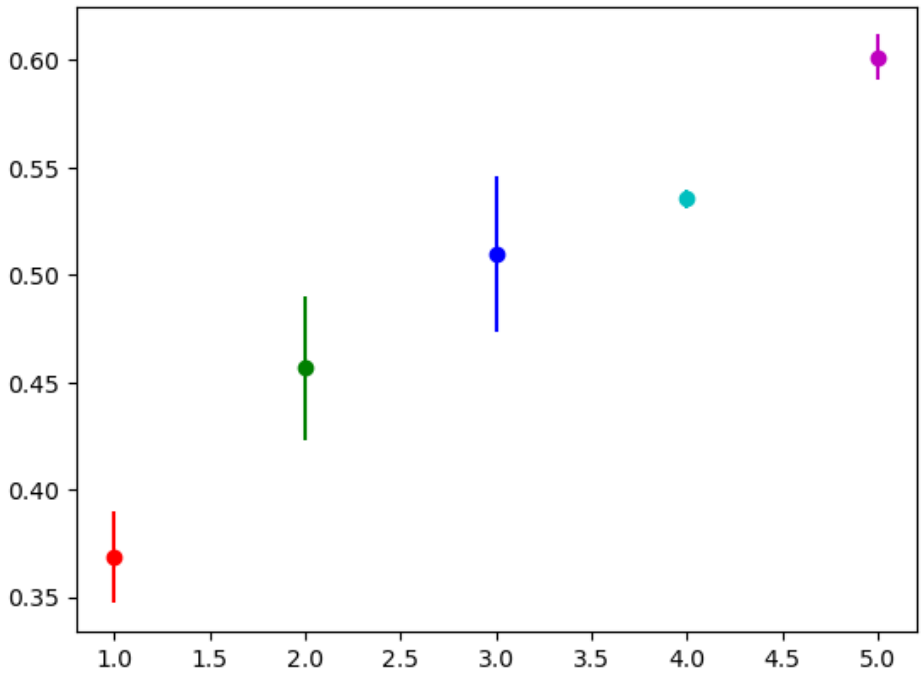


Figure 6: system size:24x240. The x-axis represents sub-system size, and the y-axis represents Entropy

From the graph, it is observed that as the size of the subsystem increases, the entropy follows a pattern resembling a half-parabola, reaching a maximum value of 0.60. for L =24, the system have 12 sub-system size, it is expected to have a half parabola shape til x = 12. However, due to the computational power of the computer, it is hard to run the Metropolis update at x = 12.

To enhance the analysis, we resale the x-axis into $\frac{l}{L}$, which l is the length of sub-system size. We demonstrate the system size $L = 8, 12, 16, 24$ to look for the variation of entropy.

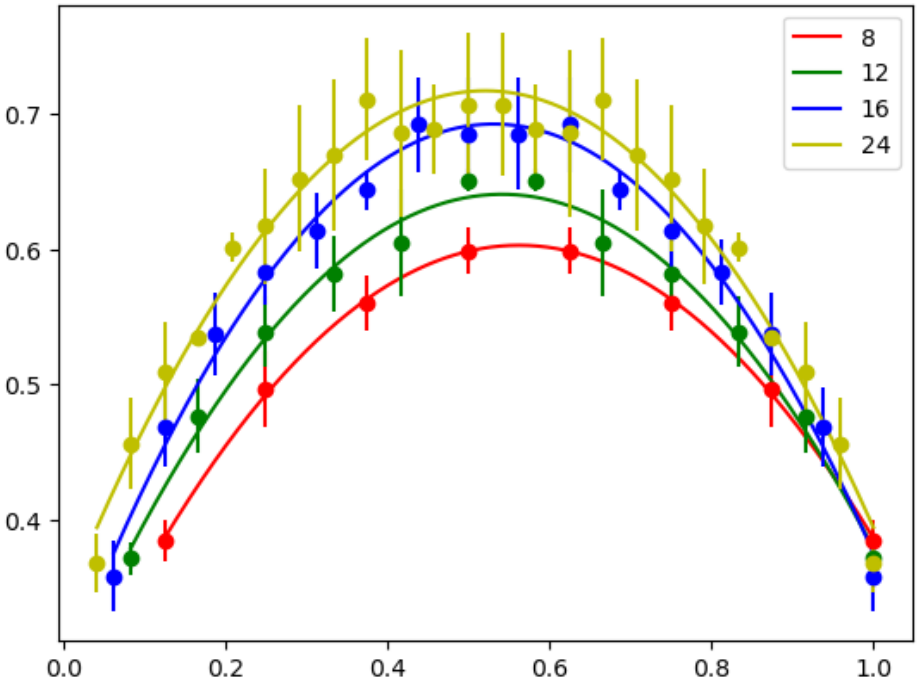


Figure 7: Wolff update:100000 steps, equilibrium:10000 steps

For every length L we measure, it demonstrate a complete parabola shape for the entropy measurement. It is due to the fact that the measurement of the first half sub-system size is symmetric to the latter after system. Therefore, in general, we only need to measure the half of the data to confirm the accuracy of the approximation. It is expected that the largest system size have a highest maximum value of entropy.
We then can fit our result into the Conformal Field Theory (CFT) predictions, before the showcase of the result, there is a brief discussion on the CFT prediction. Alba () has suggested that the linear fitting function in periodic boundary condition is given in:

$$S_A^{n=2} = \frac{c}{3} log(\frac{L}{\pi} sin(\frac{\pi l}{L})) + const. \tag{6.17}$$

As our main focus for the fitting is to verify the slope of the prediction, we will re scale the x-axis to $\frac{1}{3} log(\frac{L}{\pi} sin(\frac{\pi l}{L}))$. The expected central charge: c is 0.5. So, we plot entropy versus $\frac{1}{3} log(\frac{L}{\pi} sin(\frac{\pi l}{L}))$ with the same set of data. The result is shown as follow:

- The slope for L = 8 is: 0.5904
- The slope for L = 12 is: 0.558
- The slope for L = 16 is: 0.578
- The slope for L = 24 is: 0.519

From the data, we observe that the slopes measured for all system sizes are consistently above

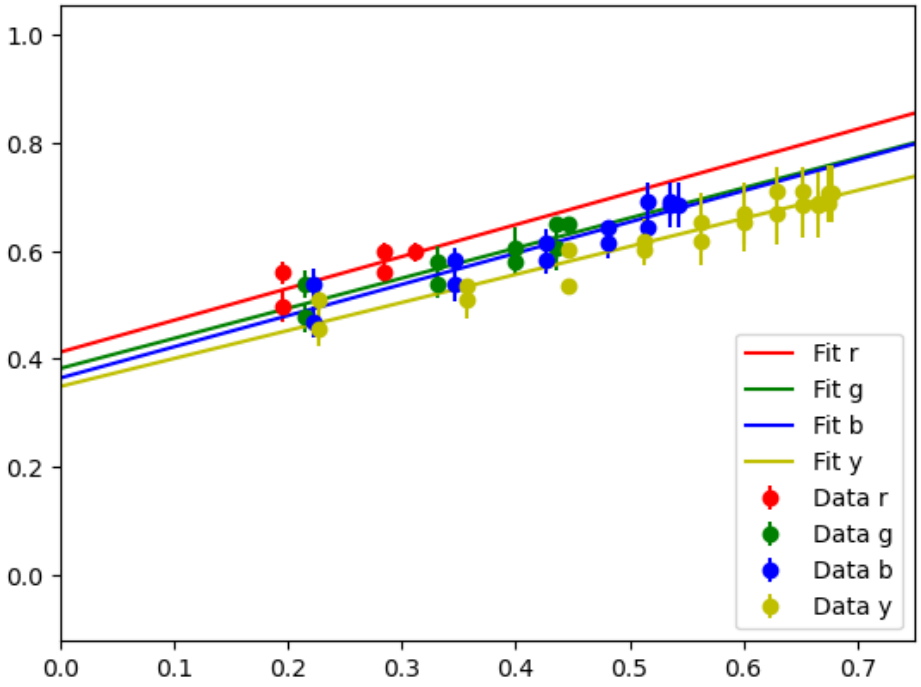


Figure 8: r:L=8, g:L=12, b:L=16, y:L=24

the theoretical value of 0.5, with the exception of L = 24, which is closer but still slightly above the expected value.

The reason for deviation can sum up by several reasons:

- Finite size limit: the theoretical value for the central charge is calculate by the large system size (say L = 256), the updated result is not large enough to get close to the theoretical value.
- Measurement uncertainty: The uncertainty (error bar) mainly contribute by the accumulated error by the update of Metropolis Algorithm and Wolff Algorithm.
- Error for small sub-system size: In our analysis, the data points corresponding to larger subsystem sizes tend to align more closely with the theoretical fit line (left-most region of the graph), and they are measured in a larger sub-system size, (for example l = 8 for L = 24). The reason is that, as the size of the subsystem increases, the entanglement entropy's leading term $(\frac{c}{3}log(\frac{L}{\pi}sin(\frac{\pi l}{L})))$ [4], which scales linearly with the subsystem size, becomes more dominant in determining the slope of the entropy scaling.
  While for a small entanglement region, the scale of the constant term will dominate the prediction, as the effect of entanglement is smaller.

To conclude, this result marks a essential role that, by updating the 1-D transverse field in MCMC method (Metropolis and Wolff Algorithm) with the periodic boundary condition in glued ensemble and independent ensemble, we can obtain the translation probabilities

between two replicas. Which match the result in the (ref. [6]).

7 Conclusion

In this project, we explored the relationship between the one-dimensional Transverse Field Ising Model (TFIM) and its mapping to the two-dimensional Classical Ising Model by the trotter-suzuki approximation. Which also enhance the generality from bridging 2-D transverse field Ising model to 3-D classical Ising model.

On the other hand, the major simulation in this project is the measurement of Renyi entropy. It verify that the Wolff Algorithm can boost up the time for simulation, and allow us to run a larger system size to approach the theoretical result.

Key result:
We have verify the classical and quantum phase transition point, (classical:T =2.269) and (T=0, h = 1) in both 2-D classical Ising model and the 1-D transverse field Ising model. Which match the behavior at phase transition.

The mapping for the 2-D transverse field Ising model demonstrate the generality for trotter-suzuki approximation. We show that, at the magnetization versus h plot, the h_c is about 2.68. Which match the prediction of theorical result.
Measuring the Renyi entropy in the structure of 1-D TFIM for two restricted boundary condition, the measured value is slightly higher than the ref [6], as the limitation of the finite system size. As the system size is closely related to the temperature, we are doing the measurement in the finite temperature.
The re scaling in the linear function show that the slope of the graph match the central charge c = 1/2 inspired by the Conformal field theory (CFT).Which mark the result that the update on the MCMC method can also reproduce and stimulate the entropy result.

Future improvement:
he Stochastic Series Expansion (SSE) method holds significant potential for further development, offering a robust and accurate approach to simulations. In contrast to the Monte Carlo Markov Chain (MCMC) methods, such as the Wolff algorithm, which need a large imaginary time axis (imL) to simulate low temperature case.

The SSE method on the other hand can avoid the long computational run time than MCMC method. It also minimize the error accumulated by the long running time.

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