THE UNIVERSITY OF HONGKONG
DEPARTMENT OF PHYSICS

Assignment 4

Course: *Computational Physics (PHYS4150/8150)* – Prof. *Zi Yang Meng*
Tutor: *Mr. Tim Lok Chau, Mr. Min Long*
Due date: *Nov. 25th, 2024*

This assignment is also a project; you are encouraged to form a group of 2 to 4 people and present your work on these questions during the classes on Nov 25th and 28th. The presentation should contain your answers to the questions, how you solved the problems, and your understanding of them.

1. **Density matrix**
   The density matrix ρ for a quantum system is $\rho = |\psi\rangle\langle\psi|$ where ψ is an arbitrary quantum state. For a single spin, an arbitrary state can be written as $|\psi\rangle = a|0\rangle + b|1\rangle$, where $|0\rangle$ and $|1\rangle$ represent the spin up and down state, respectively. The density matrix has the form $\rho = (a|0\rangle + b|1\rangle)(a^*\langle 0| + b^*\langle 1|)$. We then have

$$\begin{aligned}\rho|0\rangle &= (a|0\rangle + b|1\rangle)(a^*\langle 0| + b^*\langle 1|)|0\rangle \\ &= (a|0\rangle + b|1\rangle)(a^*\langle 0|0\rangle + b^*\langle 1|0\rangle) \\ &= (a|0\rangle + b|1\rangle)a^* = aa^*|0\rangle + ba^*|1\rangle\end{aligned}$$

   If we were only interested in information on the subsystem A. In principle, we can derive a reduced density matrix which only contains the information of A. The reduced density matrix is derived by tracing out the state from subsystem B from the density matrix ρ (the eigenbasis of B is denoted as $|b\rangle$, please do not confuse with the amplitude b in ρ) (how about now, we don't need to mention site at all?)

$$\rho_A = Tr_B(\rho) = \sum_b \langle b|\rho|b\rangle.$$

   To compute the reduced density matrix, we write the state as $|\psi\rangle = \sum_{ab} \psi_{ab}|a\rangle|b\rangle$, where $|a\rangle$ and $|b\rangle$ if the basis states from subsystems A and B separately. The density matrix has the form:

$$\rho = |\psi\rangle\langle\psi| = \sum_{aba'b'} \psi_{ab}\psi^*_{a'b'}|a\rangle|b\rangle\langle a'|\langle b'|$$

Then by definition:

$$\begin{aligned}\rho_A &= \sum_b \langle b|\rho|b\rangle \\ &= \sum_{aba'b'b''} \psi_{ab}\psi^*_{a'b'}|a\rangle\langle b''|b\rangle\langle a'|\langle b'|b''\rangle \\ &= \sum_{aba'b'b''} \psi_{ab}\psi^*_{a'b'}\delta_{bb''}\delta_{b'b''}|a\rangle\langle a'| \\ &= \sum_{ab''a'} \psi_{ab''}\psi^*_{a'b''}|a\rangle\langle a'| \\ &= [\psi][\psi]^\dagger\end{aligned}$$

where $[\psi]$ is a matrix and the matrix element is $[\psi]_{a,b} = \psi_{ab}$ and $[\psi]^\dagger_{a,b}$ is the Hermitian conjugate of $[\psi]$. In the last line, we perform the matrix multiplication for two matrices.

We calculate the reduced density matrix for a spin system as an example here. An arbitrary state can be written as $|\Psi\rangle = a|00\rangle + b|01\rangle + c|10\rangle + d|11\rangle$. We label the left spin subsystem A and the right spin subsystem B. It is easy to write the matrix $[\Psi] = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$. According to the formula above, the reduced density matrix of subsystem A is $\rho_A = [\psi][\psi]^\dagger = \begin{bmatrix} aa^* + bb^* & ac^* + bd^* \\ ca^* + db^* & cc^* + dd^* \end{bmatrix}$.

The reduced density matrix contains the entanglement information between subsystems A and B (the remaining part of the system). To extract such information from the reduced density matrix, we calculate the Rényi entropy between the subsystem and the bath.

The q-th Rényi entropy is defined as:

$$S^{(q)}_A = \frac{1}{1-q}\ln(Tr(\rho^q_A)).$$

It can be analytically reduced to the Von Neumann Entanglement entropy when $q \to 1$,

$$S^{vN}_A = -Tr(\rho_A \ln \rho_A).$$

Now, consider a one-dimensional quantum spin-1/2 chain. The Hamiltonian is defined as

$$H = J\sum_{i=1}^{N-1} \vec{S}_i\vec{S}_{i+1}, \tag{1}$$

where $\vec{S}_i$ is the operator of the i-th spin. N is the number of sites in the lattice and the antiferromagnetic Heisenberg interaction is $J = 1$. The periodic boundary condition is met by letting $\vec{S}_{N+1} = \vec{S}_1$.

For $q = 1.2, 1.5, 2, 3$ and $N = 10$, calculate the corresponding Rényi entropy as a function of subsystem size compared with the result of Von Neumann entropy

using the abovementioned formula. (i.e. compute the Rényi entropy of the subsystem, which only contains the left l_A sites of the spin chain. Vary q and plot the dependence of Rényi entropy on q, and you can compare your result with Figure 1).

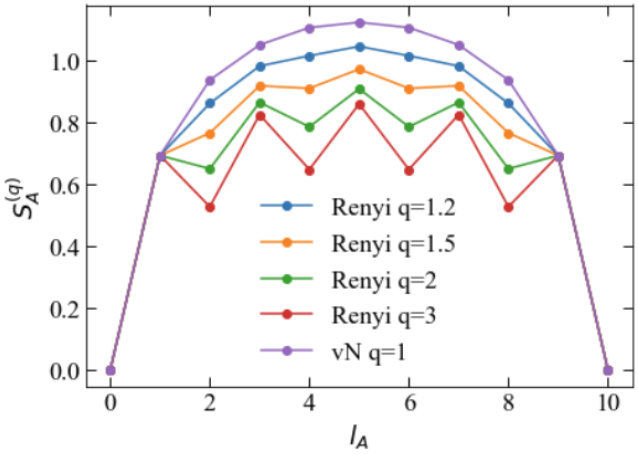


Figure 1: Rényi entropy with different q value.

2. **Transvers field Ising model**
Consider a 1D chain with **periodic boundary conditions**, with one spin lives on each site. Each spin can be either up ($\sigma_z = 1$) or down ($\sigma_z = -1$). The Hamiltonian is defined as

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

where σ_i^z is the operator measures the z component of the i-th spin. h is the strength of the transverse field, and it is on the x-direction. Also, we have $\sigma_{N+1}^z = \sigma_1^z$ from the periodic boundary condition. Here, J and h are positive, so the spin chain is ferromagnetic, and the external magnetic field points toward the positive x direction.

By properties of Pauli matrices, we have

$$H = -J\sum_{i=1}^{N}\sigma_i^z\sigma_{i+1}^z - h\sum_{i=1}^{N}(\sigma_i^+ + \sigma_i^-),$$

where σ_i^+ flips the i-th spin from down to up, and equals 0 if the i-th site is already spin up, and vice versa for σ_i^-. For example, $\sigma_1^+|\downarrow\downarrow\downarrow\downarrow\rangle = |\uparrow\downarrow\downarrow\downarrow\rangle$ and $\sigma_1^-|\downarrow\downarrow\downarrow\downarrow\rangle = 0$.

Unlike the Heisenberg model, where you need to flip two adjacent spins simultaneously, here, you only need to flip one spin each time. It is known that a quantum phase transition for the transverse field Ising model happens on $h_c = 1$.

(a) Consider $N = 10$, $h = 0, 0.5, 0.1, ..., 2.0$ and $J = 1$, find the 50-th lowest energy states, plot $E_n - E_0$ (E_0 is the ground state energy value) versus h, and

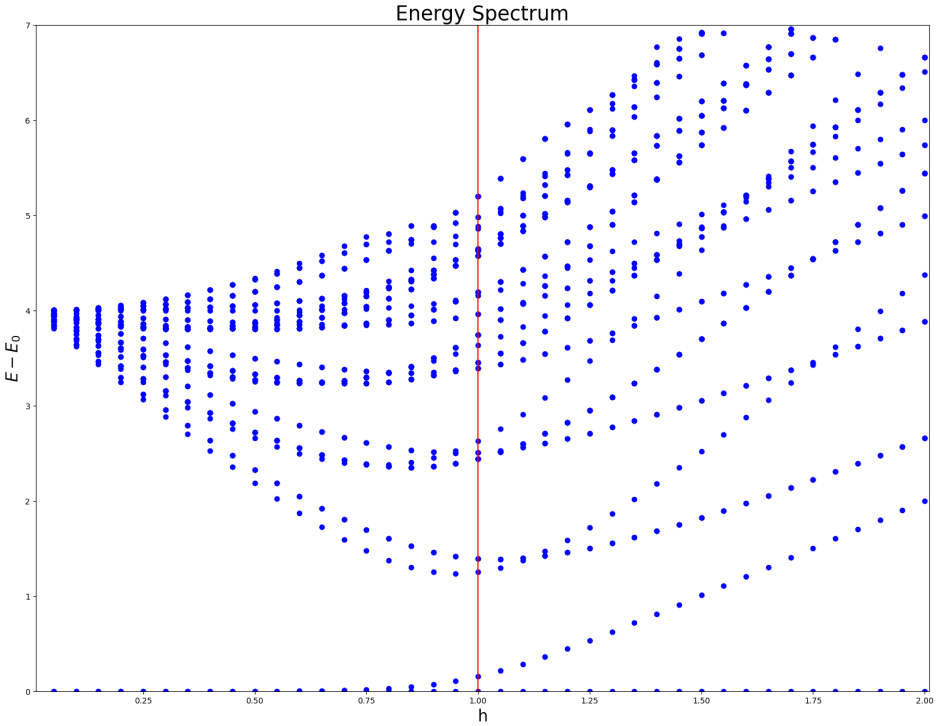


Figure 2: Energy spectrum of Transverse Field Ising Model.

you can compare your result with Figure 2. Can you interpret the information of a quantum phase transition at $h_c = 1$ from these data?

(b) Compute the second-order Rényi entropy of the TFIM at $h = h_c = 1, J = 1$ with $N = 10$, and l_A ranging from 0 to 10, and compare your result with Figure 3.

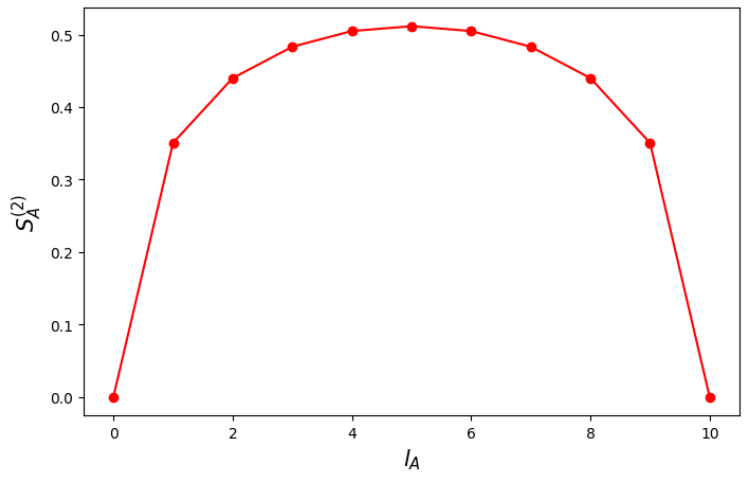
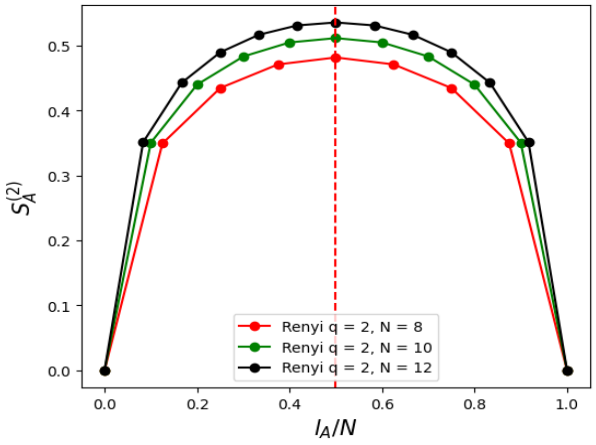


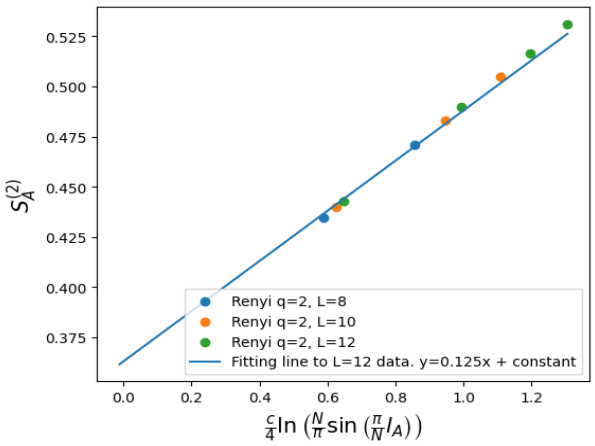
Figure 3: Rényi entropy of the Transverse field Ising Model at $h = h_c = 1$ with $N = 10$.

(c) **(Optional)** One can exactly diagonalize the longer chain and look for the scaling behaviour of the Rényi entanglement entropy. As shown in Fig.4, we plot the second-order Rényi entropy for $N = 8, 10$ and 12 versus l_A/N in the left panel and then rescale them according to the formula.

$$S_A^{(2)}(l_A) = \frac{c}{4}\ln(\frac{N}{\pi}\sin(\frac{\pi}{N}l_A)) + \text{constant}$$



(a) Rényi entropy for $N = 8, 10, 12$



(b) Rényi entropy for $N = 8, 10, 12$ with scaled rescaled x-axis. **We ignore** $\ln(\frac{N}{\pi}\sin(\frac{\pi}{N}l_A)) < 0$ **data points**

In the right panel, the data follows nicely with $c = 1/2$, which is the central charge of this quantum Ising phase transition. Please reproduce the two graphs above and comment on your findings.

Hint for part c):

- For $N = 12$, you only need to calculate Rényi entropy to $l_a = N/2$ and flip the result along the x-axis since the values of Rényi entropy are **symmetric**. It is also applicable to $N = 8, 10$.
- For the fitting line in the right panel, you can fix $c = 1/2$ in the linear fitting. You only need to do the linear fitting to $N = 12$ with $l_A = 2, 3, ..., 6$ data.