Assignment 4

Course: Computational Physics (PHYS4150/8150) – Professor: Dr. Ziyang Meng Tutor: Mr. Menghan Song, Mr. Ting-Tung Wang Due date: Nov. 24th, 2022

Exact diagonalization of the transverse field Ising model

Consider a 1D chain with periodic boundary condition, with one spin lives on each site. Each spin can be either up ($s_z = 1$) or down ($s_z = -1$). The hamiltonian is defined as

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

where s_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 $s_{N+1}^z = s_1^z$ from the periodic boundary condition. Here J and h are positive, so that the spin chain is ferromagnetic, and the external magnetic filed points toward positive x direction. By properties of Pauli matrices, we have

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

where s_i^+ flips the i-th spin from down to up, and equal 0 if the i-th site is already spin up, vice versa for s_i^- . For example, $s_1^+|\downarrow\downarrow\downarrow\downarrow\rangle=|\uparrow\downarrow\downarrow\downarrow\rangle$ and $s_1^-|\downarrow\downarrow\downarrow\downarrow\rangle=0$.

Unlike in Heisenberg model, where you need to flip two adjacent spin at the same time, here you only need to flip one spin each time.

It is known that there is a quantum phase transition for transverse field Ising model happens on $h_c = 1$. At the critical point, the degenerate ground state will split, magnetization will drop to 0, and the variance of magnetization will diverge. However, phase transition happens only in thermodynamic limit ($L \to \infty$). Due to finite size effect, the above-mentioned phenomena will be slightly difference. For example, magnetization will not drop to exactly 0. Instead, it will decay to a small finite value.

For the following part, consider N = 12, and $h = 0, 0.05, 0.1, \dots, 2.0$. Use exact diagonalization to find the following physical observables.

- 1. Find lowest 50 energy states, plot $E_n E_0$ (to set ground state energy as 0) for each h.
- 2. For ground state, measure its average absolute magnetization $\langle |m_z| \rangle = \sum_{k=0}^{2^N} |c_k|^2 |m_z(k)|$, where c_k is the k-th component of the ground state eigenvector. $m_z(k)$ is the magnetization of the k-th basis state, defined as $m_z(k) = \frac{1}{N}(n_\uparrow(k) n_\downarrow(k))$, where $n_\uparrow(k)$ counts the number of spins up in the k-th basis state, and $n_\downarrow(k)$ counts the number of spins down.
- 3. Find the variance of magnetization $\sigma_{m_z} = \langle |m_z|^2 \rangle \langle |m_z| \rangle^2$

