

Assignment

1. Derive the complexity in Big- \mathcal{O} notation for $\langle \psi | \hat{H} | \psi \rangle$ with an MPS ψ of bond dimension χ and an MPO \hat{H} of bond dimension D on chain of N sites and open index dimension d .
2. To find the m -th excited state one can add penalty terms ω_n to the Hamiltonian

$$\hat{H}' = \hat{H} + \sum_{n=0}^{m-1} \omega_n |\Psi_n\rangle \langle \Psi_n| \quad (6.1)$$

such that minimizing this $\langle \hat{H}' \rangle$ naturally avoids previously found states and gives the targeted excited state. Prove the criterion of ω_0 for the first excited states by discussing the three cases, (a) $\omega_1 < \Delta\varepsilon$, (b) $\omega_1 > \Delta\varepsilon$, (c) $\omega_1 = \Delta\varepsilon$, where $\Delta\varepsilon = \varepsilon_1 - \varepsilon_0$ is the energy gap between the first excited and the ground state.

3. Write a code in any programming language as you prefer to implement the W states $|W_3\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$ on three qubits as MPS using matrices and verify it by computing overlap to all the basis states, such as $\langle 000|W\rangle$, $\langle 001|W\rangle$, and so forth.
4. The Hamiltonian of the one-dimensional transverse-field Ising model on N sites is given by

$$H = -J \sum_{i=1}^{N-1} \sigma_i^z \sigma_{i+1}^z - h \sum_{i=1}^N \sigma_i^x, \quad (6.2)$$

where J is strength of local interaction and h is the field strength. Consider a quenched time evolution where the initial state $|\psi_0\rangle$ is the ground state of the Hamiltonian with $h \ll J$ and starting at $t = 0$ the system is applied by a quenched Hamiltonian with $h > J$. One may imagine this is like we turn on the background field at $t = 0$. You can investigate any of the following by writing a code in **iTensor** to prepare the state and simulate the dynamics:

1. What happens to the order parameter, such as $M_z = \frac{1}{N} \sum_i \langle \sigma_i^Z \rangle$, $M_x = \frac{1}{N} \sum_i \langle \sigma_i^x \rangle$, $M_z^2 = \frac{1}{N^2} \sum_{i,j} \langle \sigma_i^Z \sigma_j^Z \rangle$ as time evolves?
2. How does the correlation $C_r(i) = \langle \sigma_i^Z \sigma_{i+r}^Z \rangle$ look like at different distance r ? You may plot the expectation $C_r(t)$ as heatmap.
3. How does the overlap of the states $\langle \psi_0 | \psi(t) \rangle$ look like?
4. or any other observable you find interesting.