I. TREE TENSOR NETWORK

[Problem 2 for Guifre Vidal's lectures for Mathematica Summer School. It assumes that the student has already solved problem 1]

In this problem, you will build a real space RG scheme for quantum spin chains and a *tree tensor network* (TTN) representation of the ground state (and low energy excited states) of the critical quantum Ising model Hamiltonian

$$H = \sum_{r=1}^{N} (\sigma_{z,r} + \sigma_{x,r}\sigma_{x,r+1}) \tag{1}$$

where

$$\sigma_x \equiv \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{2}$$

are spin-1/2 Pauli matrices, r labels the N sites of the quantum spin chain, and we assume periodic boundary conditions, so that site $r = N + 1$ is actually $r = 1$.

A TTN representation is of interest because the computational cost grows as some small power of the system size N, and not as $O(\exp(N))$ as in exact diagonalization / Lanczos. This will allow us to consider much larger spin chains.

We will build a TTN approximation for the ground state $|E_0(N)\rangle$ (more generally, low energy eigenstates $|E_\alpha\rangle$) of H on N sites sequentially, by first considering smaller systems. Let us first describe the initialization step, which is slightly different from the rest.

A. Initialization step

- Use *exact diagonalization* (see problem 1) to compute the ground state $|E_0\rangle$ of H on 12 spins, see Fig. 1(a).
- Compute the reduced density matrix ρ for 6 contiguous spins (see Fig. 1(b)),

$$\rho \equiv \mathrm{tr}_{7,8,9,10,11,12}|E_0\rangle\langle E_0|. \tag{3}$$

- Compute the eigenvalue decomposition of ρ (see Fig. 1(c)),

$$\rho = \sum_{\alpha=1}^{2^6} p_\alpha |W_\alpha\rangle\langle W_\alpha|, \quad p_1 \geq p_2 \geq \cdots \geq p_{2^6} \geq 0. \tag{4}$$

- We then define the vector space of an effective site that replaces those 6 sites in terms of the first $\chi = 8$ vectors $\{|W_1\rangle, |W_2\rangle, \cdots, |W_8\rangle\}$, corresponding to the $\chi = 8$ largest eigenvalues $\{p_1, p_2, \cdots, p_8\}$.
- Our goal is to define an effective Hamiltonian on a system made of four effective sites. We distinguish two types of Hamiltonian terms: those terms J_r acting on just one effective site r (think of them as some effective magnetic field), and those terms $I_{r,r+1}$ acting on two neighboring sites r and $r + 1$(think of them as some effective interaction between those sites). We obtain the effective magnetic field J_r by projecting all the original Hamiltonian terms contained on the first 6 sites. J is a $\chi \times \chi$ matrix with components $J_{\alpha\beta} \equiv \langle W_\alpha|J|W_\beta\rangle$ that read (see Fig. 2(a))

$$(J)_{\alpha\beta} \equiv \langle W_\alpha|M|W_\beta\rangle, \qquad M \equiv \sum_{r=1}^{6} \sigma_z, r + \sum_{r=1}^{5} \sigma_{x,r}\sigma_{x,r+1} \tag{5}$$

  On the other hand, the effective interaction I is a $\chi^2 \times \chi^2$ matrix with components $I_{\alpha\alpha'\beta\beta'} \equiv \langle W_\alpha|\langle W_{\alpha'}|I|W_\beta\rangle|W_{\beta'}\rangle$ that read (see Fig. 2(b))

$$(I)_{\alpha\alpha'\beta\beta'} \equiv \langle W_\alpha|\langle W_{\alpha'}|\sigma_{x,6}\sigma_{x,7}|W_\beta\rangle|W_{\beta'}\rangle = \langle W_\alpha|\sigma_{x,6}|W_\beta\rangle\langle W_{\alpha'}|\sigma_{x,7}|W_{\beta'}\rangle. \tag{6}$$

In summary, in this initialization step we have produced an effective Hamiltonian

$$H^{(1)} = \sum_{r=1}^{4} \left(J_r^{(1)} + I_{r,r+1}^{(1)} \right) \tag{7}$$

for an effective quantum spin chain made of 4 spins, where each spin is described by a χ-dimensional vector space and we have defined $J^{(1)} \equiv J$ and $I^{(1)} \equiv I$ for convenience.

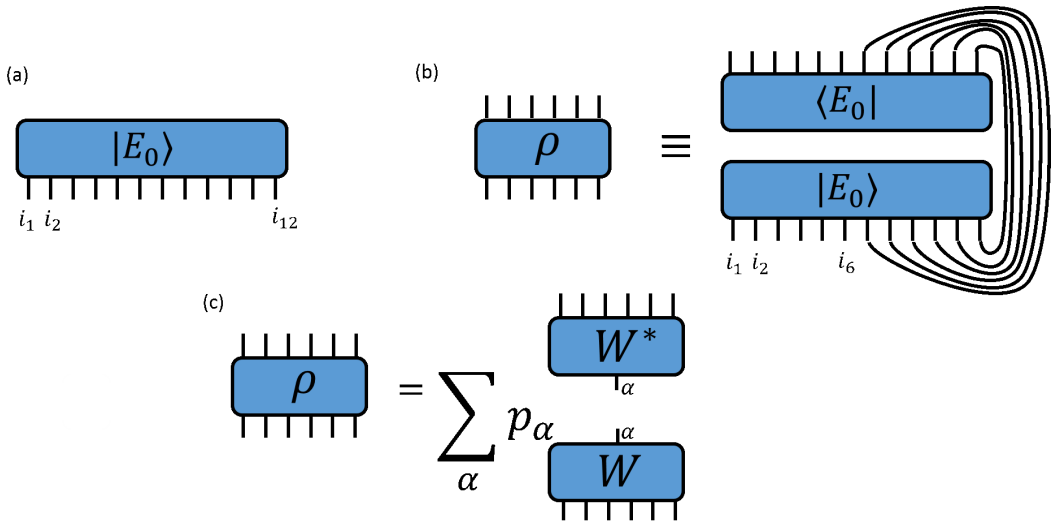

FIG. 1: (a) Representation of the ground state $|E_0\rangle$ of H on 12 spins. (b) Reduced density matrix ρ for spins $1, 2, 3, 4, 5, 6$. (c) Eigenvalue decomposition of ρ.

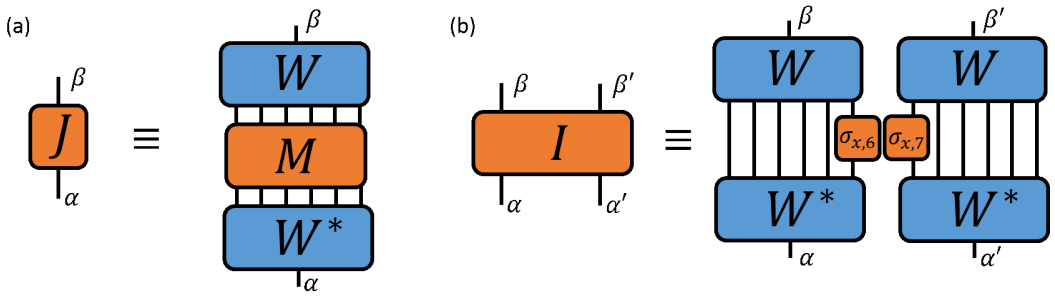

FIG. 2: (a) Effective magnetic field J. (b) Effective interation I

B. Subsequent steps

The algorithm then proceeds by iterating $Q-1$ times, labelled by $s = 1, 2, \cdots, Q-1$, the following sequence of operations. Given Hamiltonian $H^{(s)}$ at scale s,

$$H^{(s)} \equiv \sum_{r=1}^{4} \left(J_r^{(s)} + I_{r,r+1}^{(s)} \right), \tag{8}$$

we will:

- Use *exact diagonalization* (see problem 1) to compute the ground state $|E_0^{(s)}\rangle$ of $H^{(s)}$.
- Compute the reduced density matrix $\rho^{(s)}$ for 2 contiguous spins (Fig. 3),

$$\rho^s \equiv \mathrm{tr}_{3,4} |E_0^{(s)}\rangle\langle E_0^{(s)}| \tag{9}$$

- Compute the eigenvalue decomposition of $\rho^{(s)}$ (Fig. 3),

$$\rho^{(s)} = \sum_{\alpha=1}^{\chi^2} p_\alpha^{(s)} |W_\alpha^{(s)}\rangle\langle W_\alpha^{(s)}|, \quad p_1^{(s)} \geq p_2^{(s)} \geq \cdots \geq p_{\chi^2}^{(s)} \geq 0. \tag{10}$$

- We then define the vector space of an effective site that replaces those 2 sites in terms of the first χ vectors $\{|W_1^{(s)}\rangle, |W_2^{(s)}\rangle, \cdots, |W_\chi^{(s)}\rangle\}$, corresponding to the $\chi = 8$ largest eigenvalues $\{p_1, p_2, \cdots, p_\chi\}$.

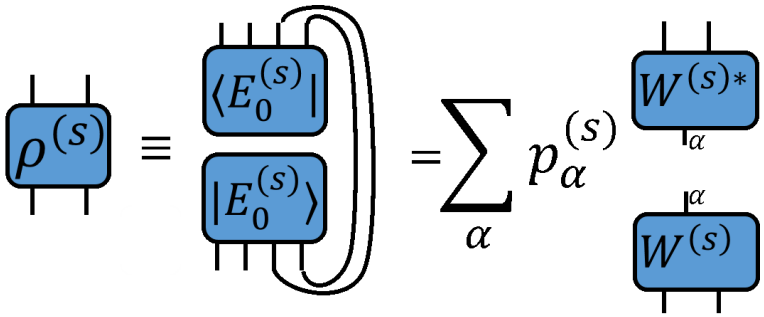

FIG. 3: Reduced density matrix $\rho^{(s)}$ and its eigenvalue decomposition.

- We then build an effective Hamiltonian $H^{(s+1)}$ at scale $s+1$,

$$H^{(s+1)} = \sum_{r=1}^{4} \left(J_r^{(s+1)} + I_{r,r+1}^{(s+1)} \right) \tag{11}$$

where the effective magnetic field $J^{(s+1)}$ is defined by (Fig. 4(a))

$$(J^{(s+1)})_{\alpha\beta} \equiv \langle W_\alpha^{(s)}| \left(J_1^{(s)} + J_2^{(s)} + I_{1,2}^{(s)} \right) |W_\beta^{(s)}\rangle, \tag{12}$$

whereas the effective interaction $I^{(s+1)}$ is given by (Fig. 4(b))

$$(I^{(s+1)})_{\alpha\alpha'\beta\beta'} \equiv \langle W_\alpha^{(s)}|\langle W_{\alpha'}^{(s)}|I_{2,3}^{(s)}|W_\beta^{(s)}\rangle|W_{\beta'}^{(s)}\rangle. \tag{13}$$

C. Final step and TTN

Finally, diagonalize the Hamiltonian

$$H^{(Q)} \equiv \sum_{r=1}^{2} \left(J_r^{(s)} + I_{r,r+1}^{(s)} \right), \tag{14}$$

on a periodic two-site chain to obtain its ground state $|E_0^{(Q)}\rangle$ as well as its low energy eigenvectors $|E_\alpha^{(Q)}\rangle$ for, say, $\alpha = 1, 2, \cdots 11$.

Fig. 5 shows how to connect the tensors in such a way as to obtain a tensor network *approximate* representation of the ground state/low energy eigenstates $|E_\alpha\rangle$ of H on 6×2^Q sites. Congratulations, you have built a tree tensor network!

D. RG transformation (optional)

You have also built a real-space RG transformation, which has produced a sequence of coarse-grained Hamiltonians $H^{(1)} \to H^{(2)} \to \cdots$. For each of these Hamiltonians, compute the low energy spectrum and use it to estimate the scaling dimensions Δ_n of the Ising CFT, as in Problem 1.

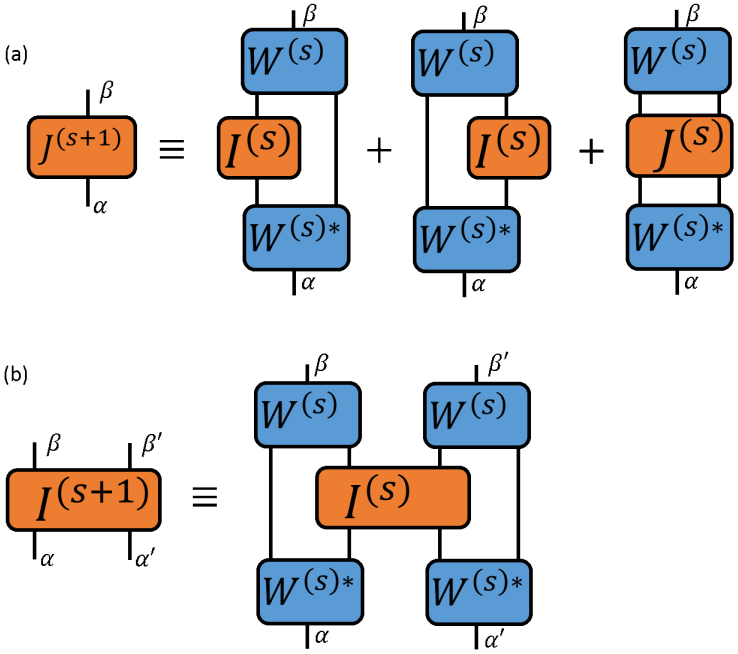

FIG. 4: (a) Effective magnetic field $J^{(s+1)}$. (b) Effective interaction $I^{(s+1)}$.

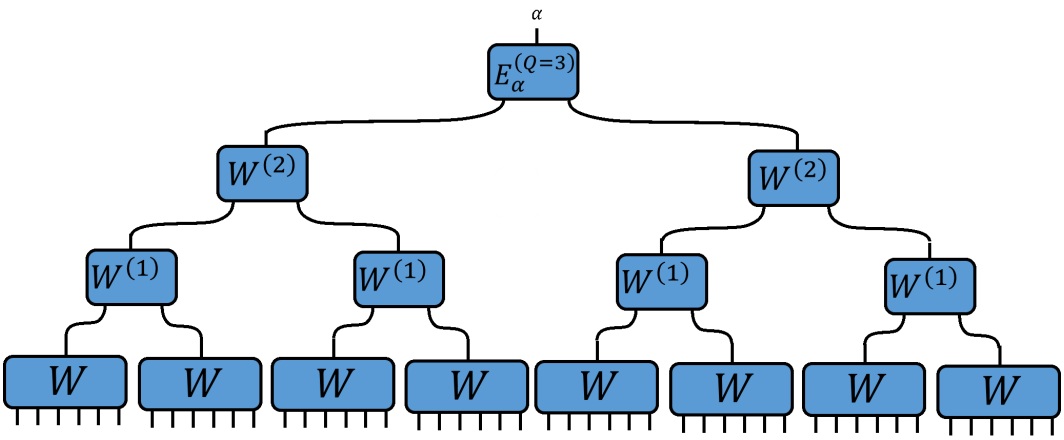

FIG. 5: Tree tensor network approximation of the state low energy eigenstates E_α (where $\alpha = 1, 2, \cdots, \chi$) of Hamiltonian H on $N = 6 \times 2^3 = 48$ spins ($Q = 3$).