Chapter 1

Model and Methods

1.1 Matrix product operator

The tSDRG method is, in essence, a renormalization of the Hamiltonian written as Matrix Product Operators (MPOs). In the computation of quantum many-body systems, matrix product representation is a powerful tool to reduce execution time and memory usage via decomposition of a big tensor representing a state or an operator into a set of small local tensors.

For a spin chain of length L with open boundary conditions (OBC), the Hamiltonian (or any operator) can be decomposed into a matrix product form written as

$$\hat{H} = \sum_{\boldsymbol{\sigma},\boldsymbol{\sigma'}} \sum_{\mathbf{b}} W_{b_1}^{\sigma_1,\sigma'_1} W_{b_1,b_2}^{\sigma_2,\sigma'_2} \cdots W_{b_{i-1},b_i}^{\sigma_i,\sigma'_i} \cdots W_{b_{L-1}}^{\sigma_L,\sigma'_L} |\boldsymbol{\sigma}\rangle\langle\boldsymbol{\sigma'}| \,, \tag{1.1}$$

where $|\boldsymbol{\sigma}\rangle = |\sigma_1\sigma_2\cdots\sigma_i\cdots\sigma_L\rangle$ represents the physical state (for example, the standard basis state of the L spins). The σ_i indices are the physical indices used to label the spin state at site i, whereas the b_i are the bond indices labeling the bonds connecting between local operators. Figure 1.1 shows diagrammatically a MPO representation of a Hamiltonian.

For our model we first rewrite the Hamiltonian in terms of the ladder operator $\hat{S}^{\pm} = \hat{S}^x \pm i\hat{S}^y$:

$$\hat{H} = \sum_{i=1} J_i [\frac{1}{2}(\hat{S}_i^+ \hat{S}_{i+1}^- + \hat{S}_i^- \hat{S}_{i+1}^+) + \hat{S}_i^z \hat{S}_{i+1}^z] \,. \tag{1.2}$$

The Hamiltonian in Eq. (1.2) for L spins with open boundary conditions has the following

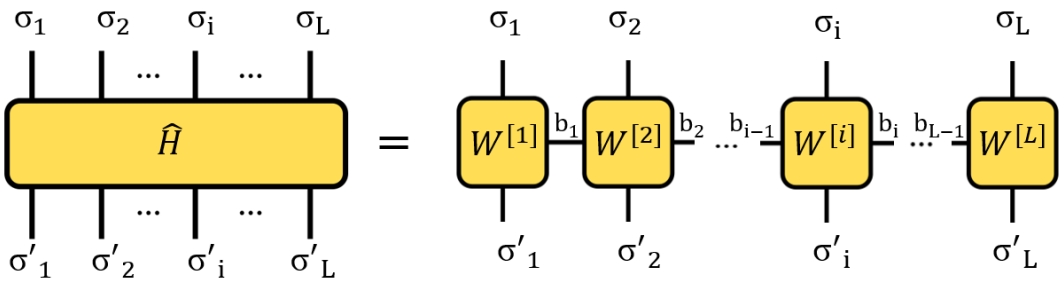


Figure 1.1: Tensor network diagram of MPO

MPO tensors:

$$W^{[1]} = \begin{pmatrix} 0 & (J_1/2)\hat{S}_1^- & (J_1/2)\hat{S}_1^+ & J_1\hat{S}_1^z & \mathbb{1} \end{pmatrix} , \tag{1.3}$$

$$W^{[i]} = \begin{pmatrix} \mathbb{1} & 0 & 0 & 0 & 0 \\ \hat{S}_i^+ & 0 & 0 & 0 & 0 \\ \hat{S}_i^- & 0 & 0 & 0 & 0 \\ \hat{S}_i^z & 0 & 0 & 0 & 0 \\ 0 & (J_i/2)\hat{S}_i^- & (J_i/2)\hat{S}_i^+ & J_i\hat{S}_i^z & \mathbb{1} \end{pmatrix} , \tag{1.4}$$

$$W^{[L]} = \begin{pmatrix} \mathbb{1} \\ \hat{S}_L^+ \\ \hat{S}_L^- \\ \hat{S}_L^z \\ 0 \end{pmatrix} . \tag{1.5}$$

For a chain with periodic boundary conditions, the MPO tensors for $i = 1 \cdots L$ are all bulk tensors as given in Eq. (1.4), where the coupling J_L links between two end sites L and 1. We can recover the Hamiltonian in Eq. (1.2) by simply multiplying the tensors $W^{[1]}W^{[2]} \cdots W^{[L]}$.

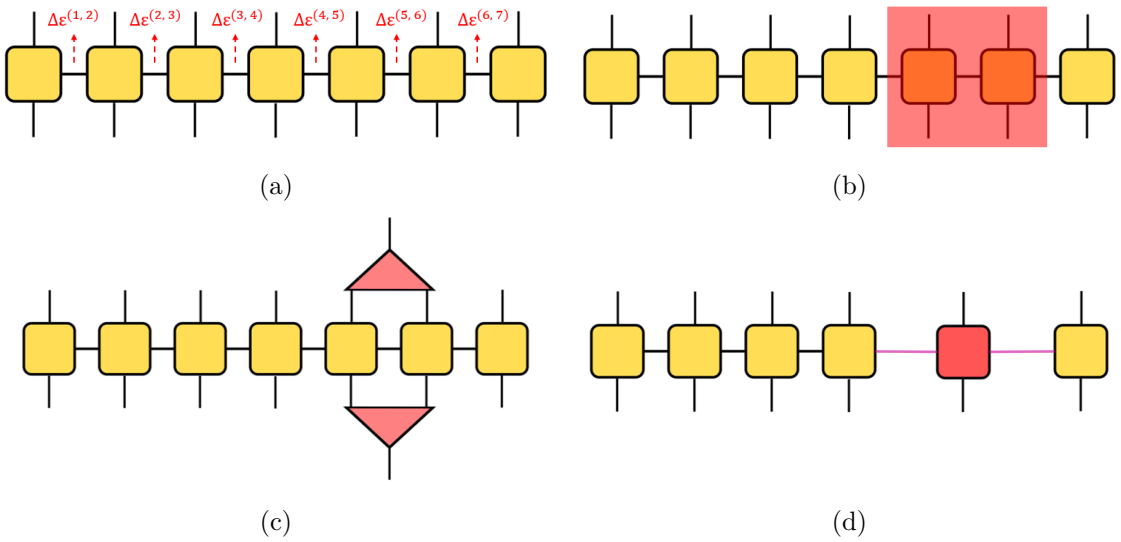


Figure 1.2: Schematic of the tree tensor network strong disorder renormalization group (a) The Hamiltonian is decomposed into MPO blocks (yellow squares). $\Delta\epsilon^{(i,j)}$ is the energy gap of local Hamiltonian. (b) The pair of nearest-neighbor MPO blocks (red-shaded square) with largest energy gap is chosen to merge. (c) Isometry tensors (red triangles) are built from χ^- lowest energy states to truncate the two MPO blocks between the two triangles. (d) Two MPO blocks are replaced with a new MPO (red square), and energy gaps of the nearest-neighbor blocks linked by the pink lines should be updated.

1.2 Tree tensor network strong disorder renormalization group

In this section, we describe the procedure of the tSDRG [1, 2]. The tSDRG procedure consists of iteratively locating a local Hamiltonian with the largest energy gap, and truncating its Hilbert space to the small subspace. Consider a spin chain of length L with two open ends. The basic steps of the tSDRG procedure are as follows:

(I) Decompose the Hamiltonian into MPO blocks $W^{[1]} \cdots W^{[L]}$.

See Section 2.2 and Figure 1.1. Here one block contains one site.

(II) Create a queue Q to store possible largest energy gaps $\Delta\epsilon^{(i,i+1)}$.

A local term in the original Hamiltonian takes the form of a two-spin Hamiltonian:

$$\hat{h}^{(i,i+1)} = J_i \vec{S}_i \cdot \vec{S}_{i+1} \,. \tag{1.6}$$

For such a two-spin local Hamiltonian, the energy eigenvalues $\epsilon^{i,i+1}$ are $-2J_i, -J_i$ and $+J_i$, corresponding to the singlet ground-state, the triplet state with $S_{\text{total}} = 1$ and the five-fold degenerate state with $S_{\text{total}} = 2$. For each $\hat{h}^{(i,i+1)}$, the largest gap is $\Delta\epsilon^{(i,i+1)} = 2J_i$. We create a queue $\mathbf{Q}$ that initially stores the set of $\Delta\epsilon^{(i,i+1)}$ for all i; that is

$$\begin{aligned}\mathbf{Q} &= [\Delta\epsilon^{(1,2)}, \Delta\epsilon^{(2,3)}, \cdots \Delta\epsilon^{(i,i+1)}, \cdots \Delta\epsilon^{(L-1,L)}] \\ &= [2J_1, 2J_2, \cdots 2J_i, \cdots 2J_{L-1}]\,.\end{aligned} \tag{1.7}$$

The gaps $\{\Delta\epsilon^{(i,i+1)}\}$ will be renormalized later under the action of the RG and the queue $\mathbf{Q}$ should be updated.

(III) Find the largest gap in max{Q}: $\Delta\epsilon_{\text{max}} \equiv \text{max}\{\mathbf{Q}\}$.

(IV) Diagonalize the local Hamiltonian $\hat{h}^{(i,i+1)}$ with the largest gap $\Delta\epsilon^{i,i+1} = \Delta\epsilon_{\text{max}}$

The local Hamiltonian $\hat{h}^{(i,i+1)}$ is encoded in the matrix element of $W^{[i]} \cdot W^{[i+1]}$ as highlighted in red in the following tensors:

$$W^{[1]} \cdot W^{[2]} = \begin{pmatrix} J_1\vec{S}_1 \cdot \vec{S}_2 & \mathbb{1} \otimes \frac{J_2}{2}\hat{S}_2^- & \mathbb{1} \otimes \frac{J_2}{2}\hat{S}_2^+ & \mathbb{1} \otimes J_2\hat{S}_2^z & \mathbb{1} \otimes \mathbb{1} \end{pmatrix}. \tag{1.8}$$

$$W^{[i]} \cdot W^{[i+1]} = \begin{pmatrix} \mathbb{1} \otimes \mathbb{1} & 0 & 0 & 0 & 0 \\ \hat{S}_i^+ \otimes \mathbb{1} & 0 & 0 & 0 & 0 \\ \hat{S}_i^- \otimes \mathbb{1} & 0 & 0 & 0 & 0 \\ \hat{S}_i^z \otimes \mathbb{1} & 0 & 0 & 0 & 0 \\ J_i\vec{S}_i \cdot \vec{S}_{i+1} & \mathbb{1} \otimes \frac{J_{i+1}}{2}\hat{S}_{i+1}^- & \mathbb{1} \otimes \frac{J_{i+1}}{2}\hat{S}_{i+1}^+ & \mathbb{1} \otimes J_{i+1}\hat{S}_{i+1}^z & \mathbb{1} \otimes \mathbb{1} \end{pmatrix}, \tag{1.9}$$

$$W^{[L-1]} \cdot W^{[L]} = \begin{pmatrix} \mathbb{1} \otimes \mathbb{1} \\ \hat{S}_{L-1}^+ \otimes \mathbb{1} \\ \hat{S}_{L-1}^- \otimes \mathbb{1} \\ \hat{S}_{L-1}^z \otimes \mathbb{1} \\ J_{L-1}\vec{S}_{L-1} \cdot \vec{S}_L \end{pmatrix}. \tag{1.10}$$

We perform an eigen-decomposition on $\hat{h}^{(i,i+1)}$:

$$\hat{h}^{(i,i+1)} = S\Lambda S^{-1}\,, \tag{1.11}$$

where Λ, S and S^{-1} are $n\times n$ matrices encoding the eigenvalues $\epsilon_n^{(i,i+1)}$ and the eigenvectors $|\Psi_n^{(i,i+1)}\rangle$ as follows:

$$S = \begin{pmatrix} |\Psi_0\rangle & |\Psi_1\rangle & \cdots & |\Psi_n\rangle \end{pmatrix}\,, \tag{1.12}$$

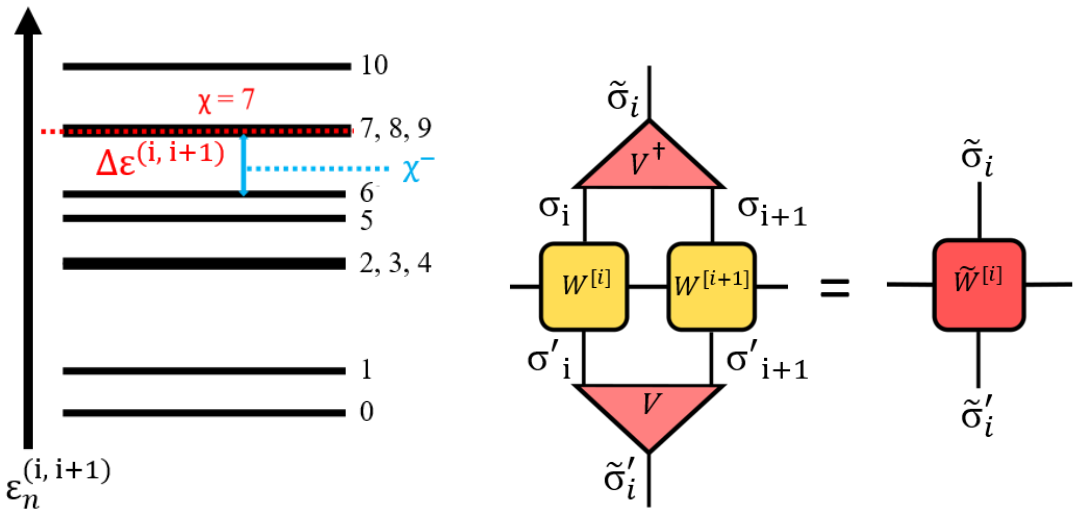
$$\Lambda = \begin{pmatrix} \epsilon_0 & 0 & \cdots & 0 \\ 0 & \epsilon_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \epsilon_n \end{pmatrix}\,, \tag{1.13}$$

$$S^{-1} = \begin{pmatrix} \langle\Psi_0| \\ \langle\Psi_1| \\ \vdots \\ \langle\Psi_n| \end{pmatrix}\,. \tag{1.14}$$

Here the superscripts $(i, i+1)$ are omitted in the matrix elements.

(V) Define the energy gap $\Delta\epsilon^{(i,i+1)}$ in the spectrum $\epsilon^{(i,i+1)}$ of the local Hamiltonian.

Here the energy gap $\Delta\epsilon^{(i,i+1)}$ is defined as the the difference between the highest energy of the χ^--lowest energy states that would be kept and the higher multiplets that would be discarded. An initial input parameter χ is given to control the number of local states to be kept. However, the actual number χ^- ($\leq \chi$) is chosen such that SU(2) symmetry is ensured (See Figure 1.3(a)).



(a) (b)

Figure 1.3: (a) Energy spectrum of a local Hamiltonian. In order to truncate the Hilbert space, we keep χ eigenstates; however the actual number χ^- of the kept state should be adjusted such that the kept states form full SU(2) multiplets. For example, if χ = 7 and the 7 lowest energy states break a full SU(2) multiplet, we should choose $\chi^- = 6$ where there is a gap to the multiplet which ensures the SU(2) symmetry. (b) Contraction of isometry tensors and MPO tensors.

(VI) Build a three-leg isometry tensor V using the χ^- lowest energy eigenstates.

The isometry tensor V and its adjoint $V^\dagger$ read:

$$V = \begin{pmatrix} |\Psi_0\rangle & |\Psi_1\rangle & \cdots & |\Psi_{\chi^-}\rangle \end{pmatrix} \tag{1.15}$$

$$V^\dagger = \begin{pmatrix} \langle\Psi_0| \\ \langle\Psi_1| \\ \vdots \\ \langle\Psi_{\chi^-}| \end{pmatrix} \tag{1.16}$$

where V is an $n \times \chi^-$ matrix and $V^\dagger$ is a $\chi^- \times n$ matrix. The isometric property satisfies that $V^\dagger V = \mathbb{1} \neq VV^\dagger$.

(VII) Renormalize the pair of blocks with the largest gap by contracting the two-block tensors with V and $V^\dagger$.

Here we perform

$$\tilde{W}^{\tilde{\sigma}_i,\tilde{\sigma}'_i}_{b_{i-1},b_{i+1}} = \sum_{\sigma_i,\sigma_{i+1}} \sum_{\sigma'_i,\sigma'_{i+1}} \sum_{b} [V^\dagger]^{\sigma_i,\sigma_{i+1}}_{\tilde{\sigma}_i} W^{\sigma_i,\sigma'_i}_{b_{i-1},b_i} W^{\sigma_{i+1},\sigma'_{i+1}}_{b_i,b_{i+1}} [V]^{\sigma'_i,\sigma'_{i+1}}_{\tilde{\sigma}'_i} \tag{1.17}$$

where $\tilde{\sigma}$ is truncated by χ^- (See Figure 1.2 (c) and Figure 1.3 (b)). We then replace the two-block MPO with the new MPO $\tilde{W}$.

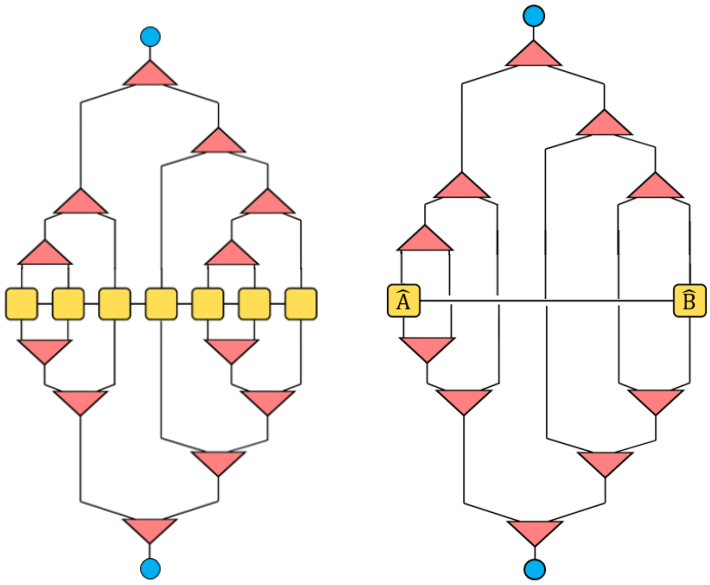
(VIII) Update the queue Q.

We remove the largest gap $\Delta\epsilon_{\max}$ from the queue $\mathbf{Q}$ and find the new gaps for the neighboring blocks to update $\mathbf{Q}$. For example, if $\Delta\epsilon_{\max} = \Delta\epsilon^{(i,i+1)}$, the queue $\mathbf{Q}$ will remove $\Delta\epsilon^{(i,i+1)}$ and become to $[\cdots, \Delta\tilde{\epsilon}^{(i-1,i)}, \Delta\tilde{\epsilon}^{(i+1,i+2)}, \cdots]$ where $\Delta\tilde{\epsilon}$ with the same trick as step (V).

(IX) Repeat steps (III) to (VIII) until there remains one single MPO block.

In the final MPO there is only one matrix element which represents the final local Hamiltonian $\hat{h}_f$.

Finally, we get a full tensor network with $\hat{h}_f$ as the top tensor (see Figure 1.4 (a)) for open boundary conditions. We can diagonalize the final local Hamiltonian $\hat{h}_f$ of top tensor to obtain the ground state energy. The expectation value of an observable $\hat{A}$ in the ground state can be obtained by replacing MPO block with operator $\hat{A}$ and contracting the tensor network (See Figure 1.4 (b)).



(a) (b)

Figure 1.4: (a) A tree tensor network constructed by isometry tensors and MPO blocks. (b) Part of the tree tensor network used to calculate the ground-state expectation value of $\hat{A}\cdots\hat{B}$; since $V^{\dagger}V = \mathbb{1}$, only those isometry tensors linking to the operators $\hat{A}$ and $\hat{B}$ are considered.

For periodic boundary conditions (PBC), all MPO blocks are $W^{[i]}$ as Eq. (1.4). In the final RG stage for a chain with PBC, there are two MPO blocks with two bonds between them, i.e. we have $W^{[i]} \cdot W^{[j]} + W^{[j]} \cdot W^{[i]}$. The final local Hamiltonian in this case is $\hat{h}_f = J_i\vec{S}_i \cdot \vec{S}_j + J_j\vec{S}_j \cdot \vec{S}_i$, where $J_{i(j)}$ and $\vec{S}_{i(j)}$ are renormalized couplings and spins.

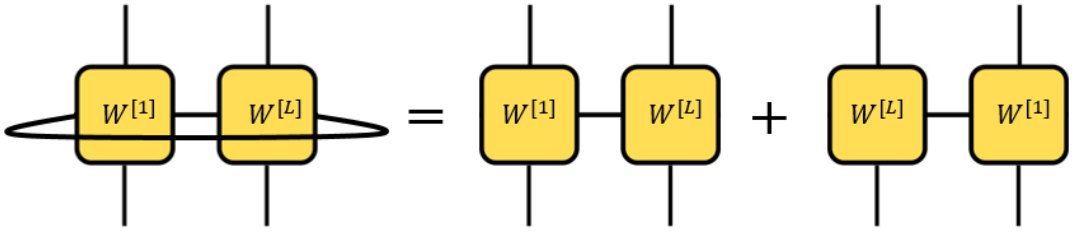


Figure 1.5: Illustration of tensor construction for periodic boundary condition.

In this work, we have largely reduced the time for code development and increased computational performance by using tensor operations from the Uni10 library [3]

Bibliographies

[1] T. Hikihara, A. Furusaki, and M. Sigrist, "Numerical renormalization-group study of spin correlations in one-dimensional random spin chains," *Phys. Rev. B*, vol. 60, pp. 12116–12124, Nov 1999.

[2] A. M. Goldsborough and R. A. Römer, "Self-assembling tensor networks and holography in disordered spin chains," *Phys. Rev. B*, vol. 89, p. 214203, Jun 2014.

[3] Y.-J. Kao, Y.-D. Hsieh, and P. Chen, "Uni10: an open-source library for tensor network algorithms," *Journal of Physics: Conference Series*, vol. 640, no. 1, p. 012040, 2015.