

V Entanglement and Matrix Product States

Overview : Area law

Efficient representation: MPS

Canonical form

Many body Hilbert space $\mathcal{H} = \mathbb{C}^{d^N}$ with local dimension d

$\rightsquigarrow S = \frac{i}{2} : |\uparrow\uparrow\uparrow\dots\uparrow\uparrow\rangle, |\downarrow\uparrow\uparrow\dots\uparrow\rangle \dots | \downarrow\downarrow\downarrow\dots\downarrow\downarrow\rangle$

$\rightsquigarrow 2^N$ states $|m_1 m_2 \dots m_N\rangle := |m_1\rangle \otimes |m_2\rangle \otimes \dots \otimes |m_N\rangle$, $m_j \in \{\uparrow, \downarrow\}$
↑ tensor product structure

Any state in the Hilbert space can be written as

$$|\Psi\rangle = \sum_{\{m_i\}} \Psi_{m_1 \dots m_N} |m_1 \dots m_N\rangle.$$

Entanglement (bipartite)

$$\begin{array}{ccc|cc} & A & & B & \\ 0 & 0 & 0 & | & 0 & 0 \end{array} \quad |\Psi\rangle \in \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

Assume that we only have access to A $M_A \otimes I$
How to characterize measurements?

$$\begin{aligned}
 \langle \Psi | M_A \otimes I | \Psi \rangle &= \sum_{i,j} \langle \psi_{ij}^* | \psi_{ij} \rangle \langle i | j | M_A | i \rangle \\
 \text{pure state} \quad &= \sum_{i,j} \langle \psi_{ij}^* | \psi_{ij} \rangle \langle i | M_A | i \rangle \underbrace{\langle j | j \rangle}_{S_{jj}} \\
 &= \sum_{i,j} \langle \psi_{ij}^* | \psi_{ij} \rangle \langle i | M_A | i \rangle \delta_{jj} \\
 &= \text{Tr}(M_A S_A),
 \end{aligned}$$

with $\text{Tr}_X(\cdot) = \sum \langle k| \cdot |k\rangle_X$ and $S_A = \sum \Psi_{ij}^* \Psi_{ij} |i\rangle\langle i|_A$
 reduced density operator / matrix $\rightarrow = \text{Tr}_B \underbrace{(\Psi)}_S (\Psi)$

From the def. we find

- (1) $S_A = S_A^+$
- (2) $S_A \geq 0$
- (3) $\text{Tr}(S_A) = 1$

(von-Neumann) entanglement entropy $S = -\text{Tr}_A S_A \cdot \log S_A$

Entangled state has mixed S_A, S_B (i.e., $S \neq 0$)

$$|\Psi\rangle = \frac{1}{\sqrt{2!}} (|ud\rangle + |du\rangle), \quad |\Psi\rangle = \frac{1}{\sqrt{2}} [|uu\rangle + |ud\rangle + |du\rangle + |dd\rangle] \\ = \frac{1}{\sqrt{2}} [|u\rangle + |d\rangle] \otimes [|u\rangle + |d\rangle]$$

Schmidt decomposition: $\hat{\equiv}$ SVD

$$|\Psi\rangle = \sum_{\alpha=1}^{\min(N_A, N_B)} \lambda_\alpha \underbrace{|\phi_\alpha\rangle_A}_{\text{Schmidt values}} \underbrace{|\phi_\alpha\rangle_B}_{\text{Schmidt states}}, \quad \lambda_1 \geq \lambda_2 \geq \dots \geq 0$$

$$\langle \phi_\alpha | \phi_{\alpha'} \rangle = \delta_{\alpha\alpha'} \quad (\text{unique up to degeneracies})$$

$$S_A = \sum \lambda_\alpha^2 |\phi_\alpha\rangle_A \langle \phi_\alpha|, \quad S_B = \sum \lambda_\alpha^2 |\phi_\alpha\rangle_B \langle \phi_\alpha|$$

and thus $S = -\sum \lambda_\alpha^2 \cdot \log \lambda_\alpha^2$. (Normalization: $\sum \lambda_\alpha^2 = 1$)

Entanglement spectrum $\{2 \cdot \ln \lambda_\alpha\}$ (eigenvalues of H_{ent} with $S_A = e^{-H_{\text{ent}}}$)

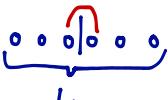
Examples: * Product state $\Rightarrow \lambda_1=1, \lambda_{i>1}=0$ and $S=0$
 $\begin{array}{cccccc} & & & & & \\ & 0 & 0 & 0 & | & 0 & 0 \end{array}$

* Maximally entangled state $\Rightarrow \lambda_1=\dots=\lambda_N=\frac{1}{\sqrt{N}}$ and $S=\log N$
 $\text{# of states in the subsystems} \stackrel{?}{=} \sum_{d=1}^N \frac{1}{\sqrt{N}} |dd\rangle \langle dd|$  $S=\frac{1}{2}, N=2^{L/2} \Rightarrow S=\frac{L}{2} \cdot \log 2$

* Random state: Entanglement close to S_{\max} [Page]
 $L = \frac{d}{2} + \frac{L}{2}$ $[S = \frac{L}{2} \log d - \frac{1}{2}]$

Area law

Ground states of (gapped) local Hamiltonians
 fulfill the area law $S \sim L^{D-1}$ [proof exists for 1D, Hastings]

1D  $S(L)=\text{const. } (L > \xi)$
 (gapless $S \sim \log L$) 

Ground states are "close" to product states \Rightarrow efficient representation

Matrix product states

Product state: $\Psi_{i_1 \dots i_L} = \phi^{[1]i_1} \dots \phi^{[L]i_L}, \phi^{[n]i_n} \in \mathbb{C}$

Matrix-product state: $\Psi_{i_1 \dots i_L} = A^{[1]i_1} \dots A^{[L]i_L}, A^{[n]i_n}$ are matrices (MPS)

Convert a generic quantum state to an MPS:

Start with Schmidt decomposition

$$|\Psi\rangle = \sum_{d_1=1}^d \Lambda_{d_1} |d_1\rangle_{[1]} |d_1\rangle_{[2 \dots N]}$$

Now define $A_{d_1}^{[1]j_1} = \langle j_1 | d_1 \rangle_{[1]}$:

$$|\Psi\rangle = \sum_{j_1=1}^d \sum_{d_1=1}^d A_{d_1}^{[1]j_1} \Lambda_{d_1}^{[1]} |j_1\rangle |d_1\rangle_{[2 \dots N]}$$

Next decompose at the second bond:

$$|\Psi\rangle = \sum_{d_2=1}^d \Lambda_{d_2}^{[2]} |d_2\rangle_{[1,2]} |d_2\rangle_{[3 \dots N]}$$

Define $A_{d_1 d_2}^{[2]j_2} = [\langle d_1 |_{[1]} \langle j_2 |] |d_2\rangle_{[1,2]}$

$$|\Psi\rangle = \sum_{d_1=1}^d \sum_{d_2=1}^d \sum_{j_1, j_2=1}^d A_{d_1}^{[1]j_1} A_{d_1 d_2}^{[2]j_2} \Lambda_{d_2}^{[2]} |j_1 j_2\rangle |d_2\rangle_{[3 \dots N]}$$

Continue the procedure until reaching the right end of the chain.

Caveat: Bond X_n increases exponentially!

Area law states have only a small number ($\ll d'$) of significant Schmidt values \rightsquigarrow Discard small ones and compress the state!

Examples

GHZ : $|\Psi\rangle = \frac{1}{\sqrt{2}} (|111111\rangle + |000000\rangle)$ has MPS has $\chi=2$

MPS representation $A^{\dagger} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$, $A^{\dagger} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$

AKLT : S=1 spin chain with $H = \sum P_{j,j+1}^{S=2} = \sum \vec{S}_j \vec{S}_{j+1} + \frac{1}{3} (S_j S_{j+1})^2 + \frac{2}{3}$

$$|\Psi_0\rangle : \text{magnetons } \circlearrowleft \text{magnetons } \circlearrowleft$$

$S=1 \quad \frac{1}{\sqrt{2}} (|1\downarrow\rangle - |1\uparrow\rangle)$

$$\odot : |+\rangle = |\uparrow\uparrow\rangle, |0\rangle = \frac{1}{\sqrt{2}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), |- \rangle = |\downarrow\downarrow\rangle$$

The MPS representation is then

$$A^{\dagger} = \sqrt{\frac{2}{3}} G^+, \quad A^0 = -\frac{1}{\sqrt{3}} G^z, \quad A^- = -\sqrt{\frac{2}{3}} G^-.$$

MPS as variational wavefunction (DMRG) : Optimize the energy
within the space of
Tensor network notation MPS with bond dim. χ

Useful diagrammatic representation of tensor networks :

Scalar $a \equiv O$, vector $a_i \equiv O$, matrix $a_{ij} \equiv O$

tensor operations : $c_{ik} = \sum_j a_{ij} b_{jk} \rightsquigarrow \begin{matrix} O \\ a \\ b \end{matrix} = \begin{matrix} O \\ a \\ b \end{matrix}$

Matrix product :

$$\text{cylinder} \approx \text{row} \times \text{column}, \quad \begin{matrix} A \\ j \end{matrix} \times \begin{matrix} A \\ i \end{matrix}$$

Overlap :

$$\langle \Psi | \phi \rangle = \begin{matrix} A & A & A & A & A \\ B^* & B^* & B^* & B^* & B^* \end{matrix}$$

Expectation value :

$$\langle \Psi | \phi | \Psi \rangle = \begin{matrix} A & A & A & A & A \\ A^* & A^* & A^* & A^* & A^* \end{matrix}$$

Some details on computing expectation values

$$|\psi\rangle = \begin{array}{c} \textcircled{1} \\ \textcircled{2} \\ \textcircled{3} \\ \textcircled{4} \end{array} \quad \langle\psi| = \begin{array}{c} \textcircled{1} \\ \textcircled{2} \\ \textcircled{3} \\ \textcircled{4} \end{array} \quad \hat{O} = \boxed{\textcircled{1}}$$
$$\langle\psi|\hat{O}|\psi\rangle = \begin{array}{c} \textcircled{1} \\ \textcircled{2} \\ \textcircled{3} \\ \textcircled{4} \end{array} \quad \begin{array}{c} \textbf{A} & \textbf{A} & \textbf{A} & \textbf{A} & \textbf{A} \\ \hline \textbf{A}^* & \textbf{A}^* & \textbf{A}^* & \textbf{A}^* & \textbf{A}^* \end{array}$$

How can we efficiently compute the expectation value?

Naive way: 1) contract tensor $\textcircled{1} \dots \textcircled{4} = \textcircled{1} \dots \textcircled{4}$

2) Compute expectation value:

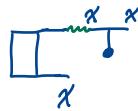


~ scales as $\exp(L)$

Smart way: Utilize MPS structure

$$[\square] \rightarrow [\square\square] \rightarrow [\square\square\square] \rightarrow [\square\square\square\square] \text{ etc.}$$

~ scales as $L \cdot X^3$



Canonical form of MPS

From now on: $A^{\text{canon}} = A^{\text{in}}$ and $L \rightarrow \infty$ / Pure states

MPS are not uniquely defined: $\begin{array}{c} A \\ \bullet \end{array} \rightarrow \begin{array}{c} X A X^{-1} \\ \bullet \end{array}$ represents same state

Bonds are directly related to the Schmidt decomposition
and $A = \Gamma \cdot \Lambda \quad (\Lambda_{d1} = \lambda_1) \quad [\text{Vidal}]$

orthonormal basis

$$|\Psi\rangle = \sum_{\lambda} |\lambda\rangle_L \lambda_d |\lambda\rangle_R$$

$$\dots \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \Gamma \dots = \sum_{\lambda} \dots \Gamma \Lambda \Gamma_{d_L} \lambda_d \Gamma_{d_R} \Gamma \dots$$

Transfer matrix

$$\Sigma_{dd'} = \langle d | d' \rangle_R = \left(\begin{array}{cccc} \Gamma \Lambda & \Gamma \Lambda & \Gamma \Lambda & \dots \\ \Gamma \Lambda & \Gamma \Lambda & \Gamma \Lambda & \dots \\ \Gamma \Lambda & \Gamma \Lambda & \Gamma \Lambda & \dots \end{array} \right) \rightsquigarrow \begin{array}{c} \Gamma \Lambda \\ \Gamma \Lambda \\ \Gamma \Lambda \end{array} \Rightarrow \Pi$$

[similar for the left]

$$\rightsquigarrow \begin{array}{c} \Lambda \Gamma \\ \Lambda \Gamma \\ \Lambda \Gamma \end{array} = \Pi \quad ($$

\Leftrightarrow Transfermatrices have left/right eigenvalue λ with eigenvector Π

Uniquely defines the MPS up to a $U(1)$ phase and $d\lambda$ in λ_d .

- Convenient to evaluate expectation values:

$$\langle \Psi | O_i | \Psi \rangle = \langle \begin{array}{c} \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \\ \bullet \\ \bullet \\ \bullet \\ \Gamma \Lambda \Gamma \Lambda \Gamma \Lambda \end{array} \rangle = \lambda^2 \left(\begin{array}{c} \Gamma \\ \bullet \\ \bullet \\ \bullet \\ \Gamma \end{array} \right) \lambda^2$$

MPS based algorithms

We know how to efficiently represent 1D ground states and can calculate expectation values.

Given a Hamiltonian H , how to obtain the ground state MPS? Time evolution?

- (1) Use ED plus successive SVD \rightsquigarrow Exponentially hard
- (2) Non-linear optimization $E_0 = \min_{\{\mathcal{B}_{AB}^S\}} \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$ \rightsquigarrow Unstable
- (3) Iterative methods: TEBD + DMRG

Time evolving block decimation (TEBD)

Real and imaginary time evolution of MPS

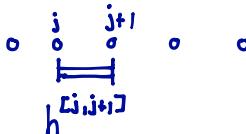
Time evolution in real time:

$$|\Psi(t)\rangle = e^{-iHt} |\Psi(t=0)\rangle$$

Time evolution in imaginary time yields GS:

$$|\Psi_0\rangle = \lim_{\tau \rightarrow \infty} \frac{e^{-H\tau} |\Psi_i\rangle}{\|e^{-H\tau} |\Psi_i\rangle\|}$$

Assume the Hamiltonian has the form $H = \sum h^{[j,j+1]}$



Decompose the Hamiltonian $H = F + G$

$$F = \sum_{\text{even } j} h^{[j,j+1]}, \quad G = \sum_{\text{odd } j} h^{[j,j+1]}$$

We observe: $[F^i, F^k] = [G^i, G^k] = 0$
 $[G, F] \neq 0$



Baker-Campbell-Hausdorff $[e^{\epsilon A} \cdot e^{\epsilon B} = e^{\epsilon(A+B) + \frac{\epsilon^2}{2}[A,B]} + \dots]$

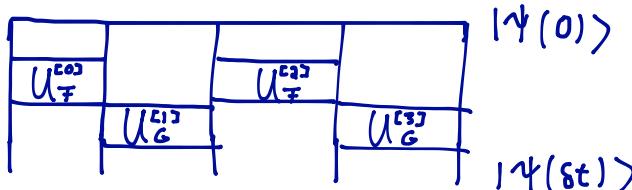
Decompose time evolution $\exp(-iHt) = [\underbrace{\exp(-iH\frac{t}{N})}_{{= \delta t}}]^N$

$$e^{-ist(F+G)} = \underbrace{e^{-istF}}_{U_F} \cdot \underbrace{e^{-istG}}_{U_G} + O(st^2)$$

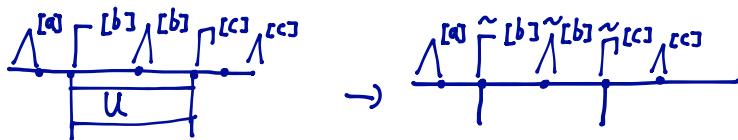
Two chains of two-site gates

$$U_F = \prod_{\text{even } j} e^{-iF^{[j,j+1]}st}, \quad U_G = \prod_{\text{odd } j} e^{-iG^{[j,j+1]}st}$$

Back to MPS:



Need an algorithm to project back to MPS form



TEBD algorithm [Vidal]

$$|\Psi\rangle = \sum_{mn\lambda\gamma} \Theta_{\lambda\gamma}^{mn} |d\rangle |m\rangle |n\rangle |\gamma\rangle$$

① "Apply U"

$$\begin{array}{ccc} \text{d} & \xrightarrow{\text{U}} & \text{d} \\ \text{---} & & \text{---} \\ \text{m} & & \text{n} \end{array} = \frac{\dim X}{\text{d}} \begin{array}{ccccccccc} \text{d} & \xrightarrow{\text{a}} & \text{b} & \xrightarrow{\text{b}} & \text{c} & \xrightarrow{\text{c}} & \text{d} \\ \text{---} & & \text{---} & & \text{---} & & \text{---} \\ \text{m} & & \text{n} & & \text{d} & & \text{d} \end{array} \frac{\dim X}{\text{d}}$$

$$|\Psi\rangle = \sum \Theta_{\lambda\gamma}^{mn} |d\rangle |m\rangle |n\rangle |\gamma\rangle \quad \begin{array}{c} |d\rangle \quad |m\rangle \quad |n\rangle \quad |\gamma\rangle \\ \boxed{0} \quad \boxed{0} \quad \boxed{0} \quad \boxed{0} \end{array}$$

$$\tilde{\Theta} = \frac{\Theta}{R} \quad [\tilde{\Theta}_{\lambda\gamma}^{mn} = U_{m'n'}^{mn} \Theta_{\lambda\gamma}^{m'n'}]$$

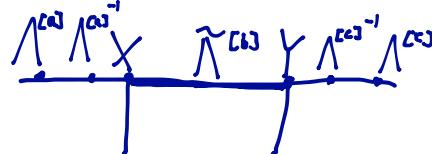
② "SVD" ($dX \times dX$ matrix)

$$\tilde{\Theta} = X \tilde{\Lambda} Y$$

$$\begin{array}{c} |\beta\rangle_L \quad \tilde{\Lambda}_\beta \quad |\beta\rangle_R \\ \boxed{0} \quad \boxed{0} \quad \boxed{0} \end{array}$$

$$[\tilde{\Theta}_{(d,m)(n\gamma)} = \sum_{\beta=1}^{dn} X_{(d,m),\beta} \tilde{\Lambda}_\beta Y_{\beta,(n\gamma)}]$$

③ „Obtain new MPS“



↙ insert identity

$$\Rightarrow \frac{\tilde{\Gamma}^{[c_1]}}{\Gamma} = \frac{(\Lambda^{[c_1]})^{-1} X}{\Gamma}, \quad \frac{\tilde{\Gamma}^{[c_2]}}{\Gamma} = \frac{Y (\Lambda^{[c_2]})^{-1}}{\Gamma}, \quad \frac{\tilde{\Gamma}^{[c_3]}}{\Gamma}$$

④ „Truncate“

Discard smallest Schmidt values/states: $dX \rightarrow X$
(i.e., keep only X rows/columns of the tensors)

Applying this algorithm iteratively to even/odd bonds,
we obtain the time evolution!

Computational time scales as $O(L \cdot d^3 X^3)$

- Computational errors:
- * truncation error: exponential growth of X when doing real time evolution
 - * Trotter error (relatively harmless): Smaller δt and higher order expansions
 - * instabilities for small Λ_S (as we need to invert it): fix by [Hastings '09]
 - * Canonical form for imaginary time evolution only when $\delta t \rightarrow 0$.

Recap MPS

$$|\Psi\rangle = \sum_{\{j_k=1\}}^d \langle j_1 \dots j_N | j_1 \dots j_N \rangle \\ = \sum A_{d_1}^{j_1} A_{d_1 d_2}^{j_2} \dots A_{d_{N-1} d_N}^{j_N} | j_1 \dots j_N \rangle$$

$$= \begin{array}{c} \square - \square - \square - \dots - \square \\ | \quad | \quad | \quad | \\ j_1 \quad j_2 \quad j_3 \quad \dots \quad j_N \end{array}$$

- An MPS with max bond dim. χ has $d^{\chi^2 \cdot N}$ variational parameters.

- The full Hilbert space has d^L states

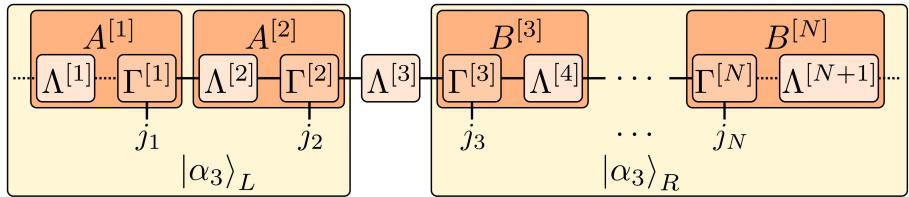
We have introduced the canonical form

$$\dots - \boxed{\Lambda^{[1]}} - \boxed{\Gamma^{[1]}} - \boxed{\Lambda^{[2]}} - \boxed{\Gamma^{[2]}} - \boxed{\Lambda^{[3]}} - \boxed{\Gamma^{[3]}} - \dots - \boxed{\Lambda^{[N]}} - \boxed{\Gamma^{[N]}} - \dots - \boxed{\Lambda^{[N+1]}} - \dots$$

$j_1 \quad j_2 \quad j_3 \quad \dots \quad j_N$

$\boxed{\Lambda^{[i]}}$... diagonal matrices containing Schmidt values

We can group them to a left (L) and right (R) canonical form:



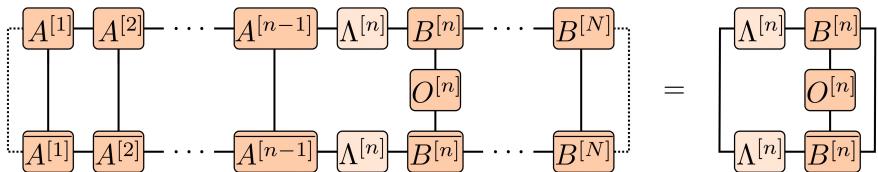
Here

$$\begin{array}{c} A^{[n]} \\ \downarrow \\ \bar{A}^{[n]} \end{array} - \frac{\omega^{n+1}}{\omega^{-n+1}} = \begin{bmatrix} \omega^{n+1} \\ \omega^{-n+1} \end{bmatrix} \quad \text{"left canonical form"}$$

and

$$\begin{array}{c} B^{[n]} \\ \downarrow \\ \bar{B}^{[n]} \end{array} = \quad \begin{bmatrix} & \\ & \end{bmatrix} \quad \text{"right canonical form"}$$

This is useful for evaluating expectation values:



Matrix product operators (MPO)

We can also represent operators in terms of matrix products:

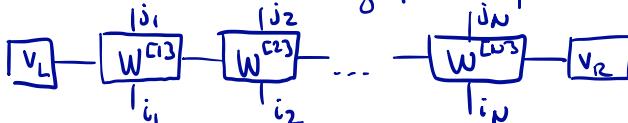
$$\hat{O} = \sum_{\substack{i_1, \dots, i_N \\ j_1, \dots, j_N}} v_L W^{[1]}{}_{i_1 j_1} W^{[2]}{}_{i_2 j_2} \dots W^{[N]}{}_{i_N j_N} v_R \quad (i_1, \dots, i_N \times j_1, \dots, j_N)$$

$W^{[n]}{}_{i_n j_n}$ are $D \times D$ matrices

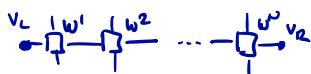
$|i_n\rangle, |j_n\rangle$ represent local basis states at site n .

v_L, v_R auxiliary vectors introduced to make the expression in the sum a scalar.

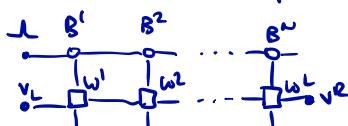
We can also write down a graphical representation of the MPO



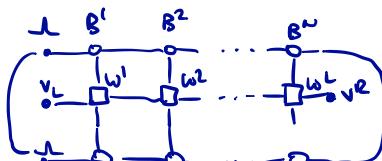
In short:



The MPO can be multiplied on an MPS



Computation of expectation values:



In order to search for a ground state using DMRG, we represent the Hamiltonian in terms of an MPO.

For systems with short ranged interactions, we can directly construct the MPO.

Let's take the Heisenberg model as an example:

$$\hat{H} = J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z) + \sum_i h_i S_i^z,$$

where h_i is a random on-site field.

Expressed as a tensor product \hat{A} reads:

$$\begin{aligned} \hat{H} = & J(S^x \otimes S^x \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} + \mathbb{1} \otimes S^x \otimes S^x \otimes \dots \otimes \mathbb{1} + \dots \\ & S^y \otimes S^y \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} + \dots + \\ & \Delta S^z \otimes S^z \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} + \dots) + \\ & h_1 S^z \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} + h_2 \mathbb{1} \otimes S^z \otimes \mathbb{1} \dots \end{aligned}$$

Such a tensorial structure can be obtained by identifying

$$W^{[n]} = \begin{pmatrix} \mathbb{1} & S^x & S^y & S^z & h_n S^z \\ 0 & 0 & 0 & 0 & JS^x \\ 0 & 0 & 0 & 0 & JS^y \\ 0 & 0 & 0 & 0 & J\Delta S^z \\ 0 & 0 & 0 & 0 & \mathbb{1} \end{pmatrix}$$

i.e. the MPO dimension $D=5$. Moreover we set $v_L = (1 \ 0 \ 0 \dots)$ and $v_R = (0 \ 0 \ \dots \ 1)^T$.

This construction works similarly for other MPO's with short ranged couplings.

Density Matrix Renormalization Group (DMRG)

DMRG is a variational principle, unlike TEBD, yet in terms of procedural steps both algorithms have similarities. One advantage of DMRG is that it does not rely on a Suzuki-Trotter decomposition. Therefore systems with longer-range couplings can be treated. For small gaps in particular, DMRG is also much faster than TEBD.

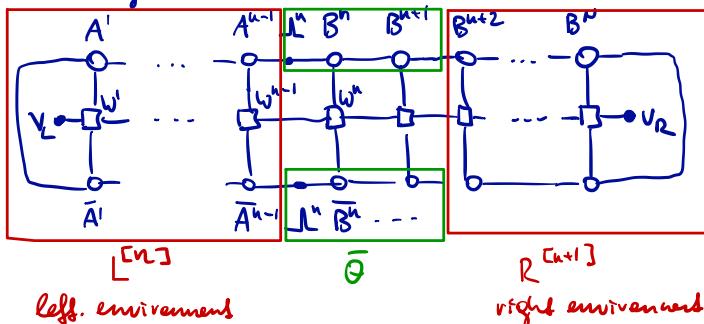
Principle idea:

Variationally optimize the tensors of two neighboring sites (say n and $n+1$), while keeping the rest of the system fixed, to minimize the ground state energy $\langle \Psi | H | \Psi \rangle$.

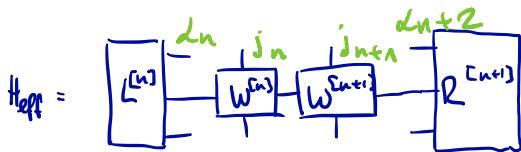
As in TEBD, we introduce the two site tensor $\Theta_{\downarrow n \downarrow n+1}^{j_n j_{n+1}}$, then we project the Hamiltonian into the basis set spanned by $|L\rangle |j_n\rangle |j_{n+1}\rangle |R\rangle$. Then we need to optimize this two site tensor by finding its ground state energy using e.g. the Lanczos algorithm.

Iteratively proceed with that by traversing the chain from left to right and back again. This is called swap.

Graphically:



We can now introduce the effective two-site Hamiltonian that we are optimizing:



Two site update:

Goal: find new tensors $\tilde{A}^{[n]}, \tilde{J}^{[n+1]}, \tilde{B}^{[n+1]}$ while keeping the others fixed.

Approach: 1) Contract tensors to obtain $\Theta_{d_n d_{n+2}}^{j_n j_{\text{int}}}$

$$\Rightarrow \text{Kontaktional Space: } |\tilde{\Psi}\rangle = \sum_{\substack{d_n j_n \\ j_{\text{int}} d_{n+2}}} \Theta_{d_n d_{n+2}}^{j_n j_{\text{int}}} |d_n j_n j_{\text{int}}, d_{n+2}\rangle$$

2) optimize energy:

$$E = \langle \tilde{\Psi} | H^{\text{eff}} | \tilde{\Psi} \rangle$$

to obtain new optimized $\tilde{\Theta}$.

\Rightarrow dimension of H^{eff} is $d^2 X^2 \times d^2 X^2$, which can get very big (i.e. $d=2$ for spin $X=1000 \Rightarrow 4 \cdot 10^6$ matrix dimension). Thus we use decores.

2) Update:

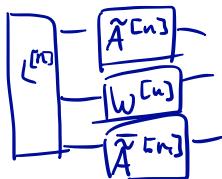
Split new $\tilde{\Theta}$ using SVD to obtain

$$\tilde{\Theta} \rightarrow \tilde{A}^{[n]} \tilde{\lambda}^{[n+1]} \tilde{B}^{[n+1]}$$

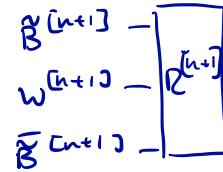
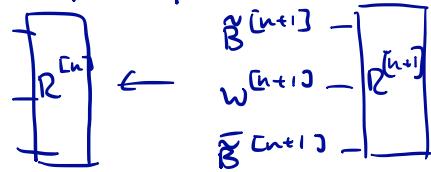
and truncate.

3) Move to the next band. Update $L^{[n+1]}$ and $R^{[n+2]}$ and start again with step 1).

Right sweep



Left sweep.



4) Make so many sweeps such that $-E^{st+1} + E^s < \epsilon$ ($\epsilon \approx 10^{-10}$) \Rightarrow within the bond dimension X we then have the optimal representation of the wave function.

$$\text{The starting environments } L_{d_1, d_1, g_1}^{[1]} = \delta_{d_1, d_1} v_{g_1}^L$$

$$R_{d_{N+1}, d_{N+1}, g_{N+1}}^{[N]} = \delta_{d_{N+1}, d_{N+1}} v_{g_{N+1}}^R$$

From that we can iteratively build the environment.