V Tensor network methods

So far, we only considered exact representations of states in the many-body Hilbert space, facing us with an exponential increase in computational complexity with the number of degrees of freedom.

Now we explore approximate representations of states $|\psi\rangle \in \mathcal{H}_L$ such that for a set of parameters $\underline{t} = (t_1, t_2, \dots, t_p)$ with $p \in \mathbb{N}$, the approximation $|\hat{\psi}(\underline{t})\rangle$ is optimal in the sense:

For a given approx. quality $\varepsilon > 0$ there exist $p \in \mathbb{N}$ with $p \sim \mathcal{O}(L^\alpha)$ for some $\alpha \in \mathbb{N}$ such that

$$\underline{t} \in V_{\mathbb{K}}^{p} \Rightarrow \text{dist}\left(|\psi\rangle, |\tilde{\psi}(\underline{t})\rangle\right) < \varepsilon$$

Questions:

(i) How do optimal parametrizations $|\tilde{\psi}(\underline{t})\rangle$ look like for which choices of $\text{dist}(x, y)$?

(ii) What do exponents α look like?

(iii) Classification of states with respect to α?

(iv) Can we construct algorithms to solve eigenvalue problem in manifold of parametrizations $|\hat{\psi}(\underline{t})\rangle$?

Consider the state $|\psi\rangle \in \mathcal{H}_2$ with $\alpha \in [0, \frac{\pi}{2})$:

$$|\psi\rangle = \cos(\alpha)\,|\uparrow\downarrow\rangle + \sin(\alpha)\,|\downarrow\uparrow\rangle$$

$$\equiv \sum_{\sigma_1\sigma_2} \psi_{\sigma_1,\sigma_2}\, |\sigma_1,\sigma_2\rangle \qquad \text{with } \sigma_{1/2} \in \{\uparrow,\downarrow\}$$

Let us interpret $\psi_{\sigma_1\sigma_2}$ as matrix :

$$\underline{\underline{\psi}} = \begin{array}{ccc} & \sigma_2 & \begin{array}{cc} \quad\uparrow & \qquad\downarrow \end{array} \\ \sigma_1 & \begin{array}{c} \uparrow \\ \downarrow \end{array} & \begin{pmatrix} 0 & \cos(\alpha) \\ \sin(\alpha) & 0 \end{pmatrix} \end{array}$$

$$\overset{\text{SVD}}{=} \begin{array}{cc} \sigma_1 & \\ \begin{array}{c} \uparrow \\ \downarrow \end{array} & \underbrace{\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}_{\underline{\underline{U}} = \begin{pmatrix} -\underline{u}_1^t- \\ -\underline{u}_2^t- \end{pmatrix}} \end{array} \underbrace{\begin{pmatrix} \cos(\alpha) & 0 \\ 0 & \sin(\alpha) \end{pmatrix}}_{\underline{\underline{S}} = \begin{pmatrix} s_1 & 0 \\ 0 & s_2 \end{pmatrix}} \begin{array}{c} \begin{array}{ccc} \uparrow & \downarrow & \sigma_2 \end{array} \\ \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{\begin{pmatrix} | & | \\ \underline{v}_1 & \underline{v}_2 \\ | & | \end{pmatrix} = \underline{\underline{V}}} \end{array}$$

This suggests to write the matrix element $\psi_{\sigma_1\sigma_2}$:

$$\psi_{\uparrow\uparrow} = \underline{u}_1^t\, \underline{\underline{S}}\, \underline{v}_1 \ ; \ \psi_{\uparrow\downarrow} = \underline{u}_1^t\, \underline{\underline{S}}\, \underline{v}_2 \ ; \ \psi_{\downarrow\uparrow} = \underline{u}_2^t\, \underline{\underline{S}}\, \underline{v}_1 \ ; \ \psi_{\downarrow\downarrow} = \underline{u}_2^t\, \underline{\underline{S}}\, \underline{v}_2$$

or for the state $|\psi\rangle$:

$$|\psi\rangle = \sum_{\sigma_1=1}^{2} \sum_{\sigma_2=1}^{2} \underline{u}^{t}_{\sigma_1} \underline{\underline{S}} \, \underline{v}_{\sigma_2} \; |\sigma_1 \, \sigma_2\rangle$$

Note :

(i) From $\underline{\underline{U}}^{\dagger} \underline{\underline{U}} = \mathbb{1}_{2\times 2}$ & $\underline{\underline{V}} \, \underline{\underline{V}}^{\dagger} = \mathbb{1}_{2\times 2}$ we can connect $\underline{\underline{S}}$ to the eigenvalues of the reduced density matrices:

$$\hat{\rho}_{<2} = \mathrm{Tr}_{\sigma_2} |\psi\rangle\langle\psi|$$

$$= \sum_{\sigma_2=1}^{2} \langle\sigma_2| \sum_{\substack{\sigma_1' \\ \sigma_1''}} \sum_{\substack{\sigma_2' \\ \sigma_2'}} \underline{u}^{t}_{\sigma_1'} \underline{\underline{S}} \, \underline{v}_{\sigma_2'} |\sigma_1' \sigma_2'\rangle\langle\sigma_1'' \sigma_2''| \underline{v}^{t}_{\sigma_2''} \underline{\underline{S}} \, \underline{u}_{\sigma_1''} |\sigma_2\rangle$$

$$= \sum_{\sigma_1' \sigma_1''} \underline{u}^{t}_{\sigma_1'} \underline{\underline{S}} \underbrace{\sum_{\sigma_2} \underline{v}_{\sigma_2} \underline{v}^{t}_{\sigma_2}}_{\mathbb{1}_{2\times 2}} \underline{\underline{S}} \, \underline{u}_{\sigma_1''} \; |\sigma_1'\rangle\langle\sigma_1''|$$

$$= \sum_{\sigma_1' \sigma_1''} \underline{u}^{t}_{\sigma_1'} \underline{\underline{S}}^{2} \underline{u}_{\sigma_1''} \; |\sigma_1'\rangle\langle\sigma_1''| \qquad (*)$$

$$\equiv \sum_{m=1}^{2} |u_m\rangle \, s_m \, \langle u_m|$$

with $|u_m\rangle = \sum_{\sigma_1} \underline{u}^{t}_{\sigma_1} \; |\sigma_1\rangle$

analogue:

$$\hat{\rho}_{1>} = \mathrm{Tr}_{\sigma_1} |\Psi\rangle\langle\Psi| = \sum_{m=1}^{2} |v_m\rangle S_m \langle v_m|$$

(∗) is eigenvalue decomposition of $\hat{\rho}_{<2}$ ($\hat{\rho}_{1>}$)

(ii) From $\underline{\underline{U}}^{\dagger}\underline{\underline{U}} = \mathbb{1}_{2\times2}$ & $\underline{\underline{V}}\,\underline{\underline{V}}^{\dagger} = \mathbb{1}_{2\times2}$ it also follows that

$$|\Psi\rangle = \sum_{m=1}^{2} S_m |u_m\rangle |v_m\rangle$$

is the Schmidt decomposition of $|\Psi\rangle$

(iii) If we sort S_m such that $S_1 > S_2$ & neglect S_2, then the approx. $|\tilde{\Psi}\rangle = S_1 |u_1\rangle |v_1\rangle$ is the best rank-1 approx. to $|\Psi\rangle$ w.r.t. $\|\cdot\|_2$ norm of the distance of the reduced density matrices:

$$\|\hat{\rho}_{<2} - \hat{\tilde{\rho}}_{<2}\|_2 = \mathrm{Tr}\left((\hat{\rho}_{<2} - \hat{\rho}_{<2})^2\right)$$

$$= \mathrm{Tr}\left(\left(\sum_{m=1}^{2} S_m |u_m\rangle\langle u_m| - S_1 |u_1\rangle\langle u_1|\right)^2\right)$$

$$= \mathrm{Tr}\left(S_2^2 |u_2\rangle\langle u_2| \right) = S_2^2$$

& analogue: $\|\hat{\rho}_{1>} - \hat{\tilde{\rho}}_{>1}\|_2 = \mathrm{Tr}\left(\left(\sum_{m=1}^{2} S_m |v_m\rangle\langle v_m| - S_1 |v_1\rangle\langle v_1|\right)^2\right)$

$$= S_2^2$$

This motivates us to introduce "local" representations of wavefunction coefficients, i.e., tensor networks!

V.1 Matrix-product states / Tensor trains

From the previous considerations, we define a matrix product state (MPS) by decomposing the coefficients $\psi_{\sigma_1 \sigma_2 \dots \sigma_L}$ of a state $|\psi\rangle \in \mathcal{H}_L$ in the many-body Hilbert space $\mathcal{H}_L = \mathcal{H}_{d_1} \otimes \dots \otimes \mathcal{H}_{d_L}$ describing $L \in \mathbb{N}$ degrees of freedom with local dimensions $d_j \in \mathbb{N}$ as:

$$\psi_{\sigma_1 \dots \sigma_L} = \underline{M}^{\sigma_1} \underline{\underline{M}}^{\sigma_2} \dots \underline{\underline{M}}^{\sigma_{L-1}} \underline{M}^{\sigma_L} \in \mathbb{K}$$

where $\underline{\underline{M}}^{\sigma_j} \in V_{\mathbb{K}}^{m_{j-1} \times m_j}$ are matrices for $j \in \{2, \dots, L-1\}$ & $\underline{M}^{\sigma_1} \in V_{\mathbb{K}}^{1 \times m_1}$, $\underline{M}^{\sigma_L} \in V_{\mathbb{K}}^{m_L \times 1}$ are row / column vectors.

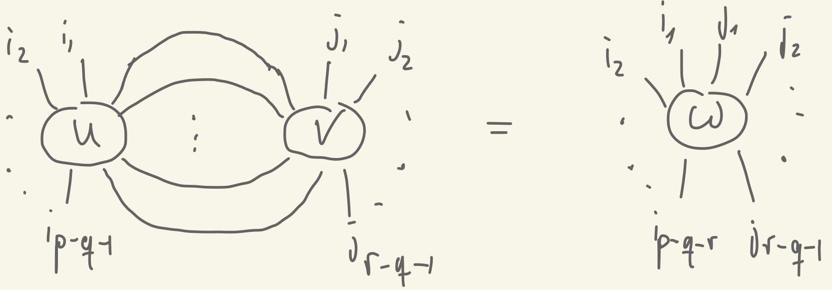
We call $m_j \in \mathbb{N}$ the bond dimension of the MPS, which specify the number of parameters used to represent

$$|\psi\rangle = \sum_{\sigma_1=1}^{d_1} \cdots \sum_{\sigma_L=1}^{d_L} \underline{\underline{M}}^{\sigma_1} \underline{\underline{M}}^{\sigma_2} \cdots \underline{\underline{M}}^{\sigma_{L-1}} \underline{\underline{M}}^{\sigma_L} |\sigma_1 \dots \sigma_L\rangle .$$

Tensor network notation

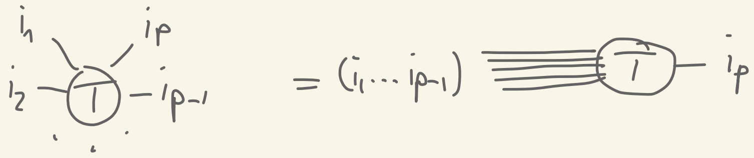
Let $T_{i_1 \dots i_p}$ be a rank-p tensor with dimensions $d_1, \dots, d_p \in \mathbb{N}$. We denote $T_{i_1 \dots i_p}$ graphically:

Contractions over a set of q shared indices of two tensors $U_{i_1 \dots i_{p-q-1} n_1 \dots n_q}$, $V_{j_1 \dots j_{r-q-1} n_1 \dots n_q}$ are represented graphically as:



$$w^{i_1\cdots i_{p-q-1}}_{j_1\cdots j_{r-q-1}} = \sum_{n_1\cdots n_q} U^{i_1\cdots i_{p-q-1}}_{n_1\cdots n_q} V^{n_1\cdots n_q}_{j_1\cdots j_{r-q-1}}$$

Fusions are defined as grouping & merging of indices:



$$T_{i_1\cdots i_{p-1} i_p} = T_{(i_1\cdots i_{p-1}) i_p}$$

Splits are the inverse operations to fusions.

Let us use that graphical notation to represent the MPS decomposition:

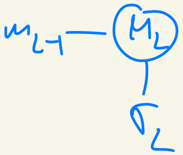
$$|\psi\rangle = \sum_{\sigma_1}\cdots\sum_{\sigma_L} \underline{M}^{\sigma_1}\, \underline{\underline{M}}^{\sigma_2} \cdots \underline{\underline{M}}^{\sigma_{L-1}}\, \underline{M}^{\sigma_L} |\sigma_1 \ldots \sigma_L\rangle$$

identify: $\underline{M}^{\sigma_1} \to$

a rank-2 tensor

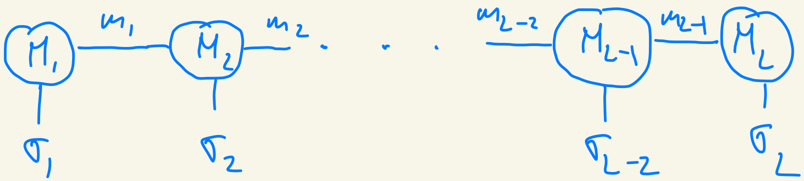
$\underline{\underline{M}}^{\sigma_j}$ $(1<j<L)$ $\to$

a rank-3 tensor

$\underline{M}^{\sigma_L} \rightarrow$ 

a rank-2 tensor

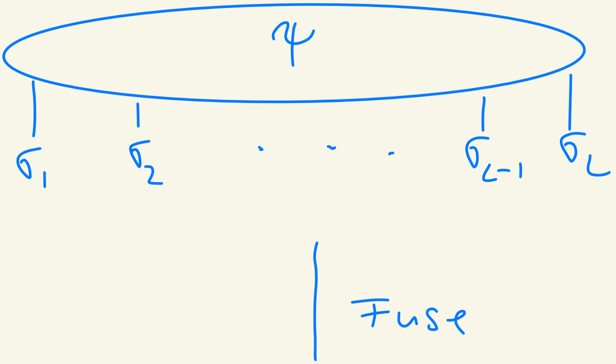
So that each coefficient $\Psi_{\sigma_1 \ldots \sigma_L}$ is given by the network of contracted tensors:

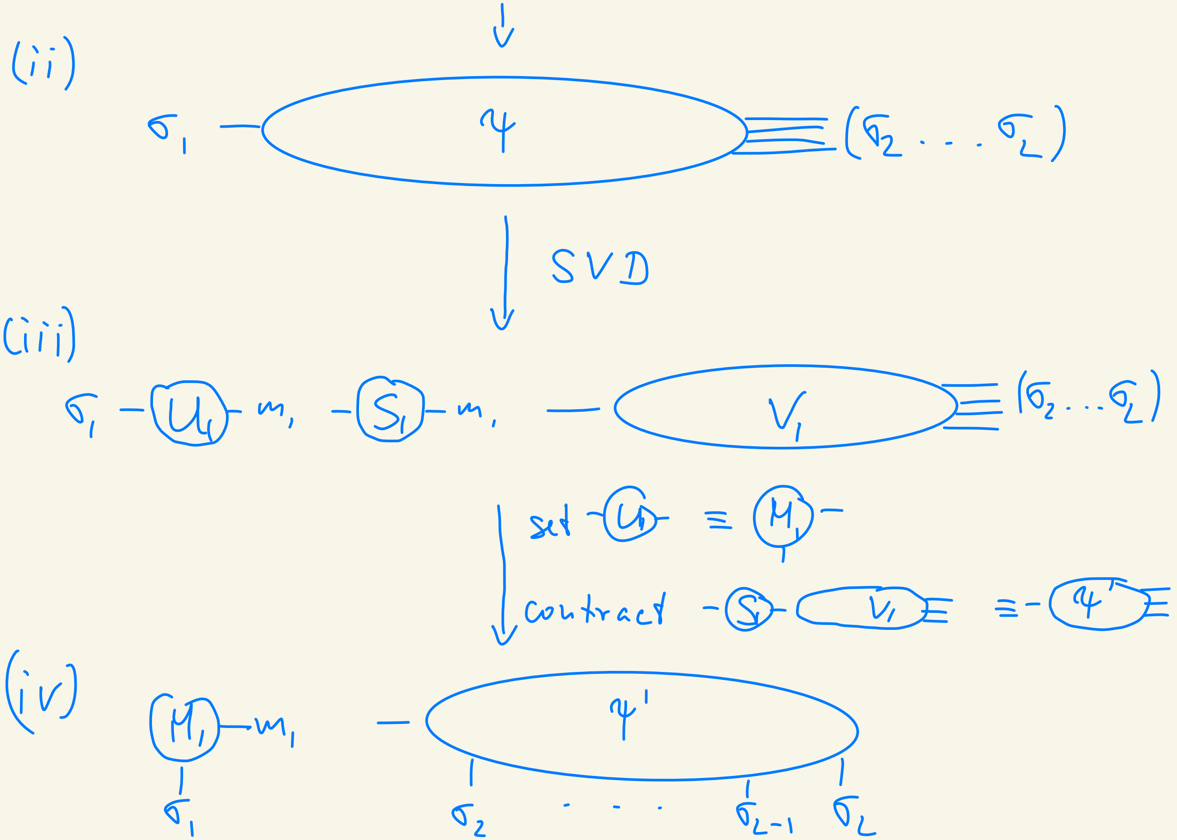


Can we always find an MPS representation for any $|\Psi\rangle \in \mathcal{H}_L$?

Yes, if we apply the decomposition scheme introduced at the example of $|\Psi\rangle = \cos(\alpha)|\uparrow\downarrow\rangle + \sin(\alpha)|\downarrow\uparrow\rangle$:

(i)





& repeat from (i) until all local degrees of freedom σ_j are factored out.

Observations:

(i) at j'th iteration, the number m_j of non-vanishing singular values $s_{j,n}$, $n \in \{1, \dots, m_j\}$ determines the bond-dimensions m_j

(ii) Let $m \equiv \max_{j \in \{1,..,L\}} m_j$ & $d = \max_{j \in \{1,..,L\}} d_j$, then

the number of coefficients per site tensor is bounded by dm^2. Thus in total the number of coefficients is bounded by:

$$2dm + \sum_{j=2}^{L-1} d_j m^2 \sim \mathcal{O}(L d m^2)$$

(iii) In each bipartition, the approximation $|\tilde{\Psi}\rangle$ with max. bond dimension $m_0 \leq m$ yields the best approx. of the reduced density matrix w.r.t. $\|\cdot\|_2$ - norm.

Mixed-canonical form & gauge fixing

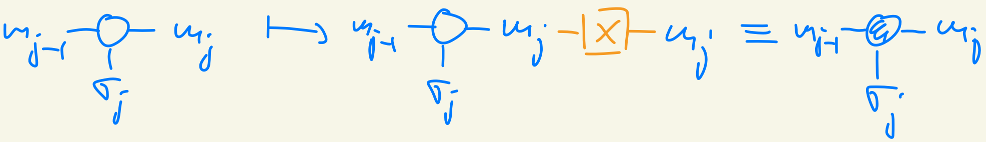
We consider a general MPS representation of a state $|\psi\rangle \in \mathcal{H}_L$ in the computational basis $\{|\sigma_1 \dots \sigma_L\rangle\}$ where σ_j's are labeling the local basis states, i.e., $\sigma_j \in \{0, \dots, d_j - 1\}$ with local dimensions $d_j \in \mathbb{N}$ for $j \in \{1, \dots, L\}$:

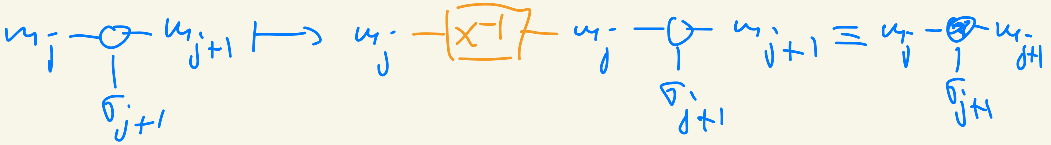
$$|\psi\rangle = \sum_{\sigma_1} \cdots \sum_{\sigma_L} \underbrace{\underline{M}^{\sigma_1} \underline{\underline{M}}^{\sigma_2} \cdots \underline{\underline{M}}^{\sigma_{L-1}} \underline{M}^{\sigma_L}}_{\psi_{\sigma_1 \dots \sigma_L} \in \mathbb{K}} |\sigma_1 \dots \sigma_L\rangle$$

with $\underline{\underline{M}}^{\sigma_j} \in \mathbb{V}_{\mathbb{K}}^{m_{j-1} \times m_j}$ matrices (or vectors at the edges).

The coefficient tensor $\psi_{\sigma_1 \dots \sigma_L}$ is invariant under gauge transformations of the form:

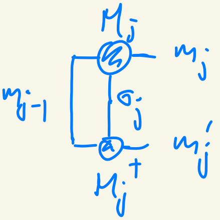
For $\underline{\underline{X}} \in \mathbb{V}_{\mathbb{K}}^{m_j \times m_j}$ an invertible matrix, the MPS is invariant under the joint trafo:





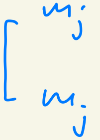
This means that MPS representations are not unique! We can fix the gauge degrees of freedom by fixing the gauge transformations:

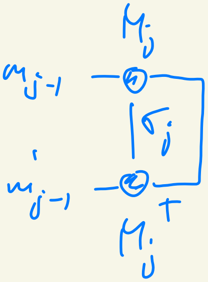
(i) left canonical gauge:



$$= \sum_{m_{j-1}} \sum_{\sigma_j} \left(M^{\sigma_j}_{m_{j-1},m_j'}\right)^\dagger M^{\sigma_j}_{m_{j-1},m_j} \overset{!}{=} \delta_{m_j,m_j'}$$

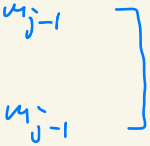
$\equiv$



(ii) 

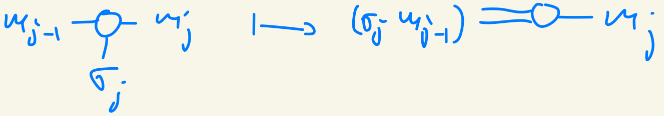
$$= \sum_{m_j} \sum_{\sigma_j} M^{\sigma_j}_{m_{j-1},m_j} \left(M^{\sigma_j}_{m_{j-1}',m_j}\right)^\dagger \overset{!}{=} \delta_{m_{j-1},m_{j-1}'}$$

$\equiv$

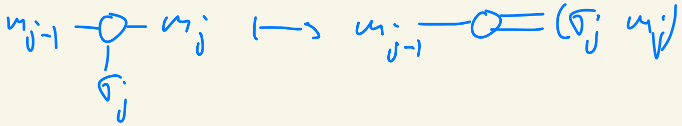


Defining:

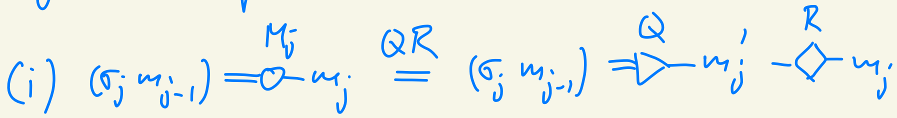
(a) Left fusion: $M^{\sigma_j}_{m_{j-1}\, m_j} \mapsto M_{(\sigma_j m_{j-1})\, m_j}$



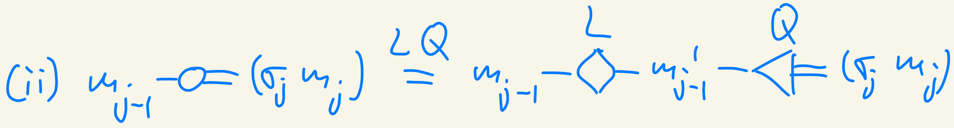
(b) Right fusion: $M^{\sigma_j}_{m_{j-1}\, m_j} \mapsto M_{m_{j-1}\, (\sigma_j m_j)}$



The gauge conditions (i)/(ii) can be satisfied by choosing $\underline{\underline{X}}$ as:



$\Rightarrow \underline{\underline{X}} = \underline{\underline{R}}^{-1}$ which always exists because $\underline{\underline{R}}$ is upper triangular



$\Rightarrow \underline{\underline{X}} = \underline{\underline{L}}^{-1}$ which always exists because $\underline{\underline{R}}$ is upper triangular

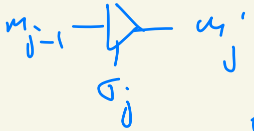
Consequences:

1) The gauge transformations taking M_j to the left-/right-canonical form are unique, because QR(LQ)-decomposition is unique

2) For each M_j there is a unique gauge-trafo $\underline{\underline{X}}$ so that all gauge degrees of freedom of the MPS-representation can be fixed demanding all site-tensors to be either left- or right-canonical!

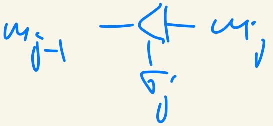
3) Replacing QR(LQ)-decomposition with the SVD, we immediately can read of $\underline{\underline{R}}^{-1}/\underline{\underline{L}}^{-1}$.

Notational agreement:

(i) Left-canonical site-tensors are represented by triangles pointing to the right: 

& denoted by $A^{\sigma_j}_{m_{j-1}\, m_j}$

(ii) Right-canonical site-tensors are represented by triangles pointing to the left:

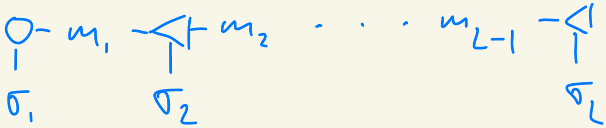


& denoted by $B^{\sigma_j}_{m_{j-1}\, m_j}$

A MPS of the form:

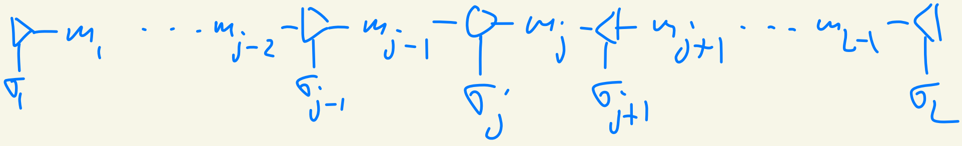
is called left-canonical

A MPS of the form:



is called right-canonical

A MPS of the form:

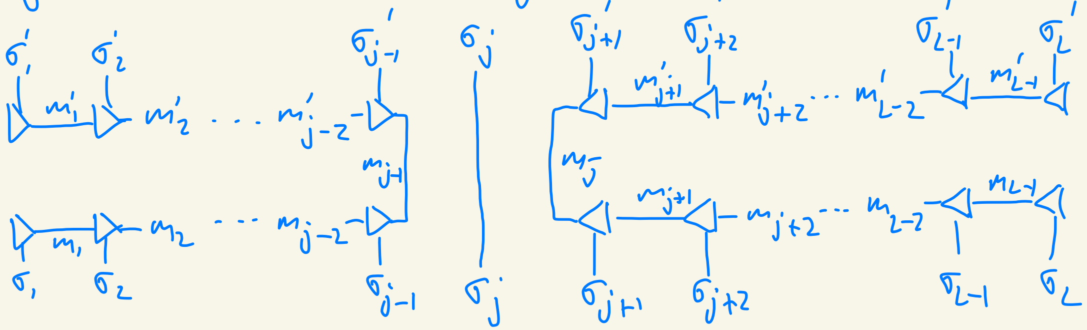


is called mixed-canonical with orthogonality center at site j.

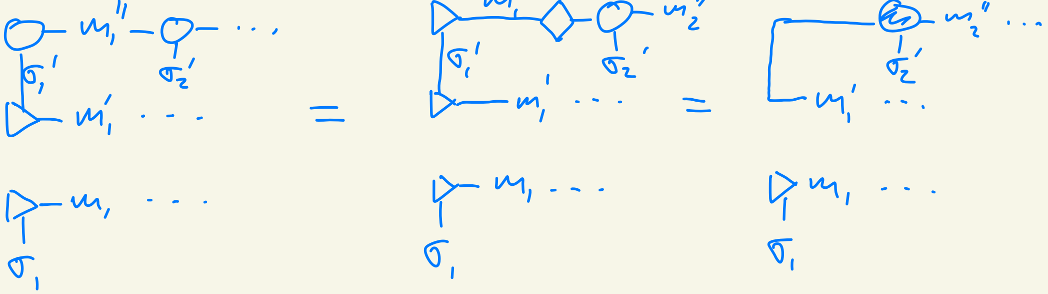
The gauge fixing projector

To formulate MPS-algorithms, it is convenient, to introduce the gauge fixing projector $\hat{\Pi}_j$.

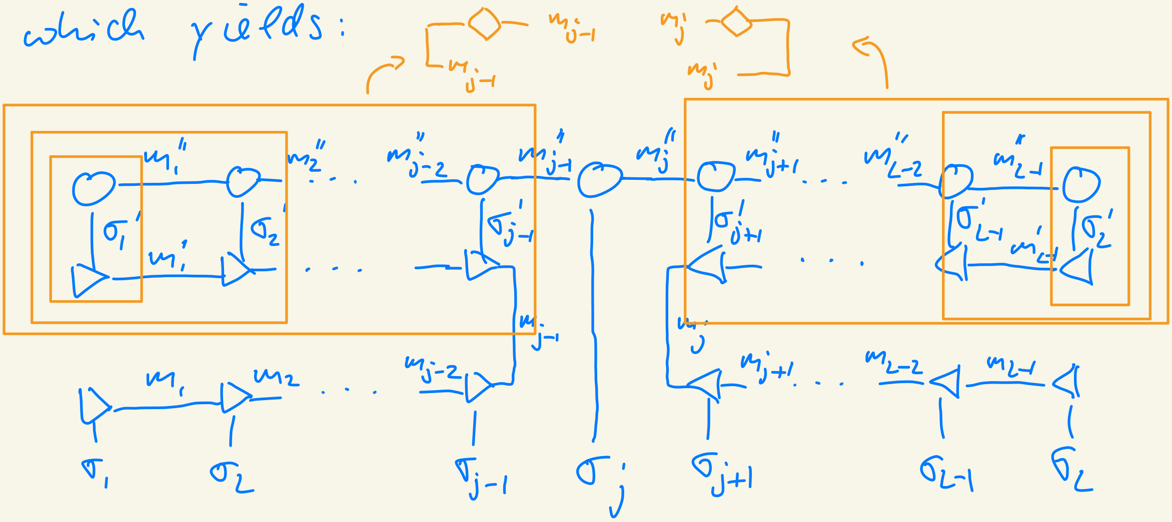
$\hat{\Pi}_j$ can be defined by :

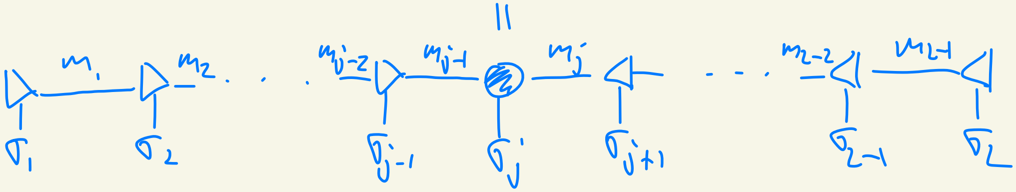


If $\hat{\Pi}_j$ acts on $|\Psi\rangle$, then we can use the gauge-trafo to show:



which yields:





It is also easy to see that $\hat{\Pi}_j^2 = \hat{\Pi}_j$.

Thus, $\hat{\Pi}_j$ is the unique operator, which transforms the MPS representation of $|\Psi\rangle$ into the mixed-canonical representation with orthogonality center at site "j".

Variational compression

Assume $|\psi\rangle$ is given as MPS with bond dimensions $m_1 \dots m_{L-1}$. We want to approximate $|\psi\rangle$ by a state $|\hat{\psi}\rangle$ with max. bond dimension $\tilde{m}$ by minimizing the distance:

$$\mathrm{dist}(|\psi\rangle, |\hat{\psi}\rangle) = \| |\psi\rangle - |\hat{\psi}\rangle \|^2$$

$$= \langle\psi|\psi\rangle + \langle\hat{\psi}|\tilde{\psi}\rangle - \langle\psi|\tilde{\psi}\rangle - \langle\tilde{\psi}|\psi\rangle$$

We minimize $\mathrm{dist}(|\psi\rangle, |\tilde{\psi}\rangle)$ by searching the stationary point w.r.t. to <u>all</u> coefficients $\tilde{M}^{\sigma_j}_{\tilde{a}_{j-1}\tilde{a}_j}$ of the guess state $\langle\tilde{\psi}|$:

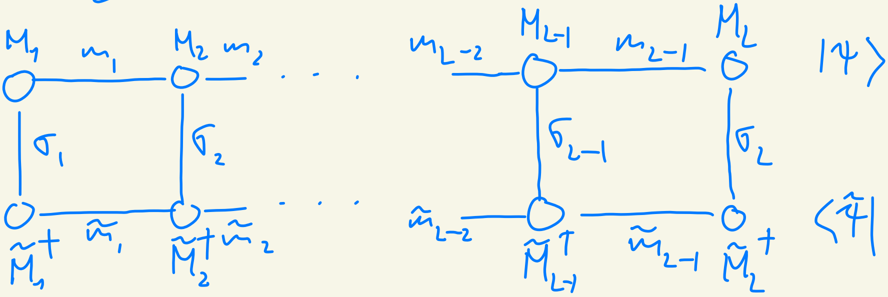
$$\langle\tilde{\psi}| \equiv \langle\tilde{\psi}(\tilde{M}^{\sigma_1 *}_{\tilde{m}_1}, \tilde{M}^{\sigma_2 *}_{\tilde{m}_1\tilde{m}_2}, \dots, \tilde{M}^{\sigma_L *}_{\tilde{m}_{L-1}})|$$

$$\Rightarrow 0 = \left(\frac{\partial}{\partial \tilde{M}^{\sigma_1}_{\tilde{m}_1}{}^*} + \frac{\partial}{\partial \tilde{M}^{\sigma_2}_{\tilde{m}_1\tilde{m}_2}{}^*} + \dots + \frac{\partial}{\partial \tilde{M}^{\sigma_L}_{\tilde{m}_{L-1}}{}^*}\right)\left(\langle\tilde{\psi}|\tilde{\psi}\rangle - \langle\tilde{\psi}|\psi\rangle\right)$$

The scalar products are evaluated by contracting a tensor-network:

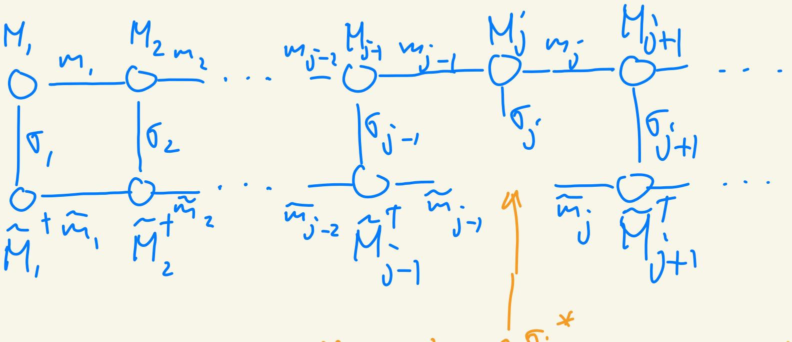
$$\langle \tilde{\Psi} | \Psi \rangle = \sum_{\sigma_1} \cdots \sum_{\sigma_L} \left(\underline{\tilde{M}}^{\sigma_L}\right)^\dagger \left(\underline{\underline{\tilde{M}}}^{\sigma_{L-1}}\right)^\dagger \cdots \left(\underline{\tilde{M}}^{\sigma_1}\right)^\dagger \underline{M}^{\sigma_1} \cdots \underline{\underline{M}}^{\sigma_{L-1}} \underline{M}^{\sigma_L}$$

$=$



Now each derivative "erases" the coefficients $\tilde{M}^{\sigma_j *}_{\tilde{m}_{j-1},\tilde{m}_j}$ if acts on:

$$\frac{\partial}{\partial \tilde{M}^{\sigma_j}_{\tilde{m}_{j-1}\tilde{m}_j}} \langle \tilde{\Psi} | \Psi \rangle =$$

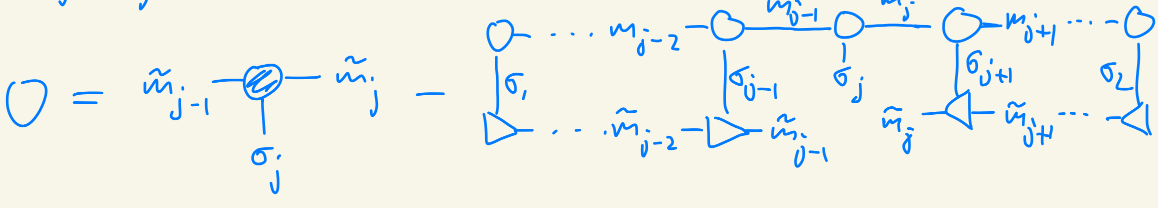


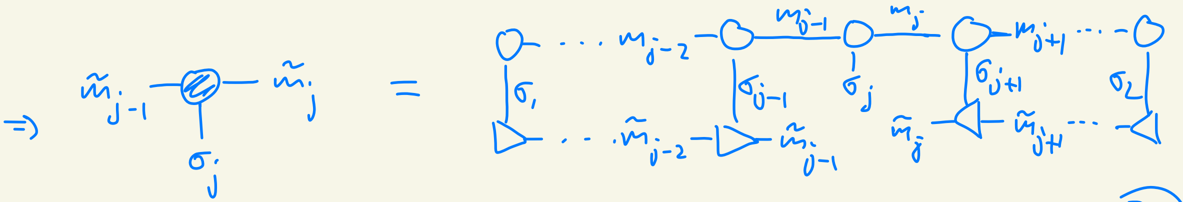
coefficients $\tilde{M}^{\sigma_j *}_{\tilde{m}_{j-1}\tilde{m}_j}$ removed from derivative!

However, solving the optimization problem for *all* derivatives is still hopeless. But we can use the fact $|\tilde{\psi}\rangle = \hat{\Pi}_j |\tilde{\psi}\rangle$ where now $\hat{\Pi}_j$ is created from the gauge-fixed tensors of $|\tilde{\psi}\rangle$. We then solve for each $j \in \{1, \dots, L\}$:

$$\frac{\partial}{\partial \tilde{M}^{\sigma_k}_{\tilde{m}_{k-1}\tilde{m}_k}} \left(\langle \tilde{\psi} | \hat{\Pi}_j | \tilde{\psi} \rangle - \langle \tilde{\psi} | \hat{\Pi}_j | \psi \rangle \right) = 0$$

Therefore, we can use the mixed-canonical representation & only solve for one set of coefficients $\tilde{M}^{\sigma_j}_{\tilde{m}_{j-1}\tilde{m}_j}$:





The left-hand side is an optimized site-tensor of the approx. $|\tilde{\Psi}\rangle$ & the right-hand side the contractions we have to perform to obtain this optimized tensor. Note that if we sweep from left to right & vice versa, we can obtain optimized tensors, reusing previous contractions of the right side.

Variational ground-state search

We apply the variational principle to find optimal approx. to the solution of the minimization problem:

$$|\tilde{\Psi}_0\rangle = \underset{|\psi\rangle \in \mathcal{M}(\underline{m})}{\text{argmin}} \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}$$

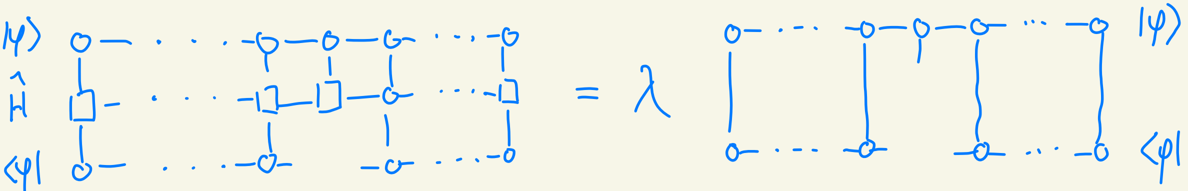
where $\mathcal{M}(\underline{m})$ is the manifold of MPS with bond dimensions $\underline{m} = (m_1, m_2, \dots, m_{L-1})$. Introducing a Lagrange-multiplier $\lambda \in \mathbb{R}$, the minimization is equivalent to solve

$$\frac{\partial}{\partial \bar{M}^{\sigma_j}_{m_{j-1}, m_j}} \left(\langle \psi | \hat{H} | \psi \rangle - \lambda \langle \psi | \psi \rangle \right) \overset{!}{=} 0$$

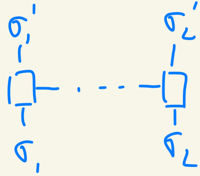
for all coefficients $\bar{M}^{\sigma_j}_{m_{j-1} m_j}$ of the bra:

$$\langle \psi | = \sum_{\sigma_1 \dots \sigma_L} \underline{\bar{M}}^{\sigma_1} \underline{\underline{\bar{M}}}^{\sigma_2} \cdots \underline{\bar{M}}^{\sigma_{L-1}} \langle \sigma_1 \dots \sigma_L | .$$

we obtain L coupled equations (for each site):



where

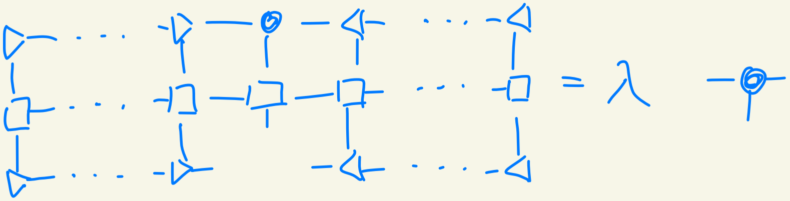


$$= \sum_{\sigma_1 \dots \sigma_L} \sum_{\sigma_1' \dots \sigma_L'} \underline{W}^{\sigma_1 \sigma_1'} \underline{\underline{W}}^{\sigma_2 \sigma_2'} \cdots \underline{W}^{\sigma_L \sigma_L'} |\sigma_1 \dots \sigma_L\rangle\langle\sigma_1' \dots \sigma_L'|$$

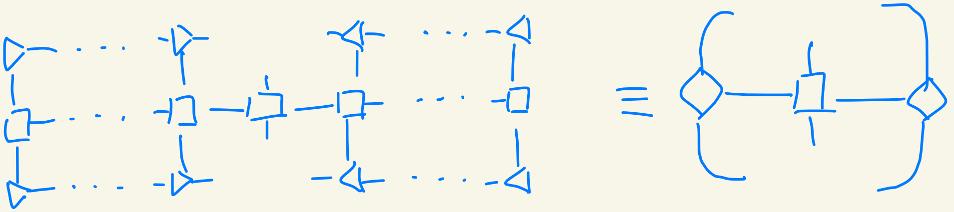
is the representation of $\hat{H}$ as matrix-product operator.

Again, we use the mixed-canonical

representation to decouple the set of equations:

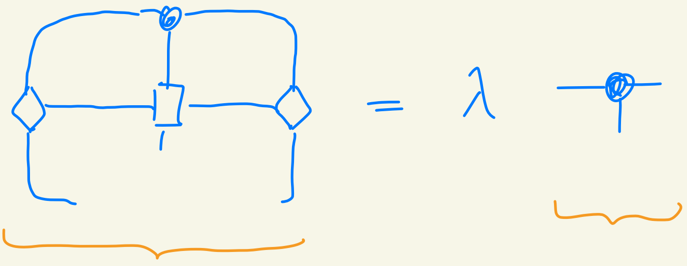


We treat the network:

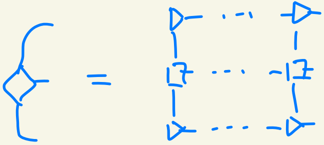


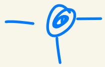
$\equiv \hat{H}^{\mathrm{eff}}_j$

as operator acting on . Then we have to solve the local eigenvalue problems:



$\hat{H}^{\mathrm{eff}}_j \, |\varphi_j\rangle$ $\qquad$ $|\varphi_j\rangle$

Note:  can be constructed iteratively when sweeping through the system!

Here, a Lanczos algorithm seems to be the method of choice to find the eigentensor  $\equiv |\psi_j\rangle$ & eigenvalue λ yielding an approx. to the overall ground state.

Note:

- Computing $\hat{H}_j^{\text{eff}} |\psi_j\rangle$ is numerical most expensive operation $\sim \mathcal{O}(m^3 d^2 w^2)$ where $w \hat{=}$ MPO-bond dimension

- Convergence locally is exponentially fast in the gap of the local Hamiltonian $\hat{H}_j^{\text{eff}}$

- Global convergence in principle also exponential, but: only in the manifold $\mathcal{M}(\underline{m})$!

- Global optimization no longer convex

because of $\hat{H}$ ⇒ Can get stuck in local minima

- Carefull choice of initial guess $|\psi\rangle$ & 2-site updates or algorithms to increase bond-dims $\underline{m}$ are crucial!

MPO - construction (the tale of FSMs)

How do we obtain MPO-representation of $\hat{H}$?

Let us look as an example at the transverse field Ising model with $L=2$ sites:

$$\hat{H} = \hat{S}^z_1 \hat{S}^z_2 - g\hat{S}^x_1 - g\hat{S}^x_2$$

$$= \hat{S}^z \otimes \hat{S}^z + (-g\hat{S}^x) \otimes \hat{\mathbb{1}} + \hat{\mathbb{1}} \otimes (-g\hat{S}^x)$$

$$= \begin{pmatrix} \mathbb{1} & \hat{S}^z & -g\hat{S}^x \end{pmatrix} \begin{pmatrix} -g\hat{S}^x \\ \hat{S}^z \\ \mathbb{1} \end{pmatrix}$$

General idea: Introduce bipartition at site j

$$\hat{H} = \sum_j \hat{S}^z_j \hat{S}^z_{j+1} - g \sum_j \hat{S}^x$$

$$= \sum_{\ell<j} \hat{S}^z_\ell \hat{S}^z_{\ell+1} + \sum_{\ell<j} (-g \hat{S}^x_\ell)$$

$$+ \sum_{\substack{\ell>j \\ \ell<L}} \hat{S}^z_\ell \hat{S}^z_{\ell+1} + \sum_{\ell>j} (-g \hat{S}^x_\ell)$$

$$+ \hat{S}^z_j \hat{S}^z_{j+1} + (-g \hat{S}^x_j)$$

Denote:

$\hat{H}^\alpha_{<j} = \hat{h}^\alpha_{<j} \otimes \underline{1}^{\otimes L-j+1}$ where $\hat{h}^\alpha_{<j} \in \mathcal{H}_{<j}$ acts only on sites $1 \dots j-1$

$\hat{H}^\alpha_{>j} = \underline{1}^{\otimes j} \otimes \hat{h}^\alpha_{>j}$ where $\hat{h}^\alpha_{>j} \in \mathcal{H}_{>j}$ acts only on sites $j+1 \dots L$

Identify:

$\hat{h}^L_{<j} = \sum_{\ell<j-1} \hat{S}^z_\ell \hat{S}^z_{\ell+1} + \sum_{\ell<j} (-g \hat{S}^x_\ell)$ acting only on left part of system

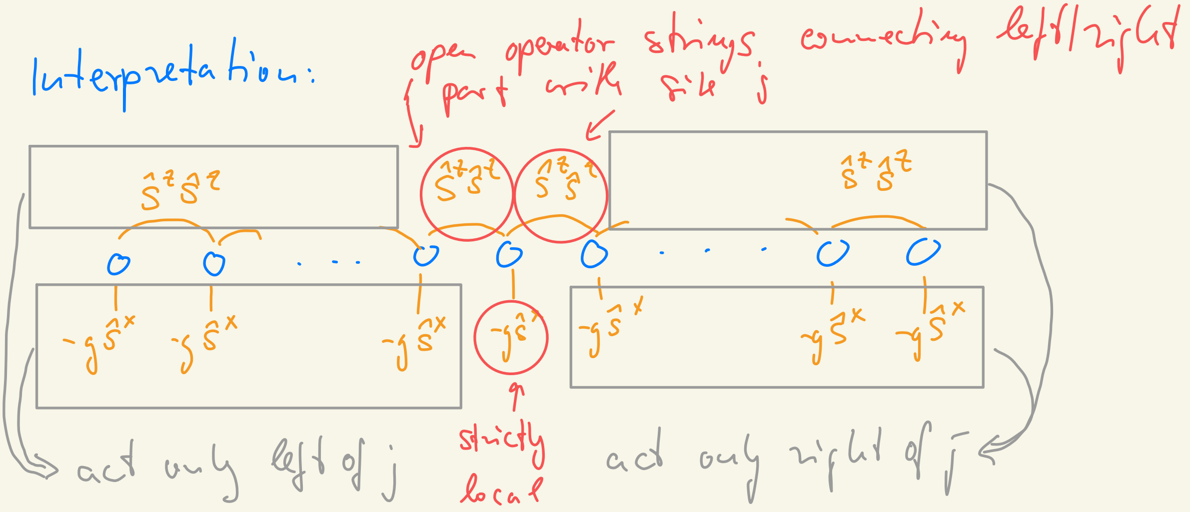
$$\hat{h}^{R}_{>j} = \sum_{\ell>j} \hat{S}^z_\ell \hat{S}^z_{\ell+1} + \sum_{\ell>j} (-g\hat{S}^x_\ell)$$

$$\hat{h}^{zz}_{<j} = \hat{S}^z_{j-1} \quad , \quad \hat{h}^{zz}_{>j} = \hat{S}^z_{j+1}$$

Then we can write:

$$\hat{H} = \begin{pmatrix} \mathbb{1}^{\otimes(j-1)} & \hat{h}^{zz}_{<j} & \hat{h}^{L}_{<j} \end{pmatrix} \begin{pmatrix} \mathbb{1} & \hat{S}^z & (-g\hat{S}^x) \\ 0 & 0 & \hat{S}^z \\ & & \mathbb{1} \end{pmatrix} \begin{pmatrix} \hat{h}^{R}_{>j} \\ \hat{h}^{zz}_{>j} \\ \mathbb{1} \end{pmatrix}$$

Interpretation:



we have:

(i) complete operator strings in left/right part of the system

(ii) open operator strings connecting left/right part of system with site j

(iii) strictly local operators

Systematic formulation using finite state machines (FSMs)

An operator is completely characterized by all non-trivial, distinct strings of local operators.

Treat operator strings (e.g. $\mathbb{1} \otimes \cdots \otimes \hat{S}^z \otimes \hat{S}^z \otimes \mathbb{1} \otimes \cdots$) as "words" formed by "alphabet" Σ, (e.g. for spins: $\Sigma = \{\mathbb{1}, \hat{S}^x, \hat{S}^y, \hat{S}^z\}$). A global operator $\hat{H}$ is then defined by the set of "words" compatible with $\hat{H}$.

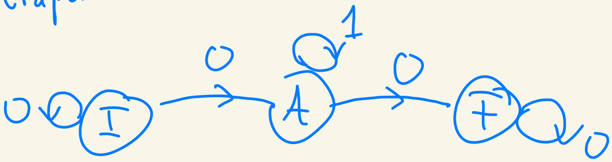
Finite state machine:

For Σ a set of symbols & Ω a set of states then $\delta : \Sigma \times \Omega \to \Omega$ an invertible map defines a FSM.

Example

Which transition function δ generates all possible combinations of $0 \dots 0\, 1 \dots 1\, 0 \dots 0$ with at arb. amount of "1" between arbitrary amount of '0'?

Graphical solution:



$\Sigma = \{0, 1\}$

$\Omega = \{I, A, F\}$

$\delta[I, 0] \mapsto I$ $\qquad \delta[A, 0] \mapsto F$ $\qquad \delta[A, 1] \mapsto A$

$\delta[I, 1] \mapsto A$ $\qquad \delta[F, 0] \mapsto F$

Write δ as matrix:

$$\begin{array}{c|ccc} & I & A & F \\ \hline I & 0 & 0 & \emptyset \\ A & \emptyset & 1 & 0 \\ F & \emptyset & \emptyset & 0 \end{array}$$

Now any sequence of length 'L' is obtained by formally multiplying matrices:

$L = 4:$

$$(0 \quad 0 \quad 0)\begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix}\begin{pmatrix}0&0&0\\0&1&0\\0&0&0\end{pmatrix}\begin{pmatrix}0\\0\\0\end{pmatrix}$$

$$= (00 \quad 00+01 \quad 00)\begin{pmatrix}00\\10+00\\00\end{pmatrix} = 0000+0010+0100+0110 + 0000$$

Now let's apply this to operators!

Consider $\hat{H} = \sum_j \left(\hat{S}^x_j \hat{S}^x_j + \hat{S}^y_j \hat{S}^y_j + \hat{S}^z_j \hat{S}^z_j\right)$.

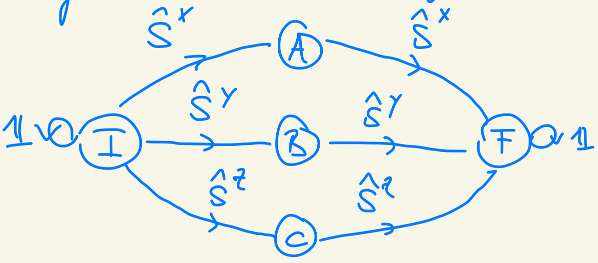
There are 3 types of operator strings:

a) $\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \hat{S}^x \hat{S}^x \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$

b) $\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \hat{S}^y \hat{S}^y \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$

c) $\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \hat{S}^z \hat{S}^z \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$

They are generated by the FSM:



$\Sigma = \{\mathbb{1}, \hat{S}^x, \hat{S}^y, \hat{S}^z\}$

$\Omega = \{I, A, B, C, F\}$

Transition function as operator-valued matrix:

$$\underline{\underline{\hat{W}}} = \begin{array}{c} \\ \\ \\ \\ \\ \\ \end{array} \begin{array}{ccccc|c} & & & & & \\ \end{array}$$

$$\underline{\underline{\hat{W}}} = \begin{array}{cc} \left(\begin{array}{ccccc} \mathbb{1} & \hat{S}^x & \hat{S}^y & \hat{S}^z & 0 \\ 0 & 0 & 0 & 0 & \hat{S}^x \\ 0 & 0 & 0 & 0 & \hat{S}^y \\ 0 & 0 & 0 & 0 & \hat{S}^z \\ 0 & 0 & 0 & 0 & \mathbb{1} \end{array}\right) & \begin{array}{c} I \\ A \\ B \\ C \\ F \end{array} \\ \begin{array}{ccccc} I & A & B & C & F \end{array} & \end{array}$$

at lattice site j take expectation value:

$$\underline{\underline{w}}^{\sigma_j \sigma_j'} = \langle \sigma_j | \underline{\underline{\hat{W}}} | \sigma_j' \rangle$$

$$= \underbrace{\begin{pmatrix} \langle \sigma_j | \mathbb{1} | \sigma_j' \rangle & \langle \sigma_j | \hat{S}^x | \sigma_j' \rangle & \langle \sigma_j | \hat{S}^y | \sigma_j' \rangle & \langle \sigma_j | \hat{S}^z | \sigma_j' \rangle & 0 \\ & & & & \langle \sigma_j | \hat{S}^x | \sigma_j' \rangle \\ & & & & \langle \sigma_j | \hat{S}^y | \sigma_j' \rangle \\ & & \underline{\underline{0}}_{4 \times 4} & & \langle \sigma_j | \hat{S}^z | \sigma_j' \rangle \\ & & & & \langle \sigma_j | \mathbb{1} | \sigma_j' \rangle \end{pmatrix}}_{\text{MPO-matrix at site } j!}$$

From this construction scheme, any operator on $\mathcal{H}_L$ can be converted into an MPO by constructing the matrices $\underline{\underline{W}}^{\sigma_j \sigma_j'}$ explicitely.