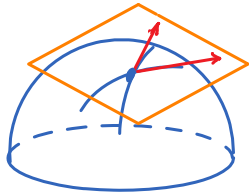
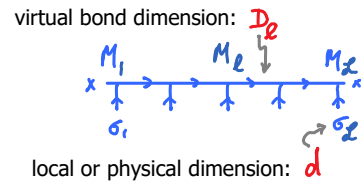


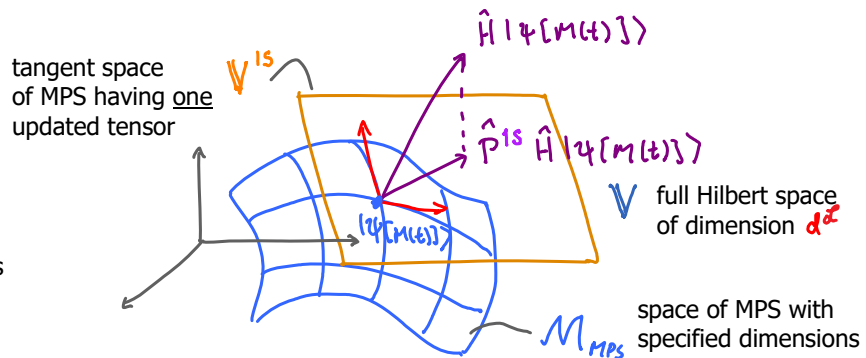
1. Motivation: why is tangent space useful?

$$|\psi[M]\rangle = \underbrace{|\sigma_1\rangle \dots |\sigma_\ell\rangle \dots |\sigma_\ell\rangle}_{|\vec{\sigma}\rangle_\ell} M_1^{\sigma_1} \dots M_\ell^{\sigma_\ell} \dots M_\ell^{\sigma_\ell}$$

Einstein summation over repeated indices is implied



Tangent space: spanned by vectors tangent to curves running within a smooth geometric structure.



Basic idea [Haegeman2011]:

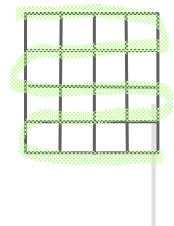
Consider Schrödinger equation: $i \frac{d}{dt} |\vec{\sigma}\rangle = \sum_{\ell=1}^L M_1^{\sigma_1} \dots \dot{M}_\ell^{\sigma_\ell} \dots M_L^{\sigma_L} = i \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle$ (1)

If a small change in an MPS $|\Psi\rangle$ is to be computed during time-evolution with a small time step, this change lives in the 'tangent space' of the manifold defined by the MPS, spanned by all states obtained by 'one-site (1s) variations of $|\Psi\rangle$, i.e. by changing only one tensor. Thus construct a projector \hat{P}^{1s} onto this space, and do time evolution using $\hat{P}^{1s} \hat{H}$.

$$i \frac{d}{dt} |\Psi(t)\rangle \simeq \hat{P}^{1s} H |\Psi(t)\rangle$$
 (2)

Basic insight: 'If you need to do a projection, do that at the outset, and then work in the projected space, without further approximations!'

This is a very fundamental and general idea. It is applicable to Hamiltonians with hopping or interactions of arbitrary range(!) (which is important for applications to 2D systems, treated via 1D snake paths). It has been elaborated in a series of publications:



[Haegeman2013] Detailed exposition of (improved version of) algorithm.

[Haegeman2014a] Mathematical foundations of tangent space approach in language of diff. geometry. (For a gentle introduction to diff. geometry, see Altland & von Delft, chapters V4, V5.)

[Lubich2015a] Concrete, explicit formula for tangent space projector. ← Breakthrough result!

[Haegeman2016] Unifying time evolution and optimization within tangent space approach.

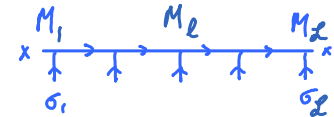
[Zauner-Stauber2018] Variational ground state optimization for uniform MPS (for infinite systems).

[Vanderstraeten2019] Review-style lecture notes on tangent space methods for uniform MPS.

[Gleis2022a], [Gleis2022], [Li2022] Research performed in the von Delft group.

This lecture follows [Gleis2022a] for construction of tangent space projector, and [Haegeman2016], for discussion of time evolution using the time-dependent variational principle (TDVP).

Consider L -site MPS with open boundary conditions:

$$|\psi[M]\rangle = |\bar{\sigma}_N\rangle M_1^{\sigma_1} \dots M_L^{\sigma_L} \dots M_L^{\sigma_L} \quad (1)$$


where $M_L^{\sigma_L}$ is matrix with elements $M_L^{\alpha\sigma_L}_{\beta}$, of dimension $D_{L-1} \times D_L$, with $D_0 = D_L = 1$

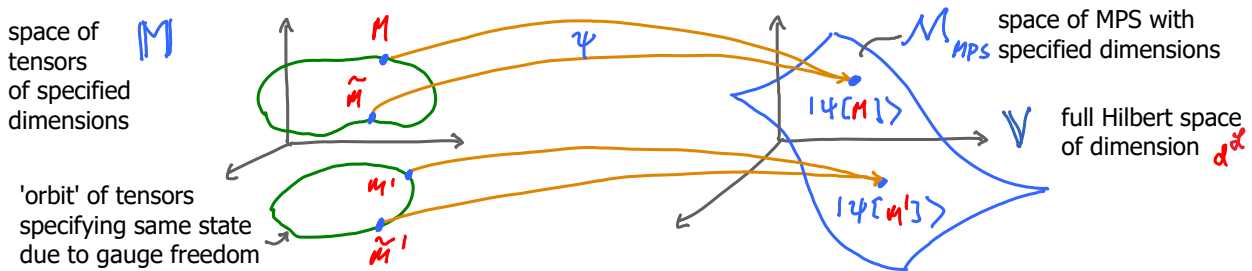
shorthand: $M := (M_1, \dots, M_L) \in \mathbb{M}$ space of tensors with specified dimensions

Gauge freedom: $|\psi[M]\rangle$ is unchanged under 'gauge transformation' on bond indices:

$$M_1 \dots M_L \mapsto \tilde{M}_1 \dots \tilde{M}_L = 1 M_1 g_1 g_1^{-1} g_2 g_2^{-1} \dots g_{L-1} g_{L-1}^{-1} M_L 1 \quad (2)$$


$$M_L^{\sigma_L} \mapsto \tilde{M}_L^{\sigma_L} \equiv g_{L-1}^{-1} M_L^{\sigma_L} g_L, \quad g_0 = g_L = 1 \quad (3)$$

with $g_L \in GL(D_L, \mathbb{C})$ group of general complex linear transformation in D_L dimensions

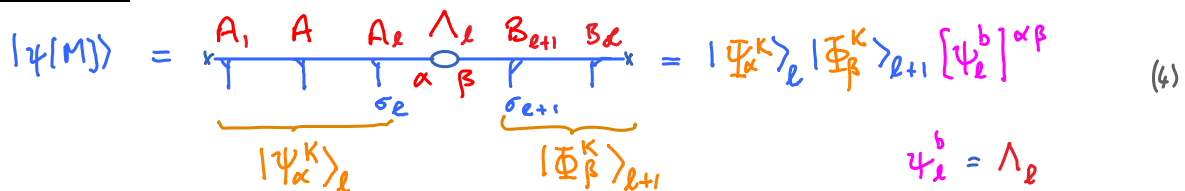


\mathcal{M}_{MPS} is a differential manifold, since it depends smoothly on the tensors in \mathbb{M} .

[Haegeman2014a] discusses this aspect in detail. In our discussion, though, it plays no role.

Gauge freedom can be exploited to bring MPS into site- or bond-canonical form:

Bond-canonical:

$$|\psi[M]\rangle = \underbrace{A_1 \dots A_L}_{|\Psi_\alpha^K\rangle_L} \underbrace{\Lambda_L}_{\alpha \beta} \underbrace{B_{L+1} \dots B_L}_{|\Phi_\beta^K\rangle_{L+1}} = |\Psi_\alpha^K\rangle_L |\Phi_\beta^K\rangle_{L+1} [\psi_L^b]^{\alpha\beta} \quad (4)$$


$\psi_L^b = \Lambda_L$

$$\text{with } A_\sigma^\dagger A_\sigma = \mathbb{1}^K, \quad \text{Diagram} = \{, \quad A_\sigma^\dagger A_\sigma = \text{diagonal} \nabla A_L \quad (5)$$


$$B_\sigma^\dagger B_\sigma = \mathbb{1}^K, \quad \text{Diagram} = \}, \quad B_\sigma^\dagger B_\sigma = \text{diagonal} \nabla B_L \quad (6)$$


requiring this fixes gauge uniquely

$\{|\Psi_\alpha^K\rangle_L\}, \{|\Phi_\beta^K\rangle_{L+1}\}$ form orthonormal bases for 'kept' (K) subspaces representing left- and right parts of chain.

$${}_l \langle \Psi^{\kappa \alpha'} | \Psi^{\kappa}_{\alpha} \rangle_l = [\mathbb{1}_l^{\kappa}]^{\alpha'}_{\alpha} \quad \begin{array}{c} \xrightarrow{\alpha} \\ \text{---} \\ \xleftarrow{\alpha'} \end{array} = \{ \quad \quad \quad \} \quad (7)$$

$${}_l \langle \Phi^{\kappa \alpha'} | \Phi^{\kappa}_{\beta} \rangle_l = [\mathbb{1}_l^{\kappa}]^{\beta'}_{\beta} \quad \begin{array}{c} \xleftarrow{\beta} \\ \text{---} \\ \xrightarrow{\beta'} \end{array} = \} \quad (8)$$

1-site-canonical:

$$|\psi[M]\rangle = \underbrace{\text{---} \text{---} \text{---} \text{---}}_{|\Psi^{\kappa}_{\alpha}\rangle_{l-1}} \xrightarrow{\alpha} \text{---} \xleftarrow{\beta} \underbrace{\text{---} \text{---} \text{---} \text{---}}_{|\Phi^{\kappa}_{\beta}\rangle_{l+1}} = |\Psi^{\kappa}_{\alpha}\rangle_{l-1} |\sigma_l\rangle |\Phi^{\kappa}_{\beta}\rangle_{l+1} [\psi_l^{1s}]^{\alpha \sigma_l \beta} \quad (9)$$

2-site-canonical:

$$|\psi[M]\rangle = \underbrace{\text{---} \text{---} \text{---} \text{---}}_{|\Psi^{\kappa}_{\alpha}\rangle_{l-1}} \xrightarrow{\sigma_l, \sigma_{l+1}} \text{---} \xleftarrow{\beta} \underbrace{\text{---} \text{---} \text{---} \text{---}}_{|\Phi^{\kappa}_{\beta}\rangle_{l+2}} = |\Psi^{\kappa}_{\alpha}\rangle_{l-1} |\sigma_l\rangle |\sigma_{l+1}\rangle |\Phi^{\kappa}_{\beta}\rangle_{l+2} [\psi_l^{2s}]^{\alpha \sigma_l \sigma_{l+1} \beta} \quad (10)$$

Relation between 1-site- and bond-canonical: $\psi_l^{1s} = C_l = \frac{A_l}{\text{---}} \frac{\Lambda_l}{\text{---}} = \frac{\Lambda_{l-1}}{\text{---}} \frac{B_l}{\text{---}} \quad (11)$

Relation between 1-site- and 2-site-canonical: $\psi_l^{2s} = \frac{A_l}{\text{---}} \frac{C_{l+1}}{\text{---}} = \frac{C_l}{\text{---}} \frac{B_{l+1}}{\text{---}} \quad (12)$

Matrix elements of Hamiltonian, represented as MPO:

bond (b): $\langle \Psi^{\kappa}_{\alpha'} | \langle \Phi^{\kappa}_{\beta} | \hat{H} | \Psi^{\kappa}_{\alpha} \rangle | \Phi^{\kappa}_{\beta} \rangle = \begin{array}{c} \xrightarrow{\alpha} \\ \text{---} \\ \xleftarrow{\alpha'} \end{array} \begin{array}{c} \xrightarrow{\beta} \\ \text{---} \\ \xleftarrow{\beta'} \end{array} =: \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_l^b \quad (13)$

1-site (1s): $\langle \Psi^{\kappa}_{\alpha'} | \langle \sigma_l | \langle \Phi^{\kappa}_{\beta} | \hat{H} | \Psi^{\kappa}_{\alpha} \rangle | \sigma_l \rangle | \Phi^{\kappa}_{\beta} \rangle = \begin{array}{c} \xrightarrow{\alpha} \\ \text{---} \\ \xleftarrow{\alpha'} \end{array} \begin{array}{c} \xrightarrow{\sigma_l} \\ \text{---} \\ \xleftarrow{\sigma'_l} \end{array} \begin{array}{c} \xrightarrow{\beta} \\ \text{---} \\ \xleftarrow{\beta'} \end{array} =: \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_l^{1s} \quad (14)$

2-site (2s): $\langle \Psi^{\kappa}_{\alpha'} | \langle \sigma_l \sigma_{l+1} | \langle \Phi^{\kappa}_{\beta} | \hat{H} | \Psi^{\kappa}_{\alpha} \rangle | \sigma_l \rangle | \sigma_{l+1} \rangle | \Phi^{\kappa}_{\beta} \rangle = \begin{array}{c} \xrightarrow{\alpha} \\ \text{---} \\ \xleftarrow{\alpha'} \end{array} \begin{array}{c} \xrightarrow{\sigma_l} \\ \text{---} \\ \xleftarrow{\sigma'_l} \end{array} \begin{array}{c} \xrightarrow{\sigma_{l+1}} \\ \text{---} \\ \xleftarrow{\sigma'_{l+1}} \end{array} \begin{array}{c} \xrightarrow{\beta} \\ \text{---} \\ \xleftarrow{\beta'} \end{array} =: \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_l^{2s} \quad (15)$

Related by:

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_l^b = \begin{array}{c} A_l \\ \text{---} \\ A_l^\dagger \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_l^{1s} = \begin{array}{c} B_{l+1} \\ \text{---} \\ B_{l+1}^\dagger \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_{l+1}^{1s} \quad (16)$$

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_l^{1s} = \begin{array}{c} A_{l-1} \\ \text{---} \\ A_{l-1}^\dagger \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_{l-1}^{2s} = \begin{array}{c} B_{l+1} \\ \text{---} \\ B_{l+1}^\dagger \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \end{array} H_l^{2s} \quad (17)$$

$$|\psi[M]\rangle = \underbrace{\begin{array}{c} A_1 \quad A \quad A_L \\ \downarrow \quad \downarrow \quad \downarrow \\ \text{---} \end{array}}_{|\Psi_\alpha^K\rangle_L} \underbrace{\begin{array}{c} \wedge_L \\ \downarrow \\ \text{---} \end{array}}_{\sigma_L} \underbrace{\begin{array}{c} B_{L+1} \quad B_{L+1} \quad B_L \\ \downarrow \quad \downarrow \quad \downarrow \\ \text{---} \end{array}}_{|\Phi_\beta^K\rangle_{L+1}}$$

for simplicity: assume all virtual bonds have same dimension, D

Definition of kept spaces:

left 'kept' (K) space of site l : $V_l^K = \text{span} \{ |\Psi_\alpha^K\rangle \} \subset V_1 \otimes \dots \otimes V_l$ (1)

right 'kept' (K) space of site l : $W_{l+1}^K = \text{span} \{ |\Phi_\beta^K\rangle_{l+1} \} \subset V_{l+1} \otimes \dots \otimes V_L$ (2)

Action of isometries: generates new kept spaces:

$$A_l: \underbrace{V_{l-1}^K \otimes V_{\sigma_l}}_{\text{'left parent (P) space'}} \rightarrow V_l^K, \quad |\Psi_\alpha^K\rangle_{l-1} |\sigma\rangle_{\sigma_l} [A_l]^{\alpha\sigma_l}_{\alpha'} = |\Psi_{\alpha'}^K\rangle_l$$

Dimensions: $D \cdot d \rightarrow D$

rectangular matrix
 $(D \cdot d) \times D$

open triangles: 'kept'

$$B_{l+1}: \underbrace{V_{\sigma_{l+1}} \otimes W_{l+2}^K}_{\text{'right parent (P) space'}} \rightarrow W_{l+1}^K, \quad [B_{l+1}]^{\sigma_{l+1}\beta'}_{\beta} |\sigma\rangle_{\sigma_{l+1}} |\Phi_\beta^K\rangle_{l+2} = |\Phi_{\beta'}^K\rangle_{l+1}$$

Dimensions: $d \cdot D \rightarrow D$

$D \times (d \cdot D)$

Isometric conditions, $A_l^\dagger A_l \stackrel{(2.5)}{=} \mathbb{1}_l^K$, $B_{l+1}^\dagger B_{l+1} \stackrel{(2.6)}{=} \mathbb{1}_l^K$ ensure orthonormality of kept basis states. (2.7, 8)

$$\begin{array}{|c|} \hline \text{---} \\ \hline \end{array} \begin{array}{|c|} \hline \text{---} \\ \hline \end{array} = \begin{array}{|c|} \hline \text{---} \\ \hline \end{array}, \quad \begin{array}{|c|} \hline \text{---} \\ \hline \end{array} \begin{array}{|c|} \hline \text{---} \\ \hline \end{array} = \begin{array}{|c|} \hline \text{---} \\ \hline \end{array} \quad (5)$$

The image spaces of A_l and B_{l+1} are smaller than their parent spaces.

Let \bar{A}_l and \bar{B}_{l+1} be their complements, mapping onto 'discarded' (D) spaces orthogonal to kept ones,

such that $A_l = A_l \oplus \bar{A}_l$ and $B_l = B_{l+1} \oplus \bar{B}_{l+1}$ are unitary maps on their parent spaces. (6)

$$\begin{array}{|c|} \hline D \\ \hline \text{---} \\ \hline \end{array} \begin{array}{|c|} \hline \bar{D} \\ \hline \text{---} \\ \hline \end{array} \quad \begin{array}{|c|} \hline D \\ \hline \text{---} \\ \hline \end{array} \begin{array}{|c|} \hline \bar{D} \\ \hline \text{---} \\ \hline \end{array} \quad \left. \begin{array}{|c|} \hline D \\ \hline \text{---} \\ \hline \end{array} \right\} (D \cdot d)$$

Definition of 'discarded' (D) spaces:

$$\bar{A}_l: \underbrace{V_{l-1}^K \otimes V_{\sigma_l}}_{\text{'left parent space'}} \rightarrow V_l^D, \quad |\Psi_\alpha^K\rangle_{l-1} |\sigma\rangle_{\sigma_l} [\bar{A}_l]^{\alpha\sigma_l}_{\alpha'} = |\Psi_{\alpha'}^D\rangle_l$$

Dimensions: $D \cdot d \rightarrow D \cdot d - D = \bar{D}$

$(D \cdot d) \times (D \cdot d - D)$

filled triangles: 'discarded'

Dimensions: $D \cdot d \rightarrow D \cdot d - D = \bar{D}$

$$(D \cdot d) \times (D \cdot d - D)$$

$$\bar{B}_{l+1} : \underbrace{V \otimes W^K}_{\sigma_{l+1} \text{ 'right parent space' } l+2} \rightarrow W_{l+1}^D, \quad [\bar{B}_{l+1}]_{\beta}^{\sigma_{l+1} \beta'} |\Phi_{\beta'}^K\rangle_{l+2} |\sigma_{l+1}\rangle = |\Phi_{\beta}^D\rangle_{l+1} \quad (8)$$

Dimensions: $d \cdot D \rightarrow d \cdot D - D = \bar{D}$



$$(d \cdot D - D) \times (d \cdot D)$$

(9)

Unitarity implies: $A_l^\dagger A_l = \begin{pmatrix} A_l^\dagger & \bar{A}_l^\dagger \\ A_l & \bar{A}_l \end{pmatrix} \begin{pmatrix} A_l \\ \bar{A}_l \end{pmatrix} = \begin{pmatrix} A_l^\dagger A_l & A_l^\dagger \bar{A}_l \\ \bar{A}_l^\dagger A_l & \bar{A}_l^\dagger \bar{A}_l \end{pmatrix} = \begin{pmatrix} \mathbb{1}_l^K & 0 \\ 0 & \mathbb{1}_l^D \end{pmatrix} = \mathbb{1}_{l-1}^K \otimes \mathbb{1}_d \quad (10)$

'orthogonality':

$$A_l^\dagger A_l = \mathbb{1}_l^K, \quad \bar{A}_l^\dagger \bar{A}_l = \mathbb{1}_l^D, \quad \bar{A}_l^\dagger A_l = 0, \quad A_l^\dagger \bar{A}_l = 0 \quad (11)$$

$$\begin{matrix} \text{Diagram 1} \\ \text{Diagram 2} \\ \text{Diagram 3} \\ \text{Diagram 4} \end{matrix} = \begin{matrix} \text{Diagram 5} \\ \text{Diagram 6} \\ \text{Diagram 7} \\ \text{Diagram 8} \end{matrix} \quad (12)$$

$$\begin{matrix} \text{Diagram 9} \\ \text{Diagram 10} \\ \text{Diagram 11} \\ \text{Diagram 12} \end{matrix} = \begin{matrix} \text{Diagram 13} \\ \text{Diagram 14} \\ \text{Diagram 15} \\ \text{Diagram 16} \end{matrix} \quad (13)$$

'When K meets K, or D meets D, they yield unity;

when K meets D or D meets K, they yield zero.' (14)

Unitarity implies: $A_l A_l^\dagger = \begin{pmatrix} A_l & \bar{A}_l \end{pmatrix} \begin{pmatrix} A_l^\dagger \\ \bar{A}_l^\dagger \end{pmatrix} = \begin{pmatrix} \mathbb{1}_l^K & 0 \\ 0 & \mathbb{1}_l^D \end{pmatrix} = \mathbb{1}_l^P = \mathbb{1}_{l-1}^K \otimes \mathbb{1}_d \quad (15)$

'completeness':

$$A_l A_l^\dagger + \bar{A}_l \bar{A}_l^\dagger = \mathbb{1}_{l-1}^K \otimes \mathbb{1}_d \quad (16)$$

$$\begin{matrix} \text{Diagram 17} \\ \text{Diagram 18} \end{matrix} = \begin{matrix} \text{Diagram 19} \end{matrix} \quad (17)$$

$$\begin{matrix} \text{Diagram 20} \\ \text{Diagram 21} \end{matrix} = \begin{matrix} \text{Diagram 22} \end{matrix} \quad (18)$$



Similarly: $B_{l+1} B_{l+1}^\dagger = \mathbb{1}_l^P$ and $B_{l+1}^\dagger B_{l+1} = \mathbb{1}_l^P = \mathbb{1}_d \otimes \mathbb{1}_{l+1}^K$ imply: (19)

'orthogonality':

$$B_{l+1} B_{l+1}^\dagger = \mathbb{1}_l^K, \quad \bar{B}_{l+1} \bar{B}_{l+1}^\dagger = \mathbb{1}_l^D, \quad \bar{B}_l B_{l+1}^\dagger = 0, \quad B_l \bar{B}_l^\dagger = 0, \quad (20)$$


 $=$

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 $\cdot (2i)$

'completeness': $B_{\ell+1}^\dagger B_{\ell+1} + \bar{B}_{\ell+1}^\dagger \bar{B}_{\ell+1} = \mathbb{1}_d \otimes \mathbb{1}_{\ell+1}^K$, (22)

Structure of spaces explored by bond-, 1s or 2s schemes can be elucidated by introducing local projectors:

Left K projector (cf. MPS-II.1): $l \in [0, L]$

$$\hat{P}_l^K := |\Psi^{K\alpha}\rangle_l \langle \Psi^{K\alpha}| = \text{diagram}, \quad \hat{P}_0^K := 1$$

(sum over α implied)

Right K projector: $l \in [1, L+1]$

$$\hat{Q}_l^K := |\Phi^{K\beta}\rangle_l \langle \Phi^{K\beta}| = \text{diagram}, \quad \hat{Q}_{L+1}^K := 1$$

(sum over β implied)

(1)

Left D projector (cf. MPS-II.1): $l \in [0, L]$

$$\hat{P}_l^D := |\Psi^{D\alpha}\rangle_l \langle \Psi^{D\alpha}| = \text{diagram}, \quad \hat{P}_0^D := 0$$

(sum over α implied)

Right D projector: $l \in [1, L+1]$

$$\hat{Q}_l^D := |\Phi^{D\beta}\rangle_l \langle \Phi^{D\beta}| = \text{diagram}, \quad \hat{Q}_{L+1}^D := 0$$

(sum over β implied)

(2)

(3)

Projector properties: $\hat{P}_l^X \hat{P}_l^{\bar{X}} = \delta^{X\bar{X}} \hat{P}_l^X, \quad \hat{Q}_l^X \hat{Q}_l^{\bar{X}} = \delta^{X\bar{X}} \hat{Q}_l^X \quad (X \in \{K, D\})$ (4)

For example: $\hat{P}_l^K \hat{P}_l^K = \text{diagram} \stackrel{(2.7)}{=} \text{diagram} = \text{diagram} = \hat{P}_l^K$ (5)

$$\hat{P}_l^D \hat{P}_l^K = \text{diagram} \stackrel{(2.7)}{=} \text{diagram} \stackrel{(3.12)}{=} 0$$
 (6)

Bond projector: $\hat{P}_{l+1}^{bs} = \hat{P}_l^b = \hat{P}_l^K \otimes \hat{Q}_{l+1}^K = \text{diagram} \otimes \text{diagram}$ (7)

1s projector: $\hat{P}_l^{1s} = \hat{P}_{l-1}^K \otimes \mathbb{1}_l \otimes \hat{Q}_{l+1}^K = \text{diagram} \otimes \text{diagram} \otimes \text{diagram}$ (8)

ns projector: $\hat{P}_l^{ns} = \hat{P}_{l-1}^K \otimes \overbrace{\mathbb{1}_l \otimes \dots \otimes \mathbb{1}_{l+n-1}}^{n \text{ sites}} \otimes \hat{Q}_{l+n}^K = \text{diagram} \otimes \overbrace{\text{diagram}}^{n \text{ sites}} \otimes \text{diagram}$ (9)

Projector property: $(\hat{P}_l^b)^2 = \hat{P}_l^b, \quad (\hat{P}_l^{1s})^2 = \hat{P}_l^{1s}, \quad (\hat{P}_l^{ns})^2 = \hat{P}_l^{ns}$ (10)

follows from (2)

The projectors $\hat{P}_l^b, \hat{P}_l^{1s}, \hat{P}_l^{2s}$ mutually commute (since they are all diagonal in same basis $|\vec{\sigma}\rangle$)

However, they are not mutually orthogonal (see below).

Hamiltonian matrix elements can be obtained from full Hamiltonian via local projectors,

$$H_l^b = \hat{P}_l^b \hat{H} \hat{P}_l^b, \quad H_l^{1s} = \hat{P}_l^{1s} \hat{H} \hat{P}_l^{1s}, \quad H_l^{ns} = \hat{P}_l^{ns} \hat{H} \hat{P}_l^{ns} \quad (11)$$

For example:

$$\hat{P}_l^{1s} \hat{H} \hat{P}_l^{1s} = \text{diagram} = \langle \Psi^{K\alpha'} | \langle \sigma_l^1 | \langle \Phi^{K\beta'} | \hat{H} | \Psi^K | \sigma_l^1 | \Phi^K \rangle \quad (12)$$

Projectors for K and D sectors

$$\begin{aligned} P_{l\bar{l}}^{KK} &= \text{diagram} & P_{l\bar{l}}^{KD} &= \text{diagram} \\ P_{l\bar{l}}^{DK} &= \text{diagram} & P_{l\bar{l}}^{DD} &= \text{diagram} \end{aligned} \quad (13)$$

These fulfill numerous orthogonality relations; e.g.

$$X \in \{K, D\}$$

Same-site-indices - orthogonal:

$$P_{l\bar{l}}^{X\bar{X}} P_{l\bar{l}}^{X'\bar{X}'} = \delta^{XX'} \delta^{\bar{X}\bar{X}'} P_{l\bar{l}}^{X\bar{X}} \quad \text{e.g.} \quad \text{diagram} = \text{diagram} \quad (14)$$

D on earliest or latest site - yields zero:

$$\left. \begin{aligned} P_{l\bar{l}}^{D\bar{X}} P_{l'\bar{l}'}^{X'\bar{X}'} &= 0 \quad \text{if } l < l' \\ P_{l\bar{l}}^{X\bar{X}} P_{l'\bar{l}'}^{X'\bar{D}} &= 0 \quad \text{if } \bar{l} < \bar{l}' \end{aligned} \right\} \quad \text{e.g.} \quad \text{diagram} = 0 \quad (15)$$

two D's on same side but different sites - yield zero:

$$\left. \begin{aligned} P_{l\bar{l}}^{D\bar{X}} P_{l'\bar{l}'}^{D\bar{X}'} &\sim \delta_{l\bar{l}'} \\ P_{l\bar{l}}^{X\bar{D}} P_{l'\bar{l}'}^{X'\bar{D}} &\sim \delta_{\bar{l}\bar{l}'} \end{aligned} \right\} \quad \text{e.g.} \quad \text{diagram} = \text{diagram} \quad (16)$$

Bond, 1s and ns projectors are all KK projectors:

$$P_{l+1}^{os} = \hat{P}_l^b = P_{l,l+1}^{KK} = \text{diagram} \quad (17)$$

$$P_{l+1}^{os} = \hat{P}_l^b = P_{l,l+1}^{KK} = \text{diagram} \quad (17)$$

$$\hat{P}_l^{1s} = P_{l-1,l+1}^{KK} = \text{diagram} \quad (18)$$

$$\hat{P}_l^{ns} = P_{l-1,l+n}^{KK} = \text{diagram} \quad (19)$$

ns projectors are not orthogonal. E.g.

$$P_l^{1s} P_{l+1}^{1s} = P_{l+1}^{os} = P_l^b, \text{ e.g. } \text{diagram} = \text{diagram} \quad (20)$$

ns projector is annihilated by left D on its left or right D on its right:

$$\left. \begin{aligned} P_{l\bar{l}}^{D\bar{x}} P_{l'}^{ns} &= 0 & \text{if } l < l' \\ P_l^{ns} P_{l'\bar{l}'}^{x'D} &= 0 & \text{if } l+n \leq l' \end{aligned} \right\} \text{ e.g. } \text{diagram} = 0 \quad (21)$$

Any ns projector can be expressed through two ($n-1$)s projectors, in two different ways: E.g.

$$P_l^{1s} = \text{diagram} \quad \boxed{\begin{aligned} \Rightarrow &= \text{diagram} + \text{diagram} \\ \Leftarrow &= \text{diagram} + \text{diagram} \end{aligned}} \quad (22)$$

$$\stackrel{(3.17)}{=} \overbrace{P_{l,l+1}^{KK}}^{P_l^b} + P_{l,l+1}^{DK} = \text{diagram} + \text{diagram} \quad (23)$$

or

$$\stackrel{(3.23)}{=} \overbrace{P_{l-1,l}^{KK}}^{P_{l-1}^b} + P_{l-1,l}^{KD} = \text{diagram} + \text{diagram} \quad (24)$$

Similarly:

$$P_l^{2s} = \text{diagram} \quad (25)$$

$$\stackrel{(3.17)}{=} \overbrace{P_{l,l+2}^{KK}}^{P_l^{1s}} + P_{l,l+2}^{DK} = \text{diagram} + \text{diagram} \quad (26)$$

or

$$\stackrel{(3.23)}{=} \overbrace{P_{l-1,l+1}^{KK}}^{P_{l-1}^{1s}} + P_{l-1,l+1}^{KD} = \text{diagram} + \text{diagram} \quad (27)$$

$$\mathbb{V}^{1s} = \text{span of all states } |\Psi'\rangle \text{ differing from } |\Psi\rangle \text{ on precisely 0 or 1 sites}$$

$$= \text{span} \{ |\Psi'_\ell\rangle = x \text{---} \underset{\ell}{\underset{\uparrow}{\bigcirc}} \text{---} x, \ell \in [1, 2] \} \quad (11)$$

formal definition: $= \text{span} \left\{ \underset{\substack{\uparrow \\ \text{image}}}{\text{im}(P_\ell)} \mid \ell \in [1, L] \right\}$ (12)

$$V^{15} = \text{im}(P^{15}) \Rightarrow \text{im}(P_\ell^{15}) \subset \text{im}(P^{15}) \quad \text{for all } \ell \in [1, L] \quad (13)$$

Formally: p^{15} has the defining properties: $(p^{15})^2 = p^{15}$, $p^{15} p_l^{15} = p_l^{15}$ (14)

$\sum_{\ell=1}^{\mathcal{L}} p_{\ell}^{15}$ does not work, since summands are not

$$\sum_{\ell'} p_{\ell}^{15} p_{\ell'}^{15} = \sum_{\ell} p_{\ell}^{15} + \underbrace{\sum_{\ell \neq \ell'} p_{\ell}^{15} p_{\ell'}^{15}}_{\neq 0}$$

Define P_{ℓ}^{1s} , obtained from P_{ℓ}^{1s} by projecting out the overlap with P_{ℓ}^{1s} : (15)

$$P_{l \leq}^{1s} := P_l^{1s} (1_Y - P_{l \neq 1}^{1s}) \quad \text{subtraction generates D sectors!} \quad (16)$$

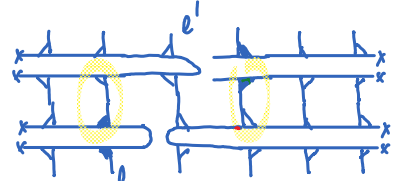
$$\begin{aligned} (4.20) \quad & \left\{ \begin{aligned} P_\ell^{1s} - P_\ell^b &= P_{\ell, \ell+1}^{DK} \\ P_\ell^{1s} - P_{\ell-1}^b &= P_{\ell-1, \ell}^{KD} \end{aligned} \right. \end{aligned} \quad \begin{aligned} (4.23) \\ (4.24) \end{aligned}$$

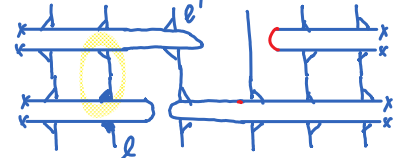
subtraction generates D sectors! (16)

(17)


 (3.17)

$$P_{l \leq}^{15} P_{l' \leq}^{15} = \delta_{ll'} P_{l \leq}^{15}$$

for all $l < l'$: $P_{l <}^{1s} P_{l' >}^{1s} = 0$ e.g.  (20)

for all $l \leq l'$: $P_{l \leq}^{1s} P_{l'}^{1s} = 0$ e.g.  (21)

Tangent space projector is defined by following sum, where l' can be freely chosen from $l' \in [1, L]$:

$$P^{1s} := \sum_{l=1}^{l'-1} \underbrace{P_{l <}^{1s}}_{P_{l, l+1}^{DK}} + P_{l'}^{1s} + \sum_{l=l'+1}^L \underbrace{P_{l >}^{1s}}_{P_{l-1, l}^{KD}} \quad \text{for any } l' \in [1, L] \quad (22)$$


$$P^{1s} = \sum_{l=1}^{l'-1} \left(\text{chain with red arrow at } l \right) + \left(\text{chain with red arrow at } l' \right) + \sum_{l=l'+1}^L \left(\text{chain with red arrow at } l \right) \quad (23)$$

Projector properties (14) hold, because the summands are mutually orthogonal projectors: For example:

$$\forall l' \in [1, L]: P^{1s} P_{l'}^{1s} = \left(\sum_{l=1}^{l'-1} P_{l <}^{1s} + P_{l'}^{1s} + \sum_{l=l'+1}^L P_{l >}^{1s} \right) P_{l'}^{1s} = P_{l'}^{1s} \quad (24)$$

hence (13) holds: $\text{im}(P_{l'}^{1s}) \subset \text{im}(P^{1s})$ for all $l' \in [1, L]$

Alternative expression for tangent space projector, expressed purely through bond projectors:

use (3.17) for l' term of (22):  (25)

$$P^{1s(23)} = \sum_{l=1}^{l'-1} \left(\text{chain with red arrow at } l \right) + \left(\text{chain with red arrow at } l' \right) + \sum_{l=l'+1}^L \left(\text{chain with red arrow at } l \right) \quad (25)$$

Another alternative expression for tangent space projector, without any D sectors: use (17), (18) in (22):

$$P^{1s} = \sum_{l=1}^{l'-1} (P_{l <}^{1s} - P_{l <}^b) + P_{l'}^{1s} + \sum_{l=l'+1}^L (P_{l >}^{1s} - P_{l >}^b) \quad \text{for any } l' \in [1, L] \quad (25)$$

$$P^{1s} = \sum_{l=1}^L P_{l <}^{1s} - \sum_{l=1}^{L-1} P_l^b = \sum_{l=1}^L \left(\text{chain with red arrow at } l \right) - \sum_{l=1}^{L-1} \left(\text{chain with red arrow at } l \right) \quad (26)$$

(26) for tangent space projector was first found in [Lubich2015a]. It is often used in the literature [Haegeman2016], [Vanderstraeten2019, Sec. 3.2], e.g. for time evolution with time-dependent variational principle (TDVP), see (TS.6).