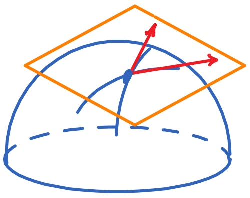
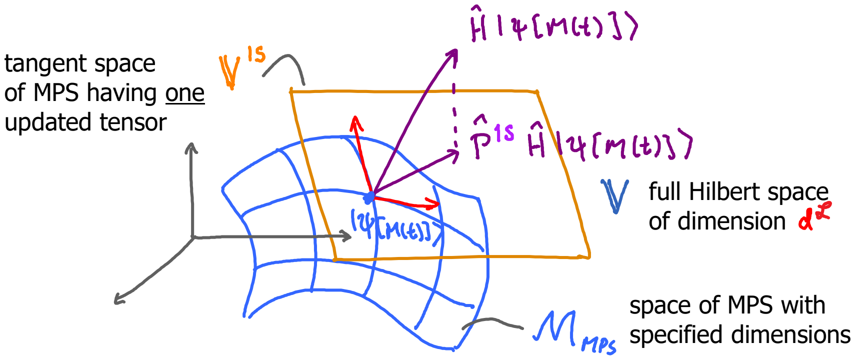
Tangent space methods I

1. Motivation: why is tangent space useful?



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



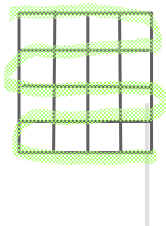
Basic idea [Haegeman2011]:

Consider Schrödinger equation: $$i \frac{d}{dt} |\Psi(t)\rangle = H |\Psi(t)\rangle \qquad (1)$$

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 $\hat P^{1s} \hat H$.

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

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).

2. MPS canonical forms

Consider $\mathcal{L}$-site MPS with open boundary conditions:

$$|\psi[M]\rangle = |\vec{\sigma}_N\rangle \, M_1^{\sigma_1} \cdots M_\ell^{\sigma_\ell} \cdots M_{\mathcal{L}}^{\sigma_{\mathcal{L}}} \qquad (1)$$

where $M_\ell^{\sigma_\ell}$ is matrix with elements $M_\ell^{\alpha\sigma_\ell}{}_\beta$, of dimension $D_{\ell-1} \times D_\ell$, with $D_0 = D_{\mathcal{L}} = 1$

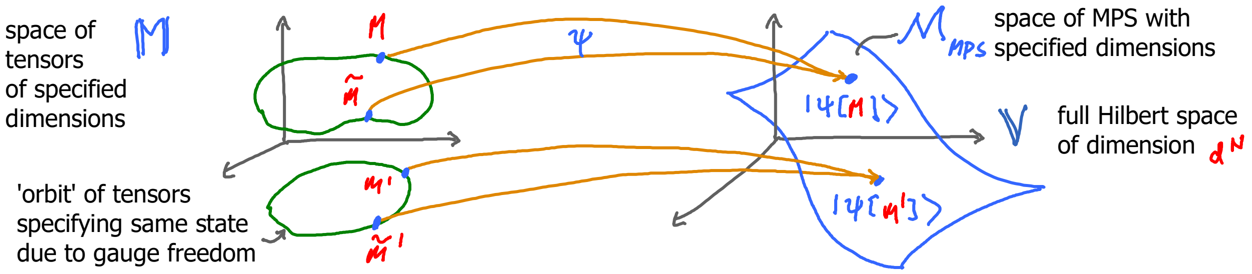
shorthand: $M := (M_1, \ldots, M_{\mathcal{L}}) \in \mathbb{M}$ space of tensors with specified dimensions

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

$$M_1 \ldots M_{\mathcal{L}} \mapsto \tilde{M}_1 \ldots \tilde{M}_{\mathcal{L}} = 1\, M_1 g_1 \; g_1^{-1} M \; g_2 \; g_2^{-1} \cdots g_{\mathcal{L}-1} \; g_{\mathcal{L}} M_{\mathcal{L}} \mathbb{1} \qquad (2)$$

$$M_\ell^{\sigma_\ell} \mapsto \tilde{M}_\ell^{\sigma_\ell} \equiv g_{\ell-1}^{-1} M_{[\ell]}^{\sigma_\ell} g_\ell \,, \qquad g_0 = g_{\mathcal{L}} = \mathbb{1} \qquad (3)$$

with $g_\ell \in GL(D_\ell, \mathbb{C})$ 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:

<u>Bond-canonical:</u>

$$|\psi[M]\rangle = \underbrace{A_1 \; A \; A_\ell}_{|\Psi^K_\alpha\rangle_\ell} \; \Lambda_\ell \; \underbrace{B_{\ell+1} \; B_{\mathcal{L}}}_{|\Phi^K_\beta\rangle_{\ell+1}} = |\Psi^K_\alpha\rangle_\ell \, |\Phi^K_\beta\rangle_{\ell+1} \, [\psi^b_\ell]^{\alpha\beta} \qquad (4)$$

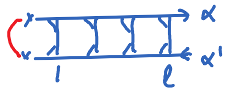
$$\psi^b_\ell = \Lambda_\ell$$

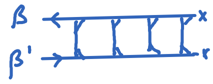
$$\text{with} \quad A^\dagger_\sigma A^\sigma = \mathbb{1}^K, \qquad A^\sigma A^\dagger_\sigma = \text{diagonal} \quad \forall A_\ell \qquad (5)$$

$$B^\sigma B_\sigma^\dagger = \mathbb{1}^K, \qquad B^\dagger_\sigma B^\sigma = \text{diagonal} \quad \forall B_\ell \qquad (6)$$

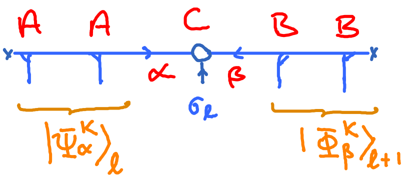
requiring this fixes gauge uniquely

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

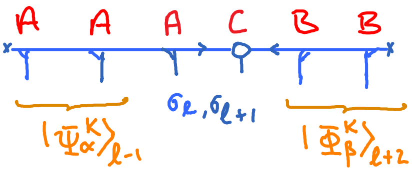
$$ {}_{\ell}\langle \Psi^{K\alpha'} | \Psi^{K}_{\alpha} \rangle_{\ell} = [\mathbb{1}^{K}_{\ell}]^{\alpha'}{}_{\alpha} $$  $=$ { (7)

$$ {}_{\ell}\langle \Phi^{K\alpha'} | \Phi^{K}_{\beta} \rangle_{\ell} = [\mathbb{1}^{K}_{\ell}]^{\beta'}{}_{\beta} $$  $=$ } (8)

1-site-canonical:

$|\psi[M]\rangle =$  $= |\Psi^{K}_{\alpha}\rangle_{\ell-1} |\sigma_{\ell}\rangle |\Phi^{K}_{\beta}\rangle^{L}_{\ell+1} [\psi_{\ell}]^{\alpha\sigma_{\ell}\beta}$ (9)

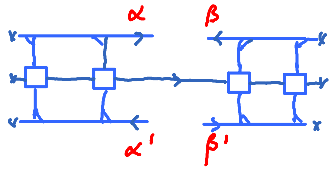
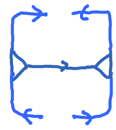
2-site-canonical:

$|\psi[M]\rangle =$  $= |\Psi^{K}_{\alpha}\rangle_{\ell-1} |\sigma_{\ell}\rangle |\sigma_{\ell+1}\rangle |\Phi^{K}_{\beta}\rangle^{L}_{\ell} [\psi^{2s}_{\ell}]^{\alpha\sigma_{\ell}\sigma_{\ell+1}\beta}$ (10)

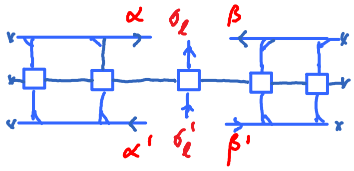
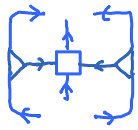
Relation between 1-site- and bond-canonical: $\psi^{1s}_{\ell} = C_{\ell} = A_{\ell}\Lambda_{\ell} = \Lambda_{\ell-1} B_{\ell}$ (11)

Relation between 1-site- and 2-site-canonical: $\psi^{2s}_{\ell} = A_{\ell} C_{\ell+1} = C_{\ell} B_{\ell+1}$ (12)

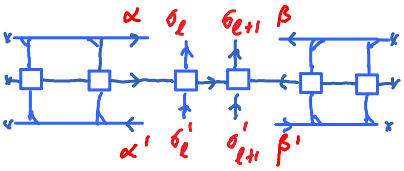
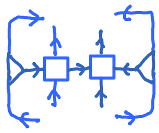
Matrix elements of Hamiltonian, represented as MPO:

bond (b): $\langle \Psi^{K}_{\alpha'} | \langle \Phi^{K}_{\beta'} | \hat{H} | \Psi^{K}_{\alpha} \rangle | \Phi^{K}_{\beta} \rangle =$  $=:$  H^{b}_{ℓ} (13)

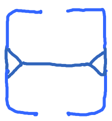
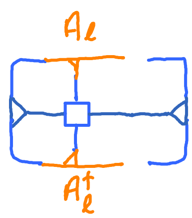
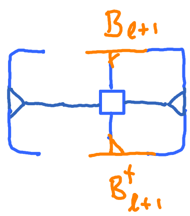
1-site (1s):

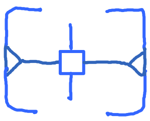
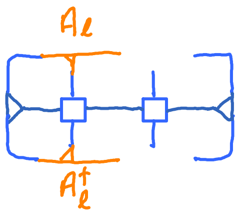
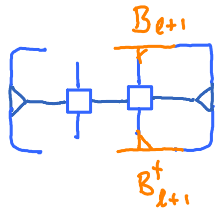
$\langle \Psi^{K}_{\alpha'} | \langle \sigma'_{\ell} | \langle \Phi^{K}_{\beta'} | \hat{H} | \Psi^{K}_{\alpha} \rangle | \sigma_{\ell} \rangle | \Phi^{K}_{\beta} \rangle =$  $=:$  H^{1s}_{ℓ} (14)

2-site (2s):

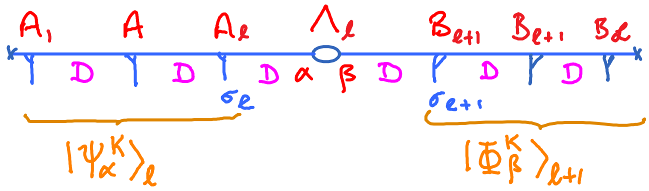
$\langle \Psi^{K}_{\alpha'} | \langle \sigma'_{\ell} | \langle \sigma'_{\ell+1} | \langle \Phi^{K}_{\beta'} | \hat{H} | \Psi^{K}_{\alpha} \rangle | \sigma_{\ell} \rangle | \sigma_{\ell+1} \rangle | \Phi^{K}_{\beta} \rangle =$  $=:$  H^{2s}_{ℓ} (15)

Related by:

 $H^{b}_{\ell} =$  $H^{1s} =$  H^{1s} (16)

 $H^{1s} =$  $H^{2b}_{\ell} =$  H^{2b}_{ℓ} (17)

3. Kept and discarded spaces

$|\psi[M]\rangle =$ 

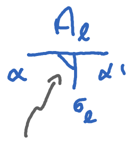
for simplicity: assume all virtual bonds have same dimension, D

Definition of kept spaces:

left 'kept' (K) space of site ℓ : $\quad \mathbb{V}^K_\ell = \mathrm{span}\{|\Psi^K_\alpha\rangle\} \subset \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_\ell$ (1)

right 'kept' (K) space of site ℓ : $\quad \mathbb{W}^K_{\ell+1} = \mathrm{span}\{|\Phi^K_\beta\rangle_{\ell+1}\} \subset \mathbb{V}_{\ell+1} \otimes \cdots \otimes \mathbb{V}_{\mathcal{L}}$ (2)

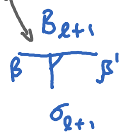
Action of isometries: generates new kept spaces:

$A_\ell : \underbrace{\mathbb{V}^K_{\ell-1} \otimes \mathbb{V}_{\sigma_\ell}}_{\text{'left parent (P) space'}} \to \mathbb{V}^K_\ell \,, \qquad |\Psi^K_\alpha\rangle_{\ell-1} |\sigma_\ell\rangle [A_\ell]^{\alpha\sigma_\ell}{}_{\alpha'} = |\Psi^K_{\alpha'}\rangle_\ell$  (3)

Dimensions: $D \cdot d \to D$

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

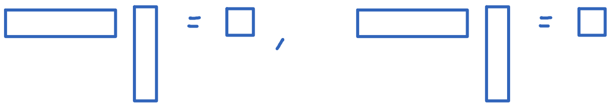
open triangles: 'kept'

$B_{\ell+1} : \underbrace{\mathbb{V}_{\sigma_{\ell+1}} \otimes \mathbb{W}^K_{\ell+2}}_{\text{'right parent (P) space'}} \to \mathbb{W}^K_{\ell+1} \,, \qquad [B_{\ell+1}]_\beta{}^{\sigma_{\ell+1}\beta'} |\Phi^K_{\beta'}\rangle_{\ell+2} |\sigma_{\ell+1}\rangle = |\Phi^K_\beta\rangle_{\ell+1}$  (4)

 $D \times (d \cdot D)$

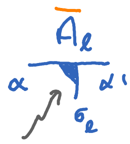
Dimensions: $d \cdot D \to D$

Isometric conditions, $\quad A^\dagger_\ell A_\ell \overset{(2.5)}{=} \mathbb{1}^K_\ell \,, \qquad B_{\ell+1} B^\dagger_{\ell+1} \overset{(2.6)}{=} \mathbb{1}^K_\ell \quad$ ensure orthonormality of kept basis states. (2.7, 8)

 (5)

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

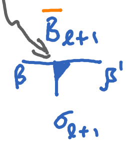
Let $\bar{A}_\ell$ and $\bar{B}_{\ell+1}$ be their <u>complements</u>, mapping onto 'discarded' (D) spaces <u>orthogonal</u> to kept ones:

$\bar{A}_\ell : \underbrace{\mathbb{V}^K_{\ell-1} \otimes \mathbb{V}_{\sigma_\ell}}_{\text{'left parent space'}} \to \mathbb{V}^D_\ell \,, \qquad |\Psi^K_\alpha\rangle_{\ell-1} |\sigma_\ell\rangle [\bar{A}_\ell]^{\alpha\sigma_\ell}{}_{\alpha'} = |\Psi^D_{\alpha'}\rangle_\ell$  (6)

Dimensions: $D \cdot d \to D \cdot d - D$

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

filled triangles: 'discarded'

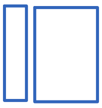
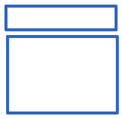
$\bar{B}_{\ell+1} : \underbrace{\mathbb{V}_{\sigma_{\ell+1}} \otimes \mathbb{W}^K_{\ell+2}}_{\text{'right parent space'}} \to \mathbb{W}^D_{\ell+1} \,, \qquad [\bar{B}_{\ell+1}]_\beta{}^{\sigma_{\ell+1}\beta'} |\Phi^K_{\beta'}\rangle_{\ell+2} |\sigma_{\ell+1}\rangle = |\Phi^D_\beta\rangle_{\ell+1}$  (7)

Dimensions: $d \cdot D \to d \cdot D - D$

 $(d \cdot D - D) \times (d \cdot D)$ (8)

Dimensions: $d\cdot D \;\to\; d\cdot D - D$  $(d\cdot D - D)\times(d\cdot D)$ (8)

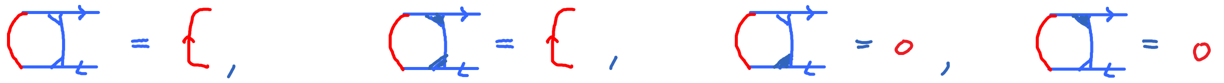
By definition, $\mathcal{A}_\ell = A_\ell \oplus \bar{A}_\ell$ and $\mathcal{B}_\ell = B_{\ell+1} \oplus \bar{B}_{\ell+1}$ are <u>unitary</u> maps on their parent spaces: (9)

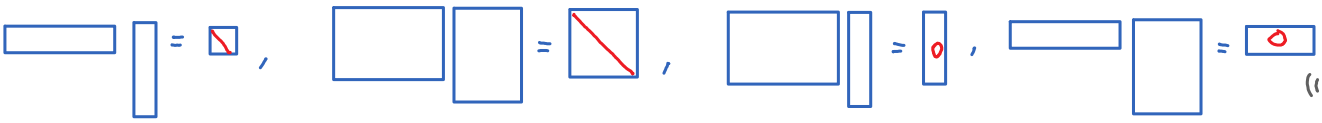
 $(D\cdot d)\times(D\cdot d)$  $(d\cdot D)\times(d\cdot D)$

Unitarity implies: $$\mathcal{A}_\ell^\dagger \mathcal{A}_\ell = \begin{pmatrix} A_\ell^\dagger \\ \hline \bar{A}_\ell^\dagger \end{pmatrix}\begin{pmatrix} A_\ell & \bar{A}_\ell \end{pmatrix} \overset{!}{=} \begin{pmatrix} A_\ell^\dagger A_\ell & A_\ell^\dagger \bar{A}_\ell \\ \bar{A}_\ell^\dagger A_\ell & \bar{A}_\ell^\dagger \bar{A}_\ell \end{pmatrix} = \overbrace{\begin{pmatrix} \mathbb{1}^K_\ell & 0 \\ 0 & \mathbb{1}^D_\ell \end{pmatrix}}^{\mathbb{1}^P_\ell} = \mathbb{1}^K_{\ell-1} \otimes \mathbb{1}_d \qquad (10)$$

'orthogonality':

$$A_\ell^\dagger A_\ell = \mathbb{1}^K_\ell, \qquad \bar{A}_\ell^\dagger \bar{A}_\ell = \mathbb{1}^D_\ell, \qquad \bar{A}_\ell^\dagger A_\ell = 0, \qquad A_\ell^\dagger \bar{A}_\ell = 0 \qquad (11)$$

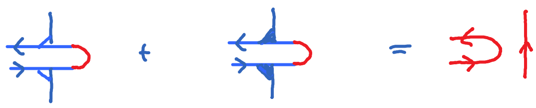
 (12)

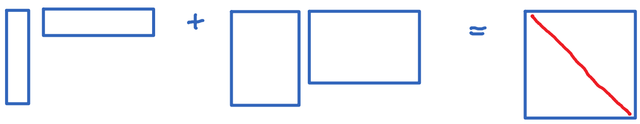
 (13)

'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: $$\mathcal{A}_\ell \mathcal{A}_\ell^\dagger = \begin{pmatrix} A_\ell & \bar{A}_\ell \end{pmatrix}\begin{pmatrix} A_\ell^\dagger \\ \hline \bar{A}_\ell^\dagger \end{pmatrix} \overset{!}{=} \begin{pmatrix} \mathbb{1}^K_\ell & \\ & \mathbb{1}^D_\ell \end{pmatrix} = \mathbb{1}^P_\ell = \mathbb{1}^K_{\ell-1} \otimes \mathbb{1}_d \qquad (15)$$

'completeness': $$A_\ell A_\ell^\dagger + \bar{A}_\ell \bar{A}_\ell^\dagger = \mathbb{1}^K_{\ell-1} \otimes \mathbb{1}_d \qquad (16)$$

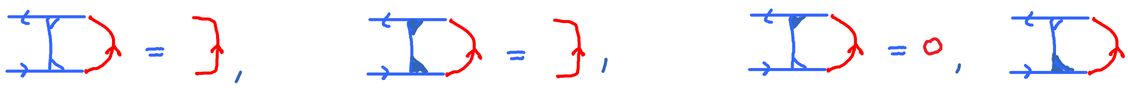
 (17)

 (18)

Similarly: $B_{\ell+1} B_{\ell+1}^\dagger = \mathbb{1}^P_\ell$ and $\mathcal{B}_{\ell+1}^\dagger \mathcal{B}_{\ell+1} = \mathbb{1}^P_\ell = \mathbb{1}_d \otimes \mathbb{1}^K_{\ell+1}$ imply: (19)

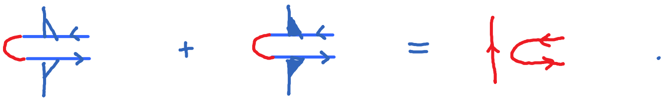
'orthogonality':

$$B_{\ell+1} B_{\ell+1}^\dagger = \mathbb{1}^K_\ell, \qquad \bar{B}_{\ell+1} \bar{B}_{\ell+1}^\dagger = \mathbb{1}^D_\ell, \qquad \bar{B}_\ell B_{\ell+1}^\dagger = 0, \qquad B_\ell \bar{B}_\ell^\dagger = 0, \qquad (20)$$

 (21)

'When K meets K, or D meets D, they yield unity; when K meets D or D meets K, they yield zero.'

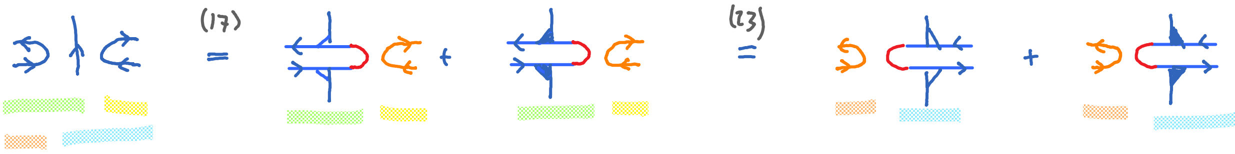
'completeness': $$B^{\dagger}_{\ell+1} B_{\ell+1} + \bar{B}^{\dagger}_{\ell+1} \bar{B}_{\ell+1} = \mathbb{1}_d \otimes \mathbb{1}^{K}_{\ell+1} \,, \tag{22}$$



(23)

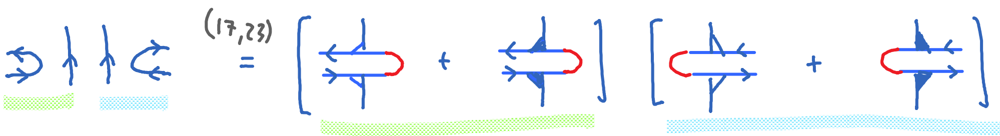
The completeness relations imply several identities that will be useful later:

1s projector can be expressed through bond projectors in two ways:

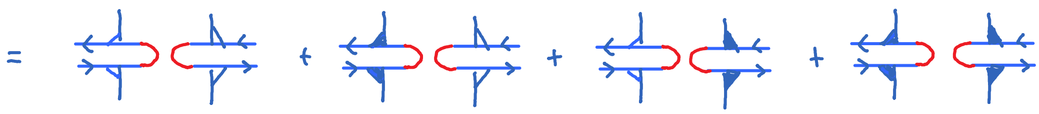


(24)

2s projector can be expressed through four bond projectors:

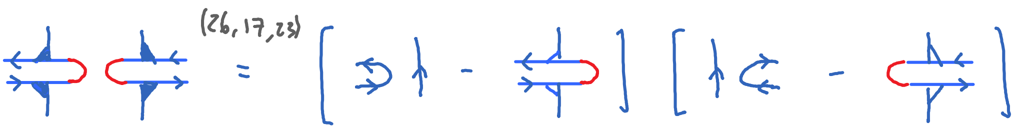


(25)

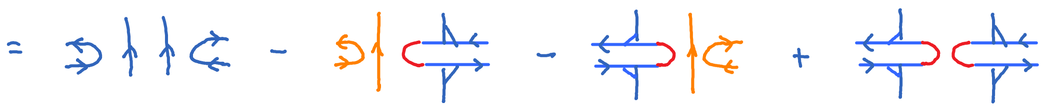


(26)

DD projector can be expressed through 2s, 1s and bond projectors that only involve K sectors:



(27)

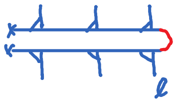


(28)

4. Kept and discarded projectors

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

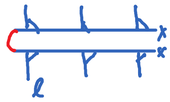
Left K projector (cf. MPS-II.1): $\ell \in [0, \mathcal{L}]$

$$\hat{P}^K_\ell := |\Psi^{K\alpha}\rangle_\ell \, {}_\ell\langle \Psi^K_\alpha| =$$ 

(sum over α implied)

$\hat{P}^K_0 := 1$

Right K projector: $\ell \in [1, \mathcal{L}+1]$

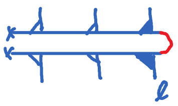
$$\hat{Q}^K_\ell := |\Phi^{K\beta}\rangle_\ell \, {}_\ell\langle \Phi^K_\beta| =$$ 

(sum over β implied)

$\hat{Q}^K_{\mathcal{L}+1} := 1$ (1)

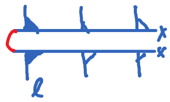
Left D projector (cf. MPS-II.1): $\ell \in [0, \mathcal{L}]$

Right D projector: $\ell \in [1, \mathcal{L}+1]$ (2)

$$\hat{P}^D_\ell := |\Psi^{D\alpha}\rangle_\ell \, {}_\ell\langle \Psi^D_\alpha| =$$ 

(sum over α implied)

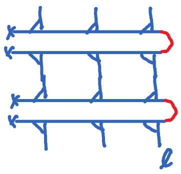
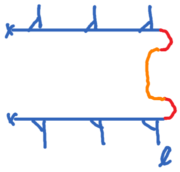
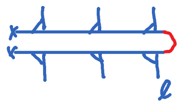
$\hat{P}^D_0 := 0$

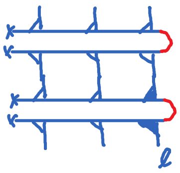
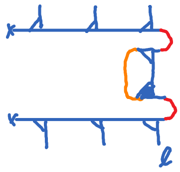
$$\hat{Q}^D_\ell := |\Phi^{D\beta}\rangle_\ell \, {}_\ell\langle \Phi^D_\beta| =$$  (3)

(sum over β implied)

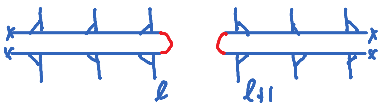
$\hat{Q}^D_{\mathcal{L}+1} := 0$

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

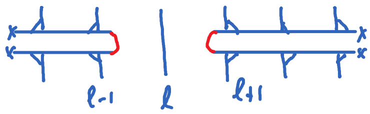
For example: $P^K_\ell P^K_\ell =$  $\overset{(2.7)}{=}$  $=$  $= P^K_\ell$ (5)

$P^D_\ell P^K_\ell =$  $\overset{(2.7)}{=}$  $\overset{(3.12)}{=} 0$ (6)

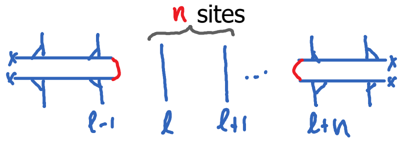
Bond projector: $\ell \in [0, \mathcal{L}]$

$$\hat{P}^b_\ell = \hat{P}^K_\ell \otimes \hat{Q}^K_{\ell+1} =$$  (7)

1s projector: $\ell \in [1, \mathcal{L}]$

$$\hat{P}^{1s}_\ell = \hat{P}^K_\ell \otimes \mathbb{1}_\ell \otimes \hat{Q}^K_{\ell+1} =$$  (8)

ns projector: $\ell \in [1, \mathcal{L}+1-n]$

$$\hat{P}^{ns}_\ell = \hat{P}^K_\ell \otimes \underbrace{\mathbb{1}_\ell \otimes \dots \otimes \mathbb{1}_{\ell+n-1}}_{n \text{ sites}} \otimes \hat{Q}^K_{\ell+2} =$$  (9)

Projector property: $\left(\hat{P}^b_\ell\right)^2 = \hat{P}^b_\ell$, $\quad \left(\hat{P}^{1s}_\ell\right)^2 = \hat{P}^{1s}_\ell$, $\quad \left(\hat{P}^{2s}_\ell\right)^2 = \hat{P}^{2s}_\ell$ (10)

follows from (2)

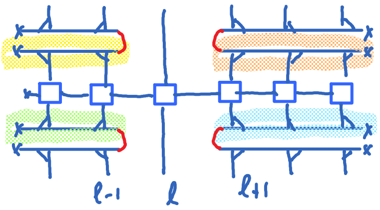
The projectors $\hat{P}^b_\ell$, $\hat{P}^{1s}_{\ell'}$, $\hat{P}^{2s}_{\ell''}$ mutually commute (since they are all diagonal in same basis $|\vec{\sigma}\rangle$)

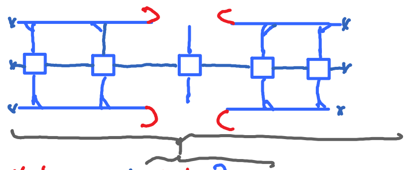
However, they are not mutually orthogonal (see below).

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

$$H^{b}_{\ell} = \hat{P}^{b}_{\ell}\,\hat{H}\,\hat{P}^{b}_{\ell}, \qquad H^{1s}_{\ell} = \hat{P}^{1s}_{\ell}\,\hat{H}\,\hat{P}^{1s}_{\ell}, \qquad H^{ns}_{\ell} = \hat{P}^{ns}_{\ell}\,\hat{H}\,\hat{P}^{ns}_{\ell} \tag{11}$$

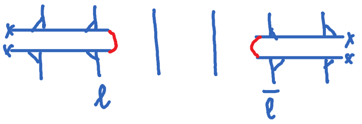
For example:

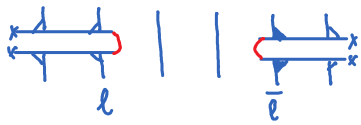
$$\hat{P}^{1s}_{\ell}\,\hat{H}\,\hat{P}^{1s}_{\ell} =$$ 

$$=$$  (12)

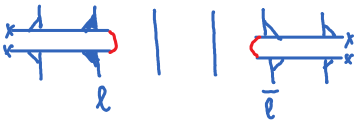
$$\langle \Psi^{K\alpha'} | \langle \sigma'_{\ell} | \langle \Phi^{K\beta'} | \hat{H} | \Psi^{K}_{\alpha} \rangle | \sigma_{\ell} \rangle | \Phi^{K}_{\beta} \rangle$$

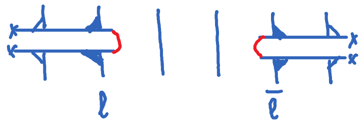
<u>Projectors for K and D sectors</u>

$P^{KK}_{\ell\bar{\ell}} =$ 

$P^{KD}_{\ell\bar{\ell}} =$ 

(13)

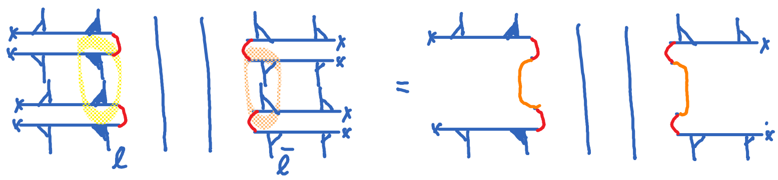
$P^{DK}_{\ell\bar{\ell}} =$ 

$P^{DD}_{\ell\bar{\ell}} =$ 

These fulfill numerous orthogonality relations; e.g.

Same-site-indices - orthogonal:

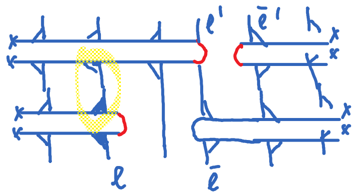
$$P^{X\bar{X}}_{\ell\bar{\ell}}\,P^{X'\bar{X}'}_{\ell\bar{\ell}} = \delta^{XX'}\,\delta^{\bar{X}\bar{X}'}\,P^{X\bar{X}}_{\ell\bar{\ell}}$$

e.g. 

D on earliest or latest site - yields zero: (14)

$$P^{D\bar{X}}_{\ell\bar{\ell}}\,P^{X'\bar{X}'}_{\ell'\bar{\ell}'} = 0 \quad \text{if} \quad \ell < \ell'$$

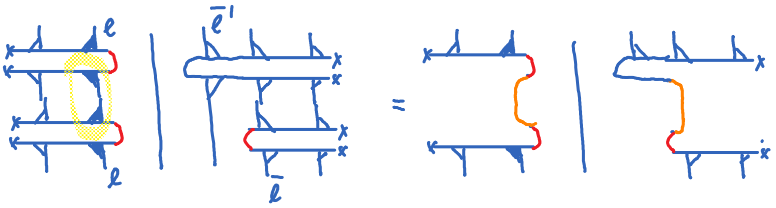
$$P^{X\bar{X}}_{\ell\bar{\ell}}\,P^{X'D}_{\ell'\bar{\ell}'} = 0 \quad \text{if} \quad \bar{\ell} < \bar{\ell}'$$

e.g.  $= 0$ (15)

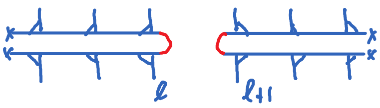
two D's on same side but different sites - yield zero:

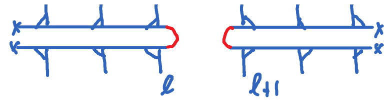
$$P^{D\bar{X}}_{\ell\bar{\ell}}\,P^{D\bar{X}'}_{\ell'\bar{\ell}'} \sim \delta_{\ell\ell'}$$

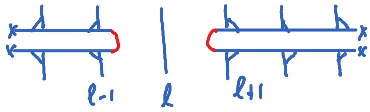
$$P^{XD}_{\ell\bar{\ell}}\,P^{X'D}_{\ell'\bar{\ell}'} \sim \delta_{\bar{\ell}\bar{\ell}'}$$

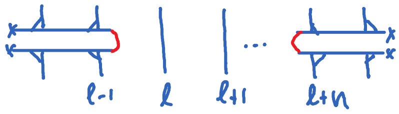
e.g.  (16)

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

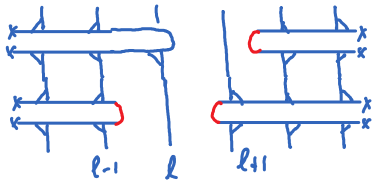
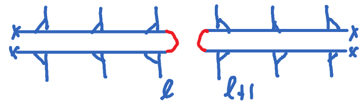
$$P^{0s}_{\ell+1} = \hat{P}^{b}_{\ell} = P^{KK}_{\ell,\ell+1} =$$  (17)

$P^{0s}_{\ell+1} = \hat{P}^{b}_{\ell} = P^{KK}_{\ell,\ell+1} =$  (17)

$\hat{P}^{1s}_{\ell} = P^{KK}_{\ell-1,\ell+1} =$  (18)

$\hat{P}^{ns}_{\ell} = P^{KK}_{\ell-1,\ell+n} =$  (19)

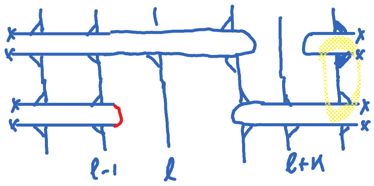
ns projectors are not orthogonal. E.g.

$P^{1s}_{\ell}\, P^{1s}_{\ell+1} = P^{0s}_{\ell+1} = P^{b}_{\ell}$, e.g.  =  (20)

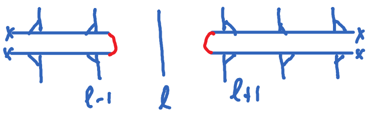
ns projector is annihilated by left D on its left or right D on its right:

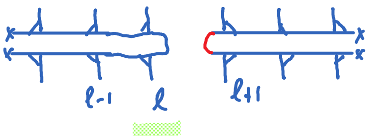
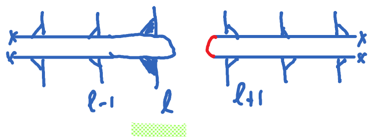
$P^{D\bar{X}}_{\ell\bar{\ell}}\, P^{ns}_{\ell'} = 0$ if $\ell < \ell'$

$P^{ns}_{\ell}\, P^{X'D}_{\ell'\bar{\ell}'} = 0$ if $\ell + n \le \ell'$

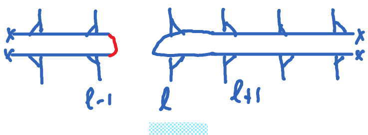
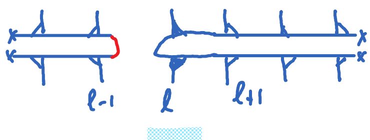
e.g.  $= 0$ (21)

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

$P^{1s}_{\ell} =$  (22)

$= \overbrace{P^{KK}_{\ell,\ell+1}}^{P^{b}_{\ell}} + P^{DK}_{\ell,\ell+1} =$  +  (23)

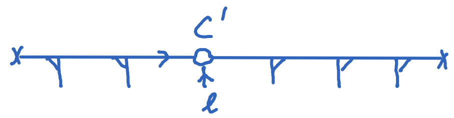
or

$= \overbrace{P^{KK}_{\ell-1,\ell}}^{P^{b}_{\ell-1}} + P^{KD}_{\ell-1,\ell} =$  +  (24)

5. Tangent space projector

Let $\mathbb{V}^{1s}$ denote the space of all 1s variations of $|\Psi\rangle$

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

$= \text{span}\{ |\Psi'\rangle =$  $, \ell \in [1, \mathcal{L}] \}$ (11)

formal definition: $= \text{span}\{ \text{im}(P^{1s}_\ell) \mid \ell \in [1, \mathcal{L}] \}$ (12)

↖ image

The 'tangent space projector' is defined by the property that its image is the tangent space:

$$\mathbb{V}^{1s} = \text{im}(P^{1s}), \quad \Rightarrow \quad \text{im}(P^{1s}_\ell) \subset \text{im}(P^{1s}) \quad \text{for all } \ell \in [1, \mathcal{L}] \tag{13}$$

Formally: P^{1s} has the defining properties: $(P^{1s})^2 = P^{1s}, \quad P^{1s} P^{1s}_\ell \overset{(13)}{=} P^{1s}_\ell$ (14)

We seek to construct P^{1s} explicitly. Note that $\sum_{\ell'=1}^{\mathcal{L}} P^{1s}_{\ell'}$ does not work, since summands are not mutually orthogonal (see below).

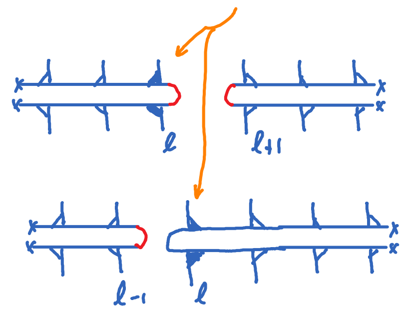
We attempt to orthogonalize them by a Gram-Schmidt type of procedure:

Define $P^{1s}_{\ell \lessgtr}$, obtained from P^{1s}_ℓ by projecting out the overlap with $P^{1s}_{\ell \pm 1}$: (15)

$$P^{1s}_{\ell \lessgtr} := P^{1s}_\ell \left(\mathbb{1}_V - P^{1s}_{\ell \pm 1} \right) \tag{16}$$

subtraction generates D sectors!

$$\overset{(4.20)}{=} \begin{cases} P^{1s}_\ell - P^b_\ell = P^{DK}_{\ell, \ell+1} & (17) \\ P^{1s}_\ell - P^b_{\ell-1} = P^{KD}_{\ell-1, \ell} & (18) \end{cases}$$



Note in (17) & (18): subtraction generates D sectors, via (3.17) & (3.24):

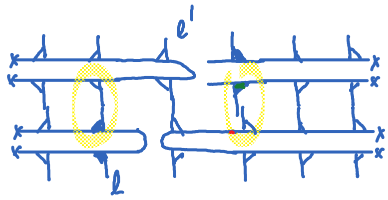
(19)

Due to the D's, the following orthogonality conditions hold:

$$P^{1s}_{\ell \lessgtr} P^{1s}_{\ell' \lessgtr} = \delta_{\ell\ell'} P^{1s}_{\ell \lessgtr}$$

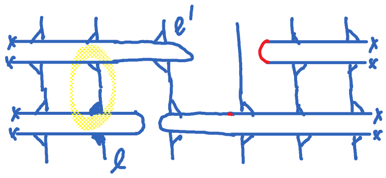
$$P^{1s}_{\ell\lessgtr}\, P^{1s}_{\ell'\lessgtr} = \delta_{\ell\ell'}\, P^{1s}_{\ell\lessgtr}$$

for all $\ell < \ell'$: $\quad P^{1s}_{\ell<}\, P^{1s}_{\ell'>} = 0 \quad$ e.g.



(20)

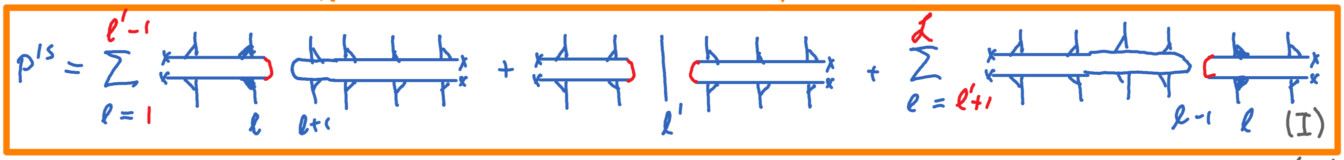
for all $\ell \lessgtr \ell'$: $\quad P^{1s}_{\ell\lessgtr}\, P^{1s}_{\ell'} = 0 \quad$ e.g.



(21)

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

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



(23)

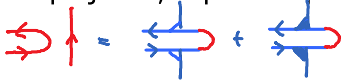
Properties (14) hold, because the summands are mutually orthogonal projectors: For example:

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

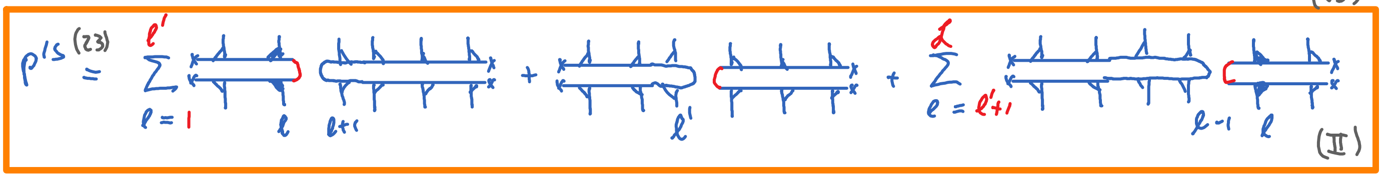
hence (13) holds: $\quad \mathrm{im}(P^{1s}_{\ell}) \subset \mathrm{im}(P^{1s}) \quad$ for all $\ell \in [1, \mathcal{L}]$

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

use (3.17) for ℓ' term of (22):



(25)

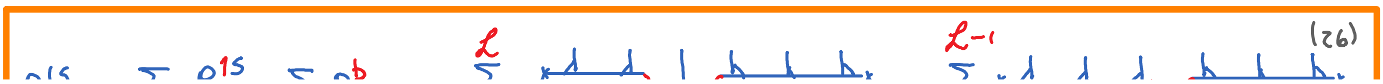


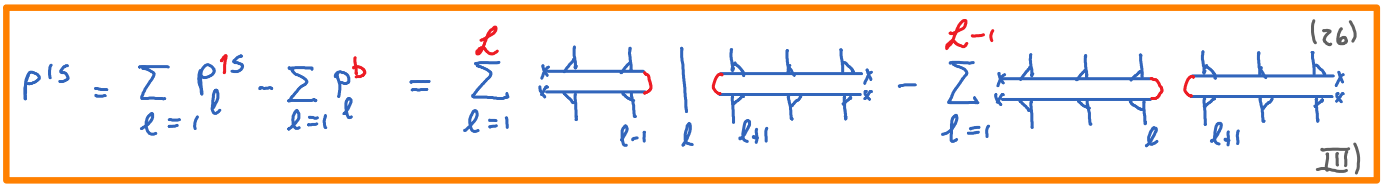
Another alternative expression for tangent space projector, expressed without any D sectors:

use (17), (18) in (22):

$$P^{1s} = \sum_{\ell=1}^{\ell'-1} \left(P^{1s}_{\ell} - P^{b}_{\ell} \right) + P^{1s}_{\ell} + \sum_{\ell=\ell'+1}^{\mathcal{L}} \left(P^{1s}_{\ell} - P^{b}_{\ell-1} \right) \qquad \text{for any } \ell' \in [1, \mathcal{L}] \qquad (25)$$

(26)





This form for tangent space projector is 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).