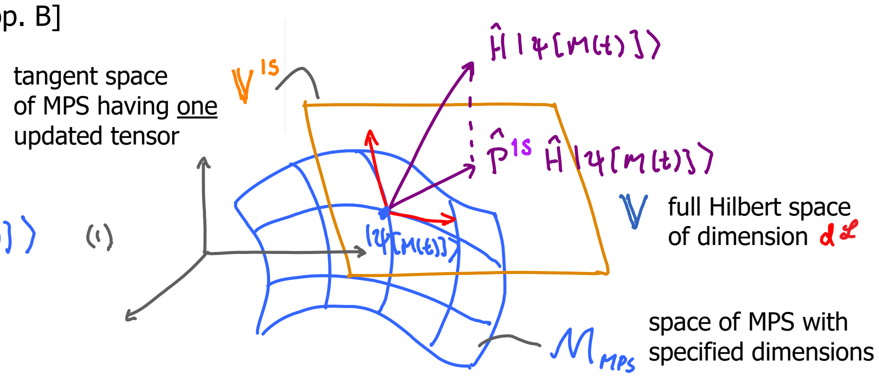
Time-dependent variational principle (TDVP)

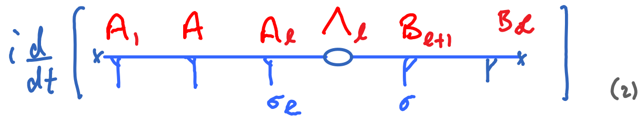
We consider time evolution using 'time-dependent variational principle' (TDVP)

1. 1-site TDVP [Haegeman2016, App. B]

Schrödinger equation for MPS:

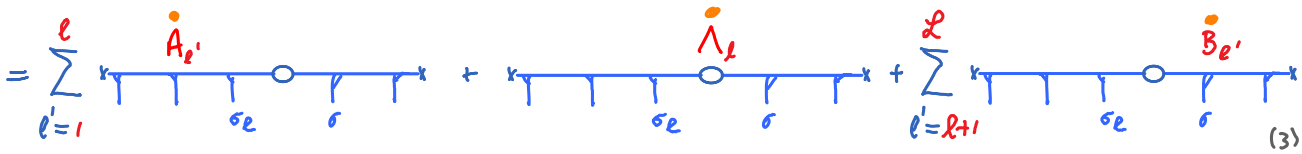


$$i\frac{d}{dt}|\Psi[M(t)]\rangle = \hat H|\Psi[M(t)]\rangle \qquad (1)$$



(2)

if we insist on using MPS with fixed bond dimensions, left side has following form:



(3)

Each term differs from $|\Psi(t)\rangle$ by precisely one site tensor or one bond tensor, so left side is a state in the tangent space, $\mathbb{V}^{1s}$ of $|\Psi(t)\rangle$. But right side of (1) is not, since since $H|\Psi(t)\rangle$ can have larger bond dimensions than $|\Psi(t)\rangle$.

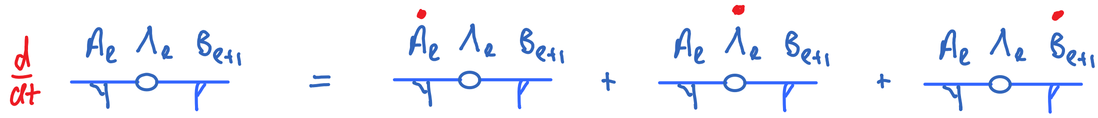
So, project right side of (1) to $\mathbb{V}^{1s}$:

$$i\frac{d}{dt}|\Psi[M(t)]\rangle \simeq \hat P^{1s}\hat H|\Psi[M(t)]\rangle \qquad (4)$$

tangent space approximation

Left and right sides of (4) are structurally consistent. To see this, consider bond ℓ

Left side of (4) contains:



(5)

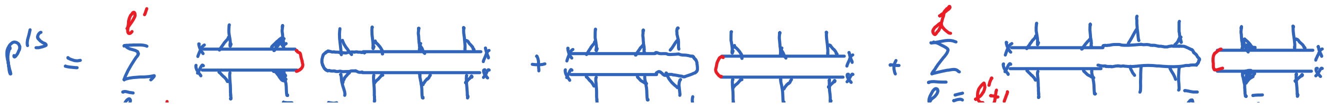
Decompose: $\dot A_\ell \Lambda_\ell = A_\ell \Lambda'_\ell + \bar A_\ell \bar\Lambda'_\ell$, $\Lambda_\ell \dot B_{\ell+1} = \Lambda''_\ell B_{\ell+1} + \bar\Lambda'' \bar B_{\ell+1}$ (6)

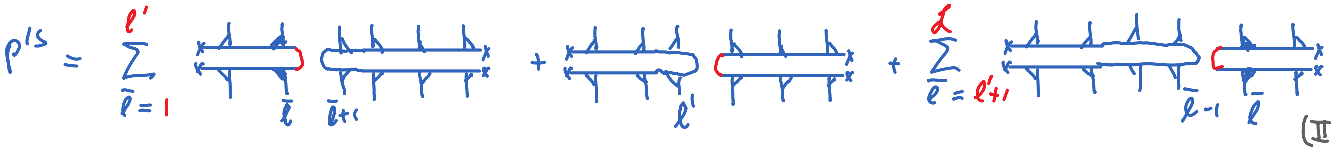
Then we find:

(7)

Right side of (4) requires tangent space projector. Consider its form (TS-I.5.25):

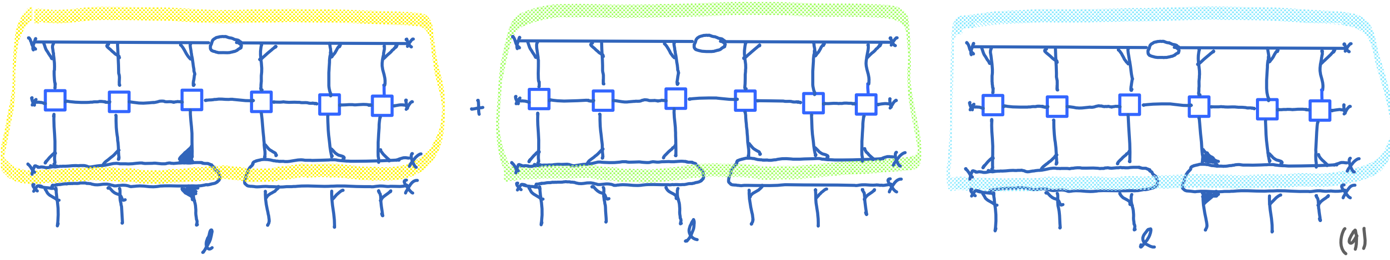
(8)





(II)

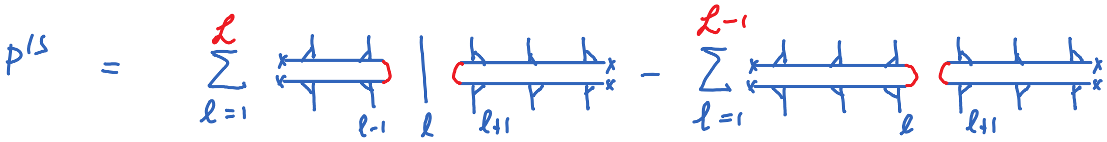
The three terms with $\bar{\ell} = \ell$, $\ell' = \ell$, $\bar{\ell} = \ell+1$, applied to $\hat{H}|\Psi(t)\rangle$, yield



(9)

matching structure of (7). Thus, P^{1s}, applied to $H|\Psi(t)\rangle$, yields terms of precisely the right structure!

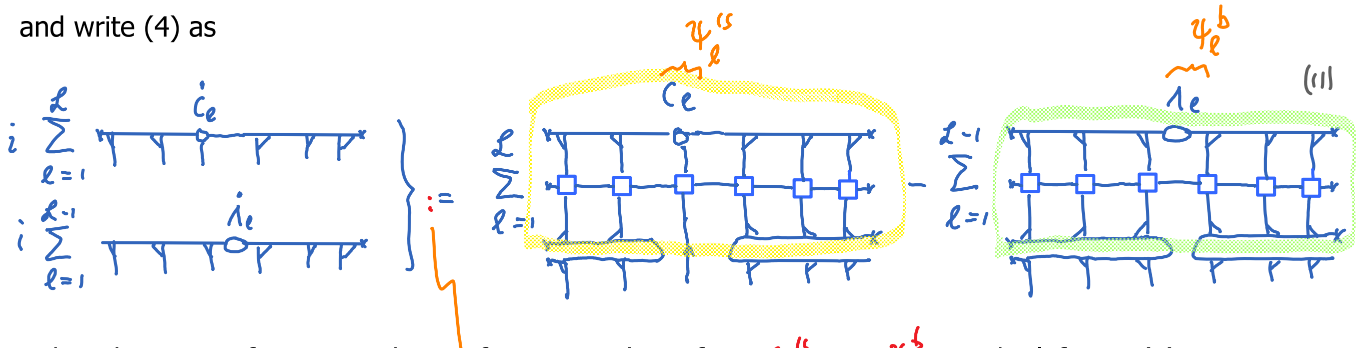
To integrate projected Schrödinger eq. (4), we write tangent space projector in the form (TS.5.26):



(10)

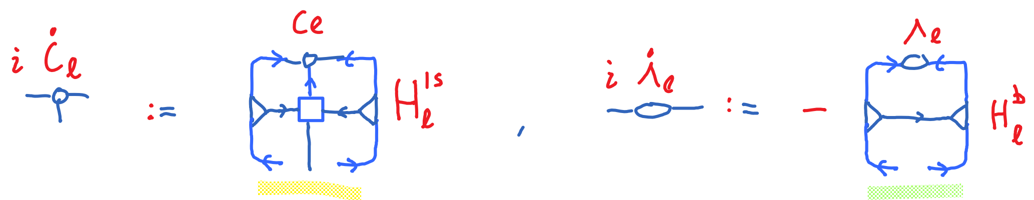
and write (4) as

or



(11)

Right side is sum of terms, each specifying an update of one ψ^{1s}_ℓ or ψ^b_ℓ on the left. Eq. (4) can be integrated one site at a time, by defining the updates through the following local Schrödinger equations:



(12)

In site-canonical form, site ℓ involves two terms linear in C_ℓ : $\quad i\dot{C}_\ell(t) = H^{1s}_\ell C_\ell(t)$ (13)

Their contribution can be integrated exactly: replace $C_\ell(t)$ by $\quad C_\ell(t+\tau) = e^{-iH^{1s}_\ell\tau} C_\ell(t)$ (14)

forward time step

In bond-canonical form, site ℓ involves two terms linear in Λ_ℓ : $\quad -i\dot{\Lambda}_\ell(t) = H^b_\ell \Lambda_\ell(t)$ (15)

Their contribution can be integrated exactly: replace $\Lambda_\ell(t)$ by $\quad \Lambda_\ell(t-\tau) = e^{iH^b_\ell\tau}\Lambda_\ell(t)$ (16)

backward(!) time step

In practice, $e^{-iH_\ell^{1s}\tau}C_\ell$ and $e^{iH_\ell^b\tau}\Lambda_\ell$ are computed by using Krylov methods.

Build a Krylov space by applying H_ℓ^{1s} multiple times to C_ℓ, set up the tridiagonal representation $[H_\ell^{1s}]_{\text{Krylov}}$ of H_ℓ^{1s} in this basis, then compute the matrix exponential in this basis, and apply result to C_ℓ.
Likewise for H_ℓ^b and Λ_ℓ.

To successively update entire chains, alternate between site- and bond-canonical form, propagating forward or backward in time with H_ℓ^{1s} or H_ℓ^b, respectively:

1. Forward sweep, for $\ell = 1, \dots, \mathcal{L}-1$, starting from $\underbrace{B_1(t)}_{C_1(t) :=} B_2(t) \dots B_{\mathcal{L}}(t)$ (17)

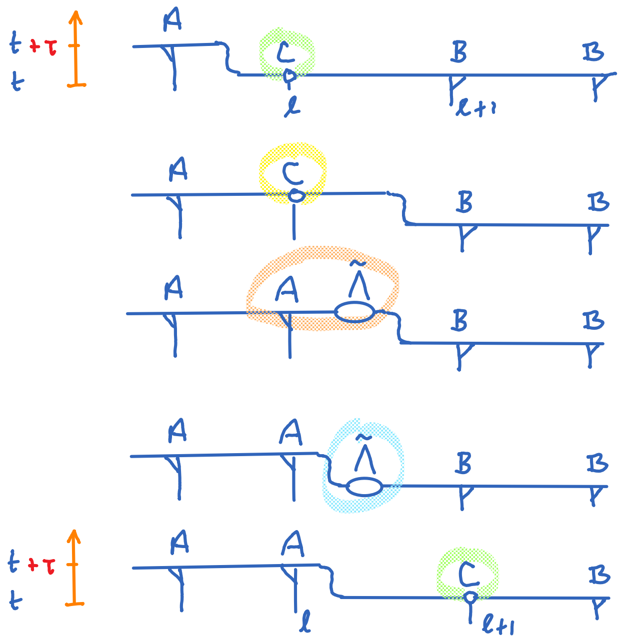
$$C_\ell(t)\, B_{\ell+1}(t)$$

$$\xrightarrow[1(a)]{H_\ell^{1s}} \underbrace{C_\ell(t+\tau)}_{1(b)}\, B_{\ell+1}(t)$$

$$= \overbrace{A_\ell(t+\tau)\, \tilde{\Lambda}_\ell(t+\tau)}\, B_{\ell+1}(t)$$

$$\xrightarrow[1(c)]{H_\ell^b} A_\ell(t+\tau)\, \underbrace{\tilde{\Lambda}_\ell(t)\, B_{\ell+1}(t)}_{1(d)}$$

$$= A_\ell(t+\tau)\, C_{\ell+1}(t) \qquad (18)$$

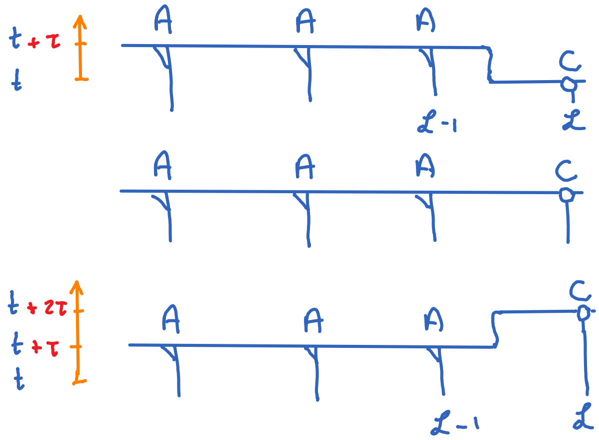


until we reach last site, and MPS described by $A_1(t+\tau) \dots A_{\mathcal{L}-1}(t+\tau)\, C_{\mathcal{L}}(t)$ (19)

2. Turn around: $C_{\mathcal{L}}(t)$

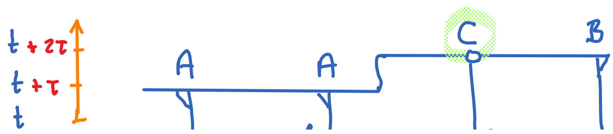
$$\xrightarrow[2(a)]{H_{\mathcal{L}}^{1s}} C_{\mathcal{L}}(t+\tau)$$

$$\xrightarrow[2(b)]{H_{\mathcal{L}}^{1s}} C_{\mathcal{L}}(t+2\tau) \qquad (20)$$



3. Backward sweep, for $\ell = \mathcal{L}-1, \dots, 1$, starting from $A_1(t+\tau) \dots A_{\mathcal{L}-1}(t+\tau)\, C_{\mathcal{L}}(t+2\tau)$ (21)

$$A_\ell(t+\tau)\, C_{\ell+1}(t+2\tau)$$



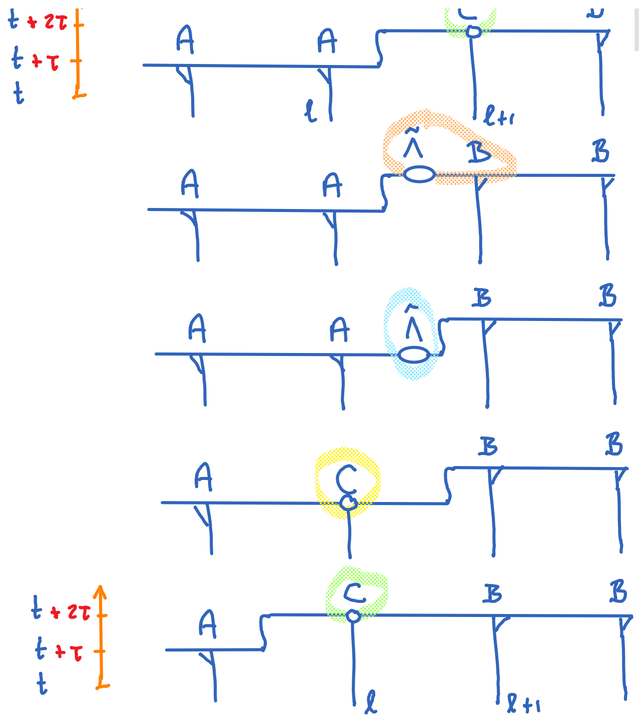
$$A_\ell(t+\tau)\,C_{\ell+1}(t+2\tau)$$

$$\underset{3(a)}{=} \quad A_\ell(t+\tau)\,\tilde{\Lambda}_\ell(t+2\tau)\,B_{\ell+1}(t+2\tau)$$

$$\xrightarrow[3(b)]{H^b_\ell} \quad A_\ell(t+\tau)\,\underbrace{\hat{\Lambda}_\ell(t+\tau)}_{3(c)}\,B_{\ell+1}(t+2\tau)$$

$$= \quad C_\ell(t+\tau)\,B_{\ell+1}(t+2\tau)$$

$$\xrightarrow[3(d)]{H^{1s}_\ell} \quad C_\ell(t+2\tau)\,B_{\ell+1}(t+2\tau)$$



(22)

until we reach first site, and MPS described by $\quad C_1(t+2\tau)\,B_2(t+2\tau)\dots B_{\mathcal{L}}(t+2\tau)$ (23)

The scheme described above involves 'one-site updates'. This has the (major!) drawback (as in one-site DMRG), that it is not possible to dynamically explore different symmetry sectors. To overcome this drawback, a 'two-site update' version of tangent space methods can be set up [Haegemann2016, App. C].

A systematic comparison of various MPS-based time evolution schemes has been performed in [Paeckel2019]. Conclusion: 2-site-update tangent space scheme is most accurate!

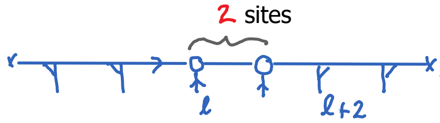
A scheme for doing 1-site TDVP while nevertheless expanding bonds, called 'controlled bond expansion (CBE), was proposed in [Li2022] (see next lecture!).

2. 2-site projectors P^{2s}

The construction of tangent space $\mathbb{V}^{1s}$ and its projector P^{1s} can be generalized to n sites [Gleis2022a].

We focus on $n = 2$ (but general case is analogous). Define space of 2-site variations:

$\mathbb{V}^{2s}$ = span of all states $|\Psi'\rangle$ differing from $|\Psi\rangle$ on at most 2 neighboring sites

$$= \mathrm{span}\left\{ |\Psi'\rangle = \right.$$ 

$$\left. , \ \ell \in [1, \mathcal{L}-1] \right\} \qquad (1)$$

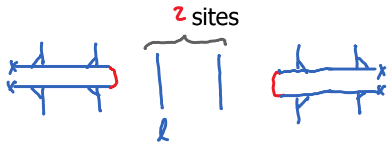
formal definition: $$= \mathrm{span}\left\{ \mathrm{im}\left(P^{2s}_\ell\right) \mid \ell \in [1, \mathcal{L}-1] \right\} \qquad (2)$$

$\uparrow$ image

Recall:

<u>local</u> 2s projector: $\ell \in [1, \mathcal{L}-1]$

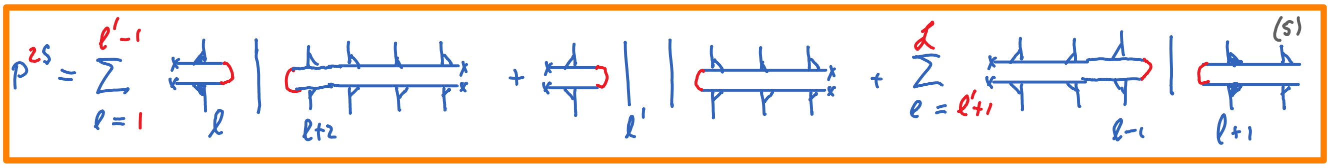
$$\hat{P}^{2s}_\ell = \qquad (3)$$ (TS-I.4.9)



<u>Global</u> 2s projector $\hat{P}^{2s}$, such that $\mathbb{V}^{2s} = \mathrm{im}\left(P^{2s}\right)$, can be found with a Gram-Schmidt scheme analogous to our construction of $\hat{P}^{1s}$, see [Gleis2022a]:

compare (TS-I.5.22) (4)

$$P^{2s} := \sum_{\ell=1}^{\ell'-1} \underbrace{P^{2s}_{\ell<}}_{P^{2s}_\ell - P^{1s}_{\ell+1} = P^{DK}_{\ell,\ell+2}} + P^{2s}_{\ell'} + \sum_{\ell=\ell'+1}^{\mathcal{L}-1} \underbrace{P^{2s}_{\ell>}}_{P^{2s}_\ell - P^{1s}_\ell = P^{KD}_{\ell-1,\ell+1}} \quad \text{for any } \ell' \in [1, \mathcal{L}-1]$$



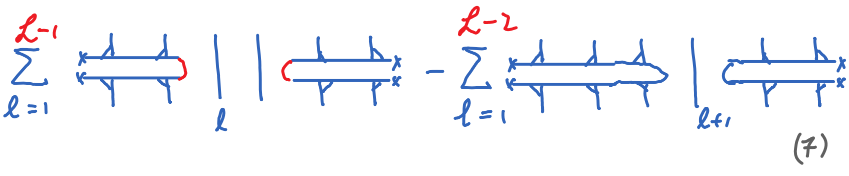
All summands are mutually orthogonal, ensuring that $(P^{2s})^2 = P^{2s}$, and that $P^{2s} P^{2s}_{\ell'} = P^{2s}_{\ell'}$.

(6)

Alternative expression:

compare (TS.5.26)

$$P^{2s} = \sum_{\ell=1}^{\mathcal{L}-1} P^{2s}_\ell - \sum_{\ell=1}^{\mathcal{L}-2} P^{1s}_{\ell+1} = $$



This projector is used for 2-site TDVP (see TS-II.3)

<u>Orthogonal n-site projectors</u>

For any given MPS $|\Psi[M]\rangle$, full Hilbert space of chain can be decomposed into mutually orthogonal subspaces:

$$\mathbb{V} = \mathbb{V}_1 \otimes \cdots \otimes \mathbb{V}_{\mathscr{L}} = \bigoplus_{n=0}^{\mathscr{L}} \mathbb{V}^{n\perp} \qquad (8)$$

with $\mathbb{V}^{0\perp} := \mathbb{V}^{0s} := \mathrm{span}\{|\Psi\rangle\}$ (9)

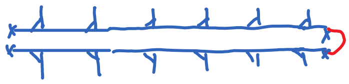
'irreducible' $\mathbb{V}^{n\perp}$ is complement of $\mathbb{V}^{(n-1)s}$ in $\mathbb{V}^{ns} = \mathbb{V}^{(n-1)s} \oplus \mathbb{V}^{n\perp}$ (10)

= span of states differing from $|\Psi\rangle$ on n contiguous sites, not expressible through subsets of $n' < n$ sites

Correspondingly, identity can be decomposed as:

$$\mathbb{1}_{\mathbb{V}} = \mathbb{1}_d^{\otimes \mathscr{L}} = \underbrace{\sum_{n=0}^{\mathscr{L}} P^{n\perp}}_{\text{completeness}} \quad , \quad \underbrace{P^{n\perp} P^{n'\perp} = \delta^{nn'} P^{n\perp}}_{\text{orthogonality}} \qquad (11)$$

where $P^{\perp n}$ is defined as the projector having $\mathbb{V}^{n\perp}$ as image: $\mathrm{im}(P^{n\perp}) = \mathbb{V}^{n\perp}$ (12)

$$P^{0\perp} = P^{0s} = |\Psi\rangle\langle\Psi| =$$  (13)

$$n \geq 1: \quad P^{n\perp} := P^{ns}\left(\mathbb{1}_{\mathbb{V}} - P^{(n-1)s}\right) = P^{ns} - P^{(n-1)s} \qquad (14)$$

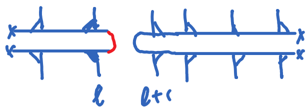
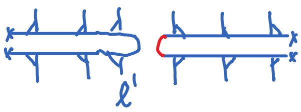
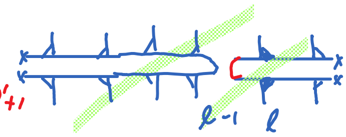
since $\mathbb{V}^{(n-1)s} \subset \mathbb{V}^{ns} \Rightarrow \mathrm{im}(P^{(n-1)s}) \subset \mathrm{im}(P^{ns})$

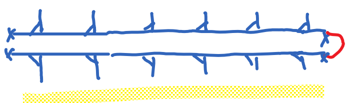
$\Rightarrow P^{ns} P^{(n-1)s} = P^{(n-1)s}$

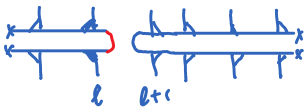
Consider n=1:

$$P^{1\perp} = P^{1s} - P^{0s}$$

(TS-I.5.26)

$= \sum_{\ell=1}^{\ell'}$  $+$  $+ \sum_{\ell=\ell'+1}^{\mathscr{L}}$ 

choose $\ell' = \mathscr{L}$ $\quad -$  (15)

$= \sum_{\ell=1}^{\mathscr{L}}$  $= \sum_{\ell=1}^{\mathscr{L}} P^{DK}_{\ell,\ell+1}$

projects onto all 1-site variations orthogonal to $|\Psi\rangle$ (16)

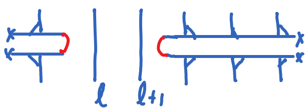
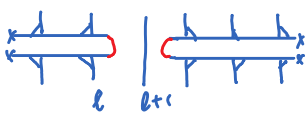
Consider n=2:

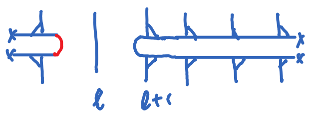
(TS.4.17) $P^{0s}_{\ell+1} = P^{b}_{\ell}$

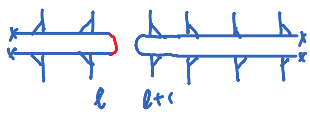
$$P^{2\perp} = P^{2s} - P^{1s} = \left(\sum_{\ell=1}^{\mathscr{L}-1} P^{2s}_{\ell} - \sum_{\ell=2}^{\mathscr{L}-1} P^{1s}_{\ell}\right) - \left(\sum_{\ell=1}^{\mathscr{L}} P^{1s}_{\ell} - \sum_{\ell=1}^{\mathscr{L}-1} P^{b}_{\ell}\right) \qquad (17)$$

move $P^{1s}_{\mathscr{L}}$ from 3rd to 2nd term

$$= \sum_{\ell=1}^{\mathscr{L}-1}\left(P^{2s}_{\ell} - P^{1s}_{\ell+1} - P^{1s}_{\ell} + P^{0s}_{\ell+1}\right) \qquad (18)$$

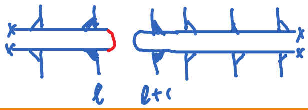
$= \sum_{\ell=1}^{\mathscr{L}-1} \Big($  $-$ 

$-$ 

$+$ 

$\Big)$ (19)

(TS.3.28)

$= \sum_{\ell=1}^{\mathcal{L}-1}$ 

$= \sum_{\ell=1}^{\mathcal{L}-1} P^{DD}_{\ell,\ell+1}$ very important result! (20)

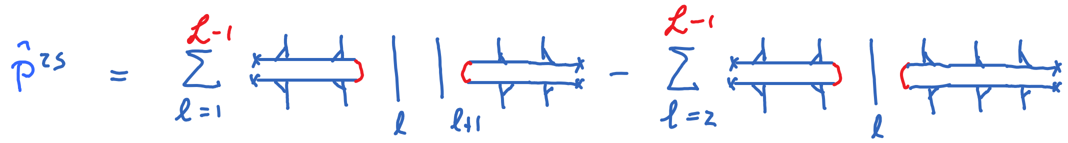
3. 2-site TDVP (optional)

[Haegeman2016, Sec. V & App. C]

2-site tangent space methods are analogous to 1-site methods, but use a 2-site projector. There is a conceptual difference, though: the main reason for using 2-site schemes is that they allow sectors with new quantum numbers to be introduced if the action of H requires this. However, states with different ranges of quantum numbers live in different manifolds, hence this procedure 'cannot easily be captured in a smooth evolution described using a differential equation. However, like most numerical integration schemes, the aforementioned algorithm is intrinsically discrete by choosing a time step, and it poses no problem to formulate an analogous two-site algorithm'. [Haegeman2016, Sec. V]. In other words: the tangent space approach is conceptually not as clean for the 2-site as for the 1-site scheme.

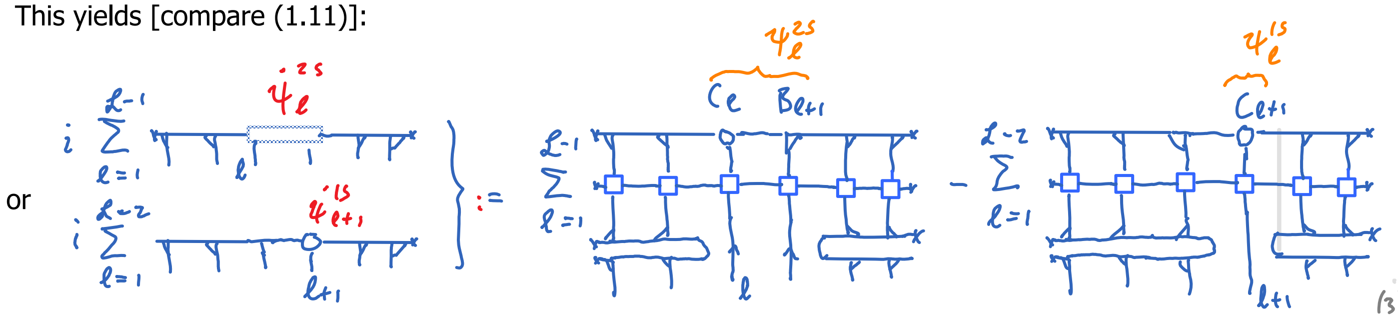
Schrödinger equation, projected onto 2-site tangent space, now takes the form (1)

$$i \frac{d}{dt} |\psi[M(t)]\rangle = \hat P^{2s} \hat H \, |\psi[M(t)]\rangle$$



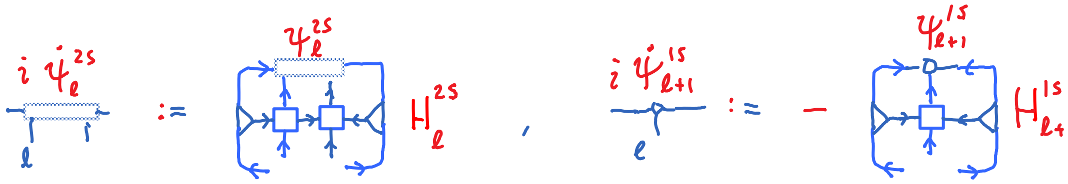
(2)

This yields [compare (1.11)]:



(3)

Right side is sum of terms, each specifying an update of one ψ^{2s}_ℓ or ψ^{1s}_ℓ on the left. Eq. (4) can be integrated one site at a time, by defining the updates through the following local Schrödinger equations:



(4)

Right side is sum of terms, each linear in a factor appearing on the left. Can be integrated one site at a time:

In 2-site-canonical form, site ℓ involves two terms linear in ψ^{2s}_ℓ : $\quad i\,\dot\psi^{2s}_\ell(t) = H^{2s}_\ell \, \psi^{2s}_\ell(t)$ (5)

Their contribution can be integrated exactly: replace $\psi^{2s}_\ell(t)$ by $\psi^{2s}_\ell(t+\tau) = e^{-iH^{2s}_\ell \tau}\, \psi^{2s}_\ell(t)$ (6)

forward time step

In 1-site-canonical form, site $\ell+1$ involves two terms linear in $\psi^{1s}_{\ell+1}$: $\quad -i\,\dot\psi^{1s}_{\ell+1}(t) = H^{1s}_{\ell+1}\, \psi^{1s}_{\ell+1}(t)$ (7)

Their contribution can be integrated exactly: replace $\psi^{1s}_{\ell+1}(t)$ by $\psi^{1s}_{\ell+1}(t-\tau) = e^{iH^{1s}_{\ell+1}\tau}\,\psi^{1s}_{\ell+1}(t)$ (8)

backward(!) time step

To successively update entire chains, alternate between 2-site- and 1-site-canonical form,
propagating forward or backward in time with H^{2s}_{ℓ} or H^{1s}_{ℓ} , respectively (analogously to 1-site scheme).

A systematic comparison of various MPS-based time evolution schemes has been performed in [Paeckel2019]. Conclusion: 2-site-update tangent space scheme is most accurate!