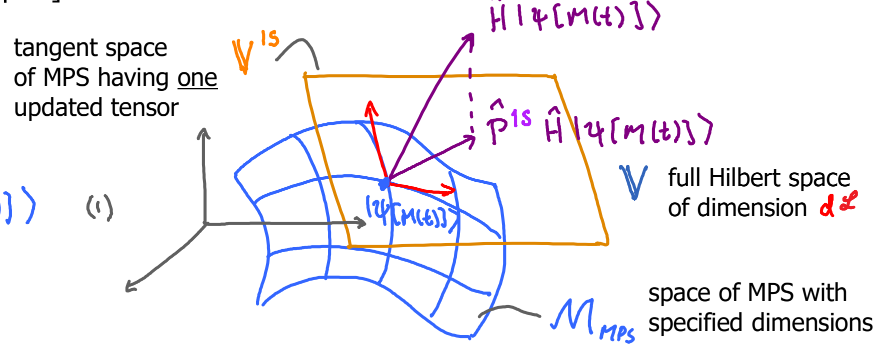
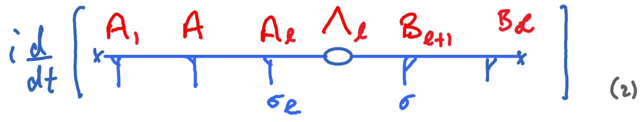
We consider time evolution using 'time-dependent variational principle' (TDVP)

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

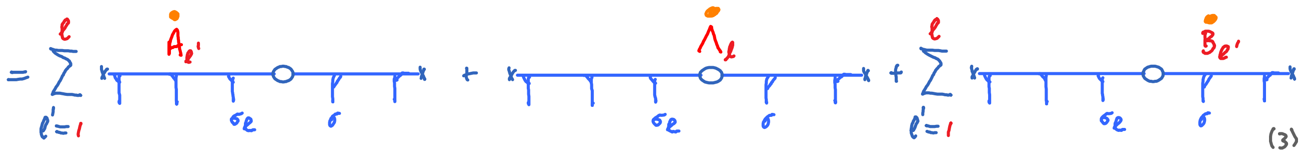
Schrödinger equation for MPS:

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




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




Each term differs from $|\Psi(t)\rangle$ by precisely one site tensor or on 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 $|\Psi(t)\rangle$.

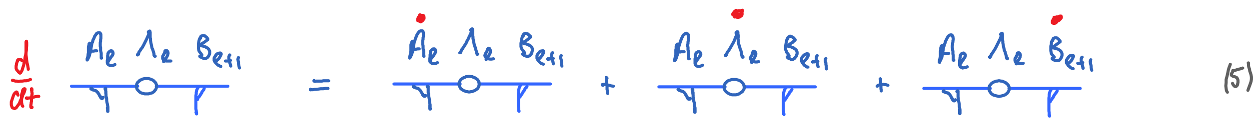
So, project right side of (1) to $\mathbb{V}^{1s}$ :

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

tangent space approximation

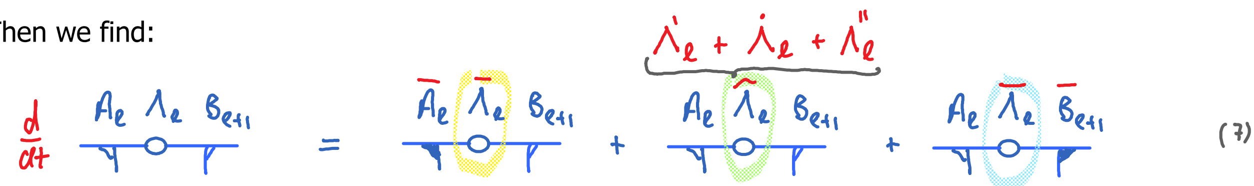
Left and right sides of (4) are structurally consistent. To see this, consider bond $\ell$

Left side of (4) contains:

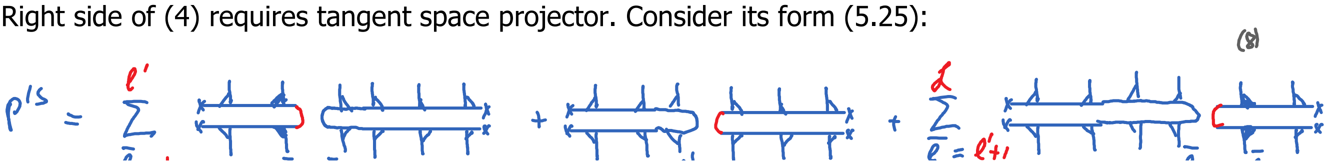


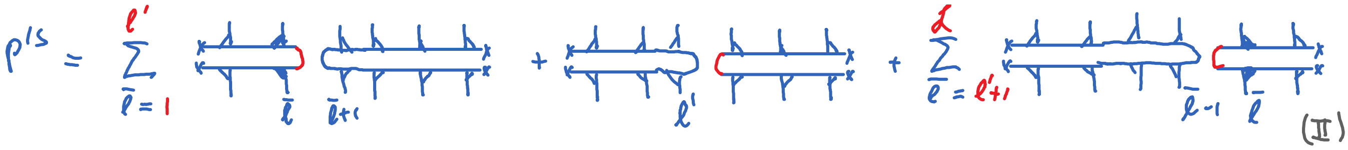

Decompose: $\dot{A}_\ell = A_\ell \Lambda'_\ell + \bar{A}_\ell \bar{\Lambda}'_\ell \quad , \quad \dot{B}_{\ell+1} = \Lambda''_\ell B_{\ell+1} + \bar{\Lambda}''\bar{B}_{\ell+1}$ (6)

Then we find:



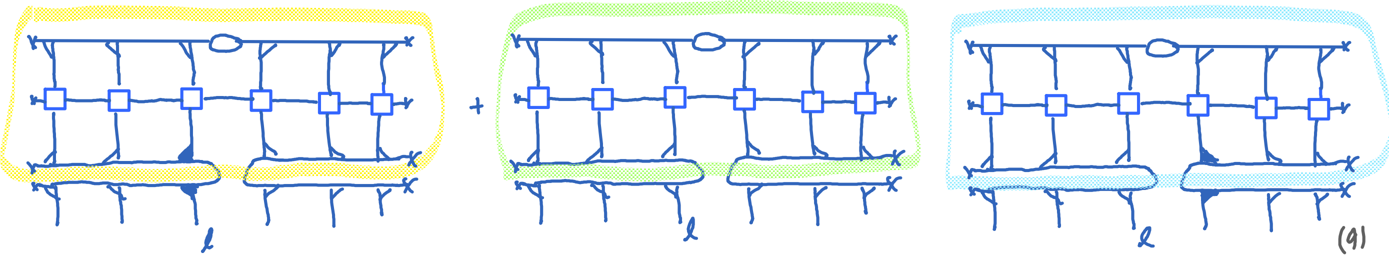

Right side of (4) requires tangent space projector. Consider its form (5.25):





(II)

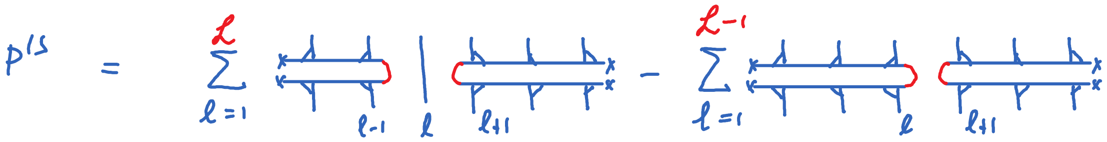
The three terms with $\bar{\ell} = \ell$, $\ell' = \ell$, $\bar{\ell} = \ell+1$, applied to $\hat{H}|\Psi(t)\rangle$, yield



(9)

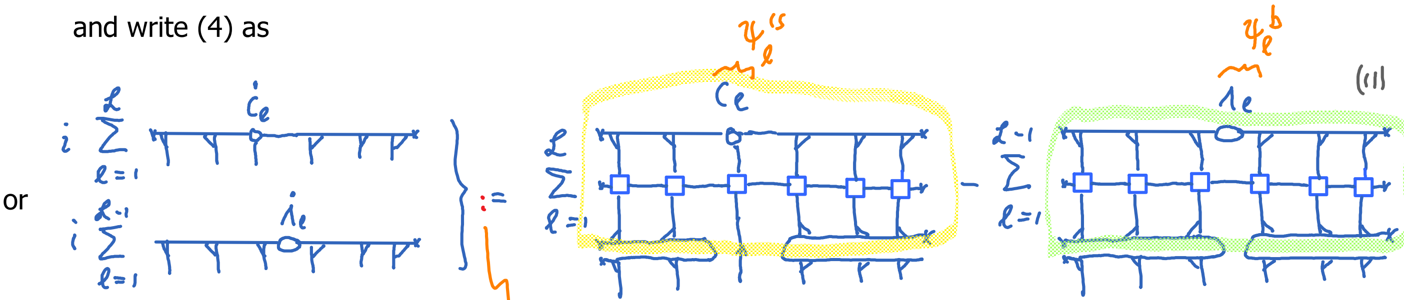
matching structure of (7). Thus, $P^{1s}$, applied to $H|\Psi(t)\rangle$, yields terms of precisely the right structure!

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



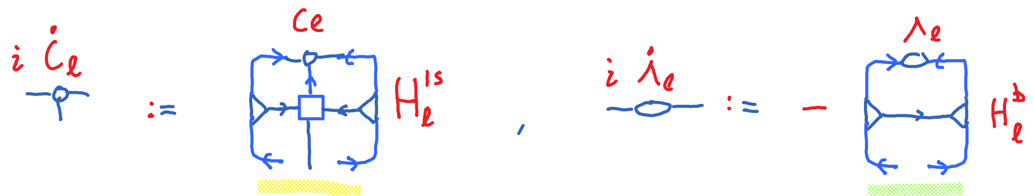
(10)

and write (4) as



(11)

Right side is sum of terms, each specifying an update of one $\psi^{1s}_\ell$ or $\psi^b_\ell$ 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 $\ell$ involves two terms linear in $C_\ell$ : $\quad i\dot{C}_\ell(t) = H^{1s}_\ell C_\ell(t)$ (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 $\ell$ involves two terms linear in $\Lambda_\ell$ : $\quad i\dot{\Lambda}_\ell(t) = -H^b_\ell \Lambda_\ell(t)$ (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

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 $H_\ell^{1s}$ multiple times to $C_\ell$, set up the tridiagonal representation $[H_\ell^{1s}]_{Krylov}$ of $H_\ell^{1s}$ in this basis, then compute the matrix exponential in this basis, and apply result to $C_\ell$.
Likewise for $H_\ell^b$ and $\Lambda_\ell$.

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

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

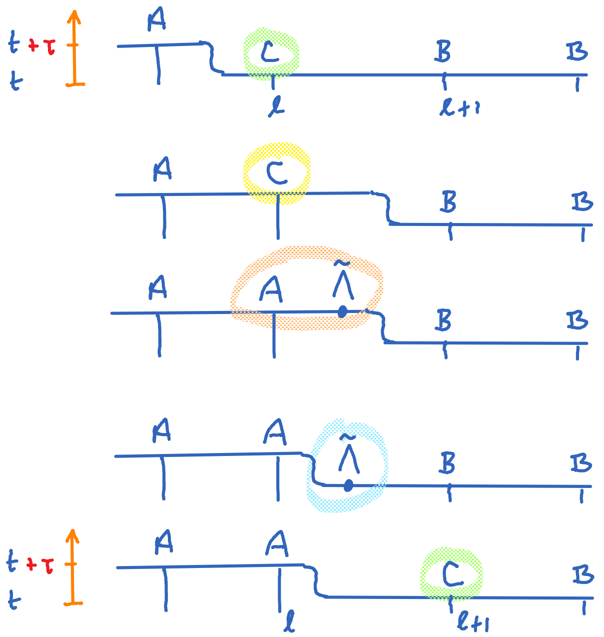
$$C_\ell(t)\,B_{\ell+1}(t)$$

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

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

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

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

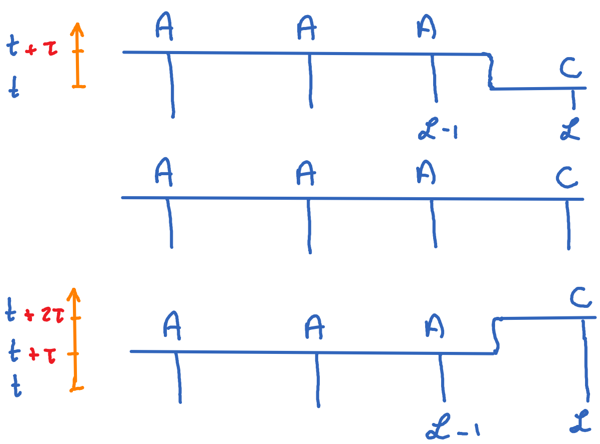



until we reach last site, and MPS described by $A_1(t+\tau)\dots A_{\mathcal{L}-1}(t+\tau)\,C_{\mathcal{L}}(t)$ (19)

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

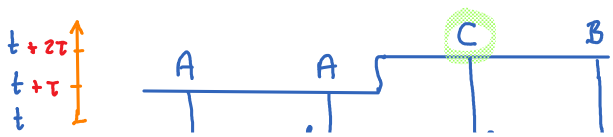
$$\xrightarrow[2(a)]{H_{\mathcal{L}}^{1s}} C_{\mathcal{L}}(t+\tau)$$

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




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)

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



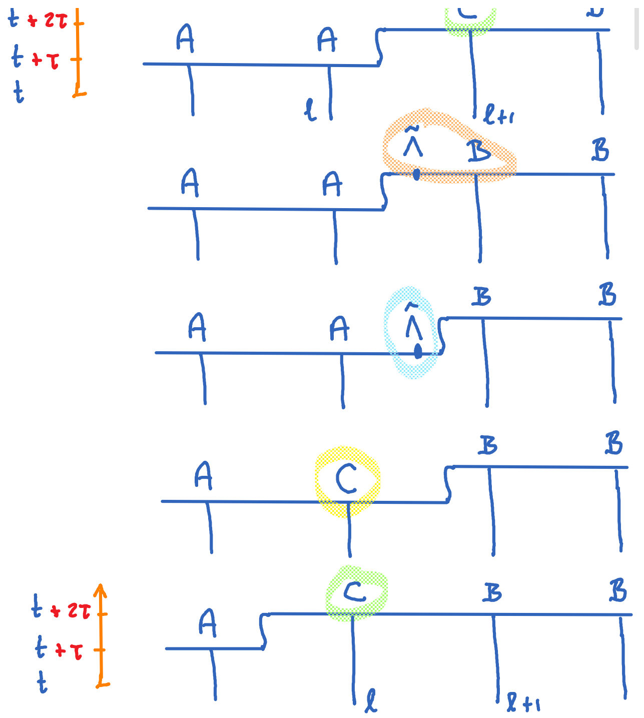
$$A_\ell(t+\tau)\,C_{\ell+1}(t+2\tau)$$

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

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

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

$$\xrightarrow[3(d)]{H_\ell^{1s}}\; C_\ell(t+2\tau)\,B_{\ell+1}(t+2\tau) \qquad (22)$$




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

The scheme described above involves 'one-site updates'. This has the drawback (as in one-site DMRG), that it is not possible to dynamically exploring 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].

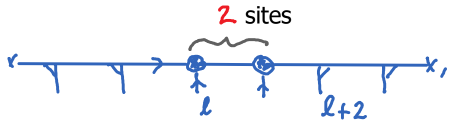
## 2. 2-site projectors $P^{2s}$



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 precisely 2 neighboring sites

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



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

image

Recall:

local 2s projector: $\hat{P}^{2s}_{\ell} =$  (3)



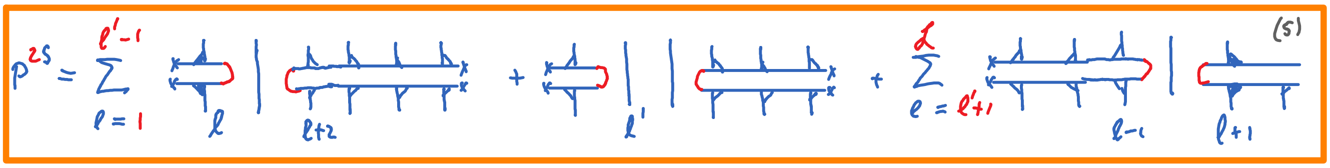
$\ell \in [1, \mathcal{L}-1]$

(TS-I.4.9)

Global 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)

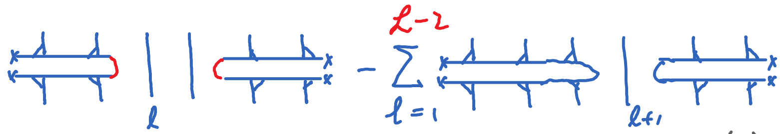
$$P^{2s} := \sum_{\ell=1}^{\ell'-1} \underbrace{P^{2s}_{\ell<}}_{P^{2s}_{\ell} - P^{1s}_{\ell+1} = P^{DK}_{\ell,\ell+2}} + P^{2s}_{\ell'} + \sum_{\ell=\ell'+1}^{\mathcal{L}-1} \underbrace{P^{2s}_{\ell>}}_{P^{2s}_{\ell} - P^{1s}_{\ell} = P^{KD}_{\ell-1,\ell+1}} \quad \text{for any } \ell' \in [1, \mathcal{L}-1]$$





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:

$$P^{2s} = \sum_{\ell=1}^{\mathcal{L}-1} P^{2s}_{\ell} - \sum_{\ell=1}^{\mathcal{L}-2} P^{1s}_{\ell+1} = \sum_{\ell=1}^{\mathcal{L}-1}$$  (7)



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

Orthogonal n-site projectors

For any given MPS , 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)

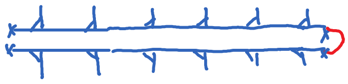
= span of states differing from $|\Psi\rangle$ on $n$ contiguous sites, not expressible through subsets of $n' < n$ sites

Correspondingly, identity can be decomposed as:

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

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)

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



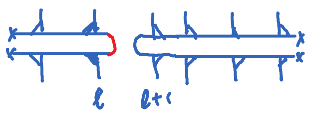
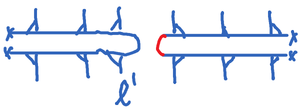
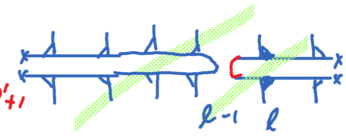
$n \geq 1$: $P^{n\perp} := P^{ns}(\mathbb{1}_{\mathbb{V}} - P^{(n-1)s}) = P^{ns} - P^{(n-1)s}$ (14)

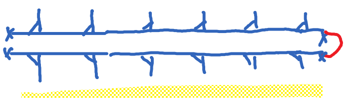
since $\mathrm{im}(\mathbb{V}^{(n-1)s}) \subset \mathrm{im}(\mathbb{V}^{ns})$

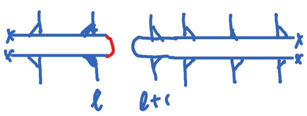
$\mathrm{im}(P^{(n-1)s}) \subset \mathrm{im}(P^{ns})$

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

$= \sum_{\ell=1}^{\mathscr{L}}$  $= \sum_{\ell=1}^{\mathscr{L}} P^{DK}_{\ell,\ell+1}$ (16)

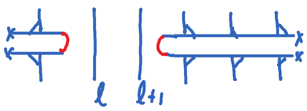
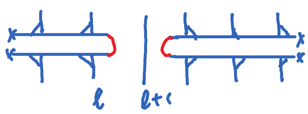
projects onto all 1-site variations orthogonal to $|\Psi\rangle$

Consider n=2:

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

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

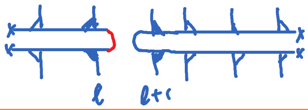
$$= \sum_{\ell=1}^{\mathscr{L}-1} \left(P^{2s}_\ell - P^{1s}_{\ell+1} - P^{1s}_\ell + P^{0s}_{\ell+1}\right) \qquad (18)$$

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

(19)

(TS-I.3.28)

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



$$\boxed{= \sum_{\ell=1}^{\mathcal{L}-1} P^{DD}_{\ell,\ell+1}} \qquad (20)$$

<u>3. 2-site TDVP</u> (optional)

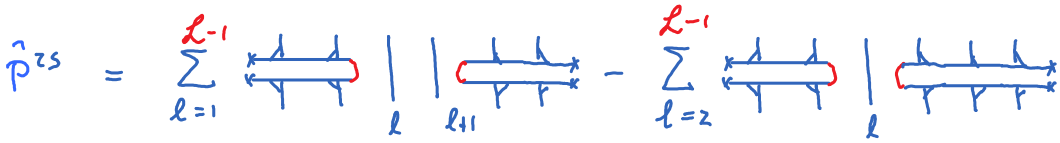
TS-II.3

[Haegeman2016, Sec. V & App. C]

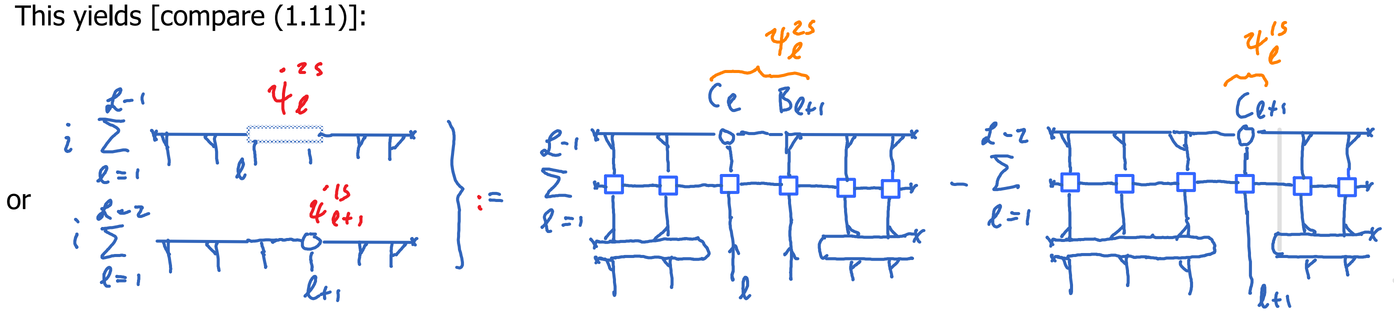
2-site tangent space methods are analogous to 1-site methods, but use a 2-site projector. There is a conceptual difference, though: the main reason for using 2-site schemes is that they allow sectors with new quantum numbers to be introduced if the action of H requires this. However, states with different 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

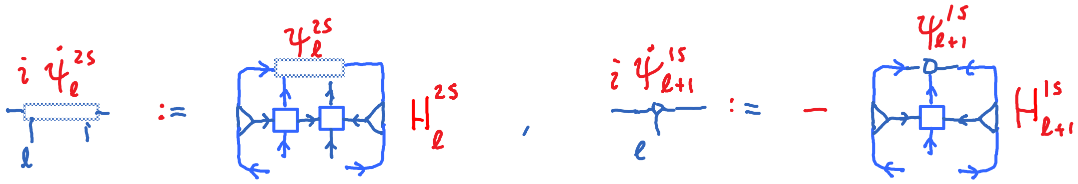
$$i\frac{d}{dt}|\psi[M(t)]\rangle = \hat{P}^{2s}\hat{H}\,|\psi[M(t)]\rangle$$



This yields [compare (1.11)]:



Right side is sum of terms, each specifying an update of one $\psi^{2s}_\ell$ or $\psi^{1s}_\ell$ on the left. Eq. (4) can be integrated one site at a time, by <u>defining</u> the updates through the following local Schrödinger equations:



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

In 2-site-canonical form, site $\ell$ involves two terms linear in $\psi^{2s}_\ell$ : $\quad i\,\dot{\psi}^{2s}_\ell(t) = H^{2s}_\ell\,\psi^{2s}_\ell(t)$ (10)

Their contribution can be integrated exactly: replace $\psi^{2s}_\ell(t)$ by $\psi^{2s}_\ell(t+\tau) = e^{-iH^{2s}_\ell\tau}\,\psi^{2s}_\ell(t)$ (11)

forward time step

In 1-site-canonical form, site $\ell+1$ involves two terms linear in $\psi^{1s}_{\ell+1}$: $\quad i\,\dot{\psi}^{1s}_{\ell+1}(t) = -H^{1s}_{\ell+1}\,\psi^{1s}_{\ell+1}(t)$ (12)

Their contribution can be integrated exactly: replace $\psi^{1s}_{\ell+1}(t)$ by $\psi^{1s}_{\ell+1}(t-\tau) = e^{iH^{1s}_{\ell+1}\tau}\,\psi^{1s}_{\ell+1}(t)$ (13)

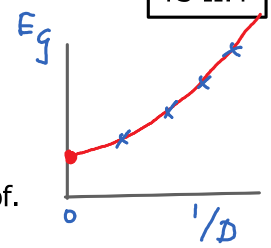
Their contribution can be integrated exactly: replace $\psi^{1s}_{\ell+1}(t)$ by $\psi^{1s}_{\ell+1}(t-\tau) = e^{iH^{1s}_{\ell+1}\tau}\,\psi^{1s}_{\ell+1}(t)$ (13)

backward(!) time step

To successively update entire chains, alternate between 2-site- and 1-site-canonical form,
propagating forward or backward in time with $H^{2s}_{\ell}$ or $H^{1s}_{\ell}$, 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!

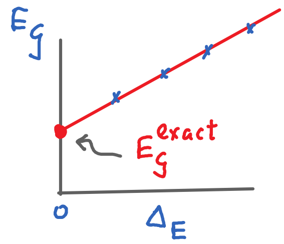
## 4. Energy variance [Hubig2018]




When doing MPS computations involving SVD truncations of virtual bonds, the results should be computed for several values of the bond dimension, $D$, to check convergence as $D \to \infty$. Often it is also necessary to extrapolate the results to $D = \infty$, e.g. by plotting results versus $1/D$ or some power thereof.

However, for some computational schemes, it is not *a priori* clear how the observable of interest scales with $D$, nor how it should be extrapolated to $D = \infty$. An example is ground state energy when computed using 1-site DMRG with subspace expansion [Hubig2015], because it does not rely on SVD truncation of bonds.

Thus, it is of interest to have a reliable error measure without requiring costly 2-site DMRG. A convenient scheme was proposed in [Hubig2018], based on a smart way to approximate the full energy variance,



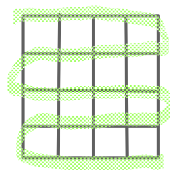

$$\Delta_E := \|(H - E)\psi\|^2 = \langle\psi|(\hat{H} - E)^2|\psi\rangle \qquad \text{(= zero for an exact eigenstate)} \quad (1)$$

$$= \langle\psi|\hat{H}^2|\psi\rangle - E^2, \qquad \text{with} \quad E = \langle\psi|\hat{H}|\psi\rangle \quad (2)$$

Then extrapolations can be done by computing quantity of interested for several $D$, but plotting the results via $\Delta_E$, and extrapolating to $\Delta_E \to 0$

If quantity of interest is energy, then extrapolation is linear, $E_g(\Delta_E) = E_g^{exact} + a \cdot \Delta_E$ (3)

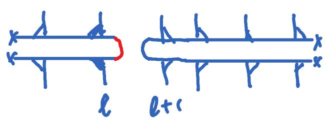
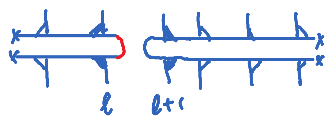
Computing $\langle\psi|\hat{H}^2|\psi\rangle$ directly is costly for large systems with long-ranged interactions, such as 2D systems treated by DMRG snakes. Also, computing $\Delta_E$ as the difference between two potentially large numbers is prone to inaccuracies. [Hubig2018] found a computation scheme in which the subtraction of such large numbers is avoided *a priori*.



Key idea: use projectors $P^{n\perp}$ onto mutually orthogonal, irreducible spaces $\mathbb{V}^{n\perp}$

Recall (2.11): $\mathbb{1}_{\mathbb{V}} = \mathbb{1}_d^{\otimes \mathcal{L}} = \sum_{n=0}^{\mathcal{L}} P^{n\perp}$, completeness (4) $\qquad P^{n\perp} P^{n'\perp} = \delta^{nn'} P^{n\perp}$ orthogonality (5)

with $P^{0\perp} = |\Psi\rangle\langle\Psi|$ (6)

(2.16) $P^{1\perp} = \sum_{\ell=1}^{\mathcal{L}}$  , $\qquad$ (2.17) $P^{2\perp} = \sum_{\ell=1}^{\mathcal{L}}$  (7)

Insert completeness into definition of variance:

$$\Delta_E \overset{(4)}{=} \langle\psi|(\hat{H} - E)\sum_{n=0}^{\mathcal{L}} P^{n\perp}(\hat{H} - E)\rangle|\psi\rangle =: \sum_{n=0}^{\mathcal{L}} \Delta_E^{n\perp} \quad (8)$$

Now two crucial simplifications occur:

$$\Delta_E^{0\perp} \overset{(5)}{=} \langle\psi|(\hat{H} - E)\underbrace{|\psi\rangle\langle\psi|}_{P^{0\perp}}(\hat{H} - E))|\psi\rangle = (E - E)(E - E) = 0 \quad (9)$$

largest contribution to variance cancels by construction!

$$\Delta_E^{0\perp} \overset{(5)}{=} \langle\psi|(\hat H - E)\underbrace{|\psi\rangle\langle\psi|}_{(6)\ P^{0\perp}}(\hat H - E))|\psi\rangle = (E-E)(E-E) = 0 \qquad (9)$$

largest contribution to variance cancels by construction!

$n>0$

$$\Delta_E^{n\perp} = \langle\psi|(\hat H - E)P^{n\perp}(\hat H - E))|\psi\rangle = \langle\psi|\hat H P^{n\perp}\hat H|\psi\rangle, \quad \text{since} \quad P^{(n>0)\perp}|\psi\rangle \overset{(5,6)}{=} 0 \qquad (10)$$

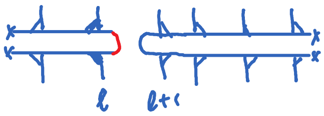
$$= \| P^{n\perp}\hat H\psi\|^2 \qquad (11)$$

In practice, approximate $\Delta_E$ by the first two nonzero terms:

$$\Delta_E \simeq \Delta_E^{2s} = \Delta_E^{1\perp}+\Delta_E^{2\perp} = \boxed{\langle\psi|\hat H P^{1s}\hat H|\psi\rangle + \langle\psi|\hat H P^{2s}\hat H|\psi\rangle} \qquad (12)$$

(11) is exact if longest-range terms in $\hat H$ are nearest-neighbor, because then $P^{(n\geq 3)\perp}\hat H|\Psi\rangle = 0$ (13)

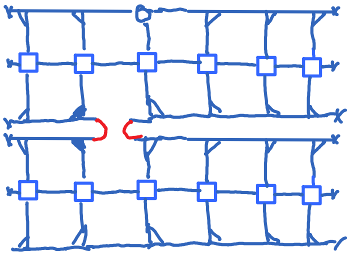
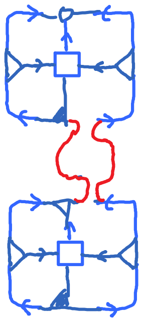
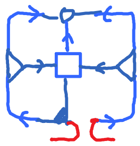
Explicit computations:

$n=1$: Recall $P^{1\perp} \overset{(2.16)}{=} \sum_{\ell=1}^{\mathcal L}$  $= \sum_{\ell=1}^{\mathcal L} P^{DK}_{\ell,\ell+1}$ (14)

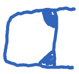


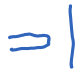
mutually orthogonal!

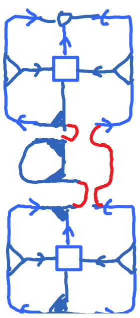
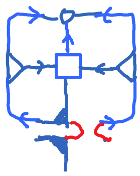
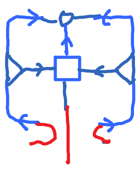
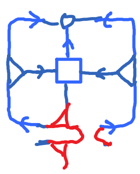
$$\Delta_E^{1\perp} = \langle\psi|\hat H \underbrace{P^{1\perp}}_{P^{1\perp}P^{1\perp}}\hat H|\psi\rangle = \|P^{1\perp}H\psi\|^2 = \sum_{\ell=1}^{\mathcal L}\|P^{DK}_{\ell,\ell+1}H\psi\|^2 \qquad (15)$$

$= \sum_{\ell=1}^{\mathcal L}$  $= \sum_{\ell=1}^{\mathcal L}$  $= \sum_{\ell=1}^{\mathcal L} \Big\|$  $\Big\|^2$ (16)

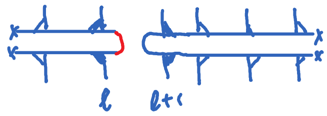
We would like to avoid computing $D$  $Dd-D$, $d$ explicitly, because of its large image dimension.

So rewrite, using isometry condition for discarded sector:  =  (17)

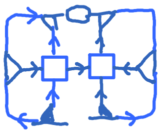
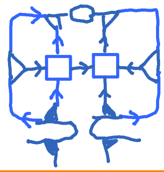
and completeness of kept together with discarded isometries:  =  −  (18)

$= \sum_{\ell=1}^{\mathcal L}$  $= \sum_{\ell=1}^{\mathcal L}\Big\|$  $\Big\|^2 = \sum_{\ell=1}^{\mathcal L}\Big\|$  $-$  $\Big\|^2$

(19)

$n = 2$ : Recall $P^{2\perp} \overset{(2.17)}{=} \sum_{\ell=1}^{\mathcal{L}-1}$  $= \sum_{\ell=1}^{\mathcal{L}} P^{DD}_{\ell,\ell+1}$ (20)

$$\Delta_E^{2\perp} = \langle\psi|\hat{H}\,\overbrace{\hat{P}^{2\perp}}^{P^{2\perp}P^{2\perp}}\,\hat{H}|\psi\rangle = \| P^{2\perp} H\psi \|^2 = \sum_{\ell=1}^{\mathcal{L}-1} \| P^{D}_{\ell,\ell+1} H\psi \|^2 \quad (21)$$

$= \sum_{\ell=1}^{\mathcal{L}-1} \Big\|$  $\Big\|^2 = \boxed{\sum_{\ell=1}^{\mathcal{L}-1} \Big\|}$  $\boxed{\Big\|^2}$ (22)

again use  (23)