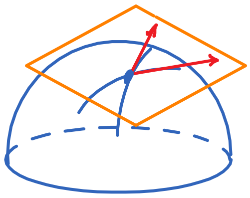
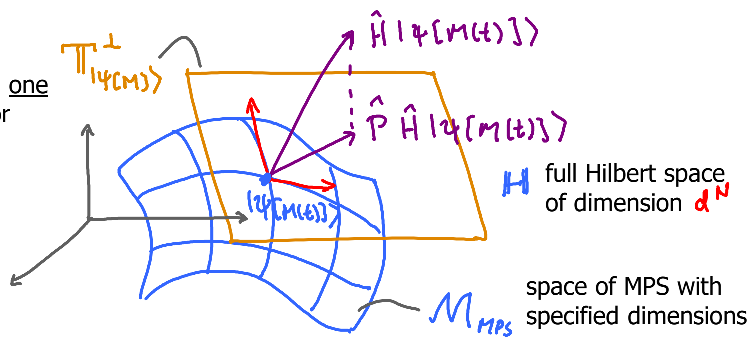
Tangent Space Methods

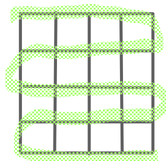


Tangent space: spanned by vectors tangent to curves running within a smooth geometric structure.



Basic idea: if a small change in an MPS is to be computed (e.g. during variational optimization or time-evolution with a small time step), this change lives in the 'tangent space' of the manifold defined by the MPS. Thus, construct a projector onto the tangent space, and implement gauge fixing conditions to remove redundancy due to gauge degrees of freedom. [Haegeman2011]

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.)

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

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

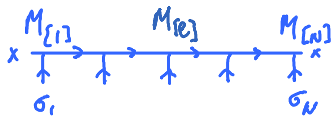
[Vanderstraeten2019] Review-style lecture notes on tangent space methods for uniform MPS.

This lecture follows [Haegeman2016], formulated for finite MPS with open boundary conditions, combined with some arguments from [Vanderstraeten2019, Sec. 3.2].

1. MPS and canonical forms (reminder)

Consider N-site MPS with open boundary conditions:

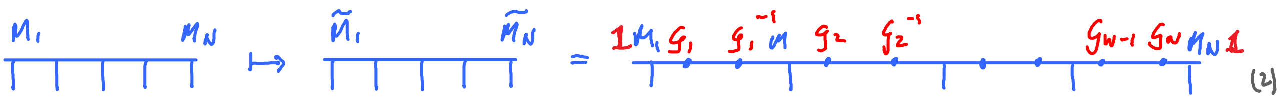
$$|\psi[M]\rangle = |\vec{\sigma}_N\rangle \, M^{\sigma_1}_{[1]} \dots M^{\sigma_\ell}_{[\ell]} \dots M^{\sigma_N}_{[N]} \qquad (1)$$



where $M^{\sigma_\ell}_{[\ell]}$ is matrix with elements $M^{\alpha\sigma_\ell}_{[\ell]\,\beta}$, of dimension $D_{\ell-1} \times D_\ell$, with $D_0 = D_N = 1$

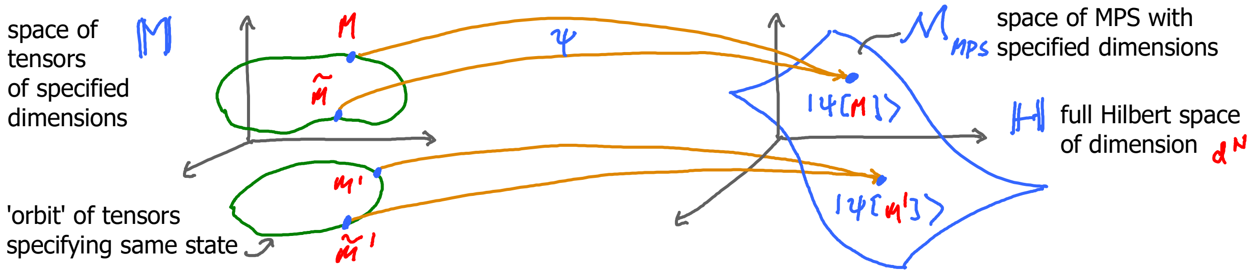
shorthand: $M := (M_{[1]}, \dots, M_{[N]}) \in \mathbb{M}$ space of tensors with specified dimensions

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



$$M^{\sigma_\ell}_{[\ell]} \mapsto \tilde{M}^{\sigma_\ell}_{[\ell]} \equiv G^{-1}_{[\ell-1]} M^{\sigma_\ell}_{[\ell]} G_{[\ell]} \,, \qquad G_{[0]} = G_{[N]} = \mathbb{1} \qquad (3)$$

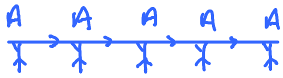
with $G_{[\ell]} \in GL(D_\ell, \mathbb{C})$ group of general complex linear transformation in D_ℓ dimensions



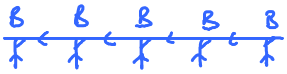
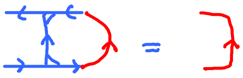
Note: $\mathbb{H}$ and $\mathbb{M}$ are vector spaces, but $\mathcal{M}_{MPS}$ is not, since sum of two MPS with same bond dimensions in general is an MPS with larger bond dimensions. $AB + \tilde{A}\tilde{B} = (A \;\; \tilde{A})\begin{pmatrix} B \\ \tilde{B} \end{pmatrix}$

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

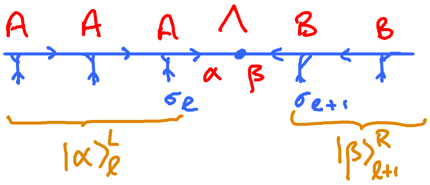
Gauge freedom can be exploited to bring MPS into left-, right-, bond- or site-canonical form:

Left-canonical: $|\Psi[M]\rangle =$  with  (4)

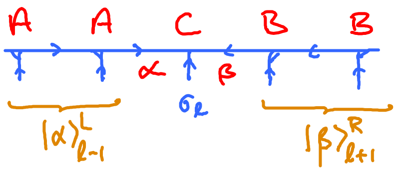
Gauge can be fixed uniquely by requiring $A^\dagger_\sigma A^\sigma = \mathbb{1}$ and $A^\sigma A^\dagger_\sigma =$ diagonal $\forall A_{[\ell]}$

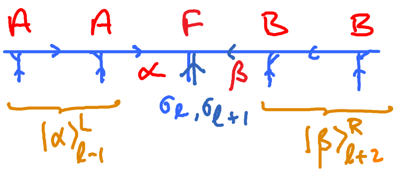
Right-canoncial: $|\Psi[M]\rangle =$  with  (5)

Gauge can be fixed uniquely by requiring $B^\sigma B_\sigma^\dagger = \mathbb{1}$ and $B^\dagger_\sigma B^\sigma =$ diagonal $\forall B_{[\ell]}$

Bond-canonical: $|\Psi[M]\rangle =$  $= |\beta\rangle^R_{\ell+1} |\alpha\rangle^L_\ell \Lambda^{\alpha\beta}_{[\ell]}$ (6)

Here $|\alpha\rangle^L_{\ell-1}$ and $|\beta\rangle^R_{\ell+1}$ are orthonormal basis for subspaces representing left- and right parts of chain.

1-site-canonical: $|\Psi[M]\rangle =$  $= |\beta\rangle^R_{\ell+1} |\sigma_\ell\rangle |\alpha\rangle^L_{\ell-1} C^{\alpha\sigma_\ell\beta}_{[\ell]}$ (7)

2-site-canonical: $|\Psi[M]\rangle =$  $= |\beta\rangle^R_{\ell+2} |\sigma_{\ell+1}\rangle |\sigma_\ell\rangle |\alpha\rangle^L_{\ell-1} F^{\alpha\sigma_\ell\sigma_{\ell+1}\beta}_{[\ell,\ell+1]}$ (8)

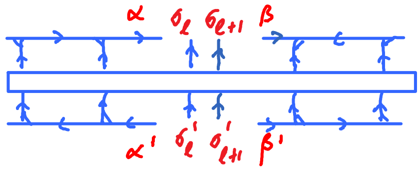
Relation between 1-site- and bond-canonical: $C_{[\ell]} = A_{[\ell]} \Lambda_{[\ell]} = \Lambda_{[\ell-1]} B_{[\ell]}$ (9)

Relation between 1-site- and 2-site-canonical: $F_{[\ell,\ell+1]} = C_{[\ell]} B_{[\ell+1]} = A_{[\ell]} C_{[\ell+1]}$ (10)

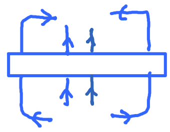
Hamiltonian matrix elements:

2-site:

$${}^{L}_{\ell-1}\langle\alpha'|\langle\sigma_\ell|\langle\sigma'_\ell|\,{}^{R}_{\ell+2}\langle\beta'|\,\hat H\,|\beta\rangle^{R}_{\ell+2}|\sigma_{\ell+1}\rangle|\sigma_\ell\rangle|\alpha\rangle^{L}_{\ell-1} =$$



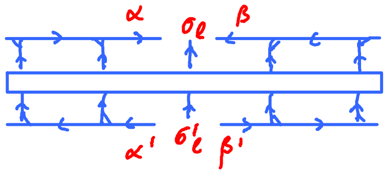
$=:$



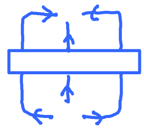
$H_{[\ell,\ell+1]}$ (11)

1-site:

$${}^{L}_{\ell-1}\langle\alpha'|\langle\sigma'_\ell|\,{}^{R}_{\ell+1}\langle\beta'|\,\hat H\,|\beta\rangle^{R}_{\ell+1}|\sigma_\ell\rangle\,|\alpha\rangle^{L}_{\ell-1} =$$



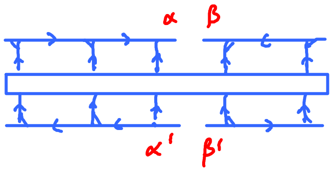
$=:$



$H_{[\ell]}$ (12)

bond:

$${}^{L}_{\ell}\langle\alpha'|\,{}^{R}_{\ell+1}\langle\beta'|\,\hat H\,|\beta\rangle^{R}_{\ell+1}|\alpha\rangle^{L}_{\ell} =$$



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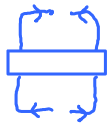
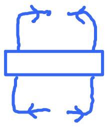
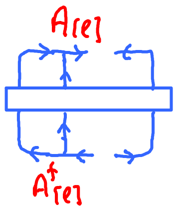


$K_{[\ell]}$ (13)

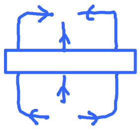
Related by:



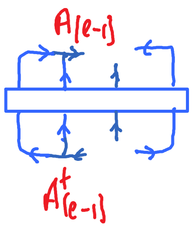
$K_{[\ell]} =$



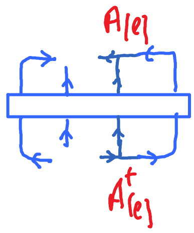
$H_{[\ell]}$ (14)



$H_{[\ell]} =$



$H_{[\ell-1,\ell]} =$



$H_{[\ell-1,\ell]}$ (15)

2. Tangent space

Time-dependent Schrödinger equation: $i\frac{d}{dt}|\psi(t)\rangle = \hat{H}|\psi(t)\rangle$ (1)

General solution is (t-dependent) vector in full many-body Hilbert space, $\mathbb{H}$, of dimension d^N.

Goal: find (approximate) solution as (t-dependent) point in space of MPS with tensors of specified dimensions:

$$|\psi[M(t)]\rangle = \overbrace{M_{[1]}(t) \cdots M_{[\ell]}(t) \cdots M_{[N]}(t)}^{} \in \mathcal{M}_{MPS} \quad (2)$$

Then $$\frac{d}{dt}|\psi[M(t)]\rangle = \sum_{\ell=1}^{N} M_{[1]} \cdots M_{[\ell-1]}\,\dot{M}_{[\ell]}\,M_{[\ell+1]} \cdots M_{[N]} =: |\Phi[\dot{M}]\rangle_{M(t)} \quad (3)$$

Here we have introduced the general notation

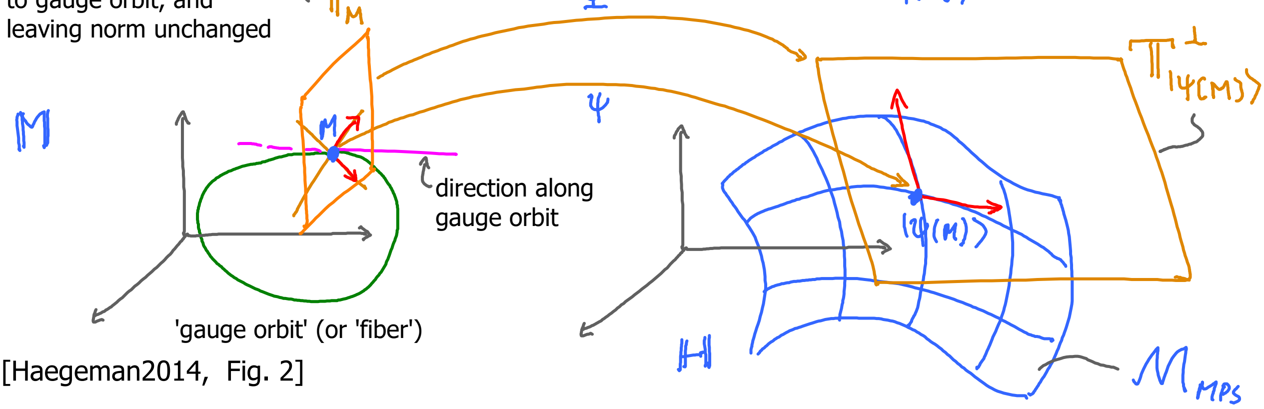
state has changed by taking out one M tensor and replacing it by a T tensor

$$|\Phi[T]\rangle_M = \sum_{\ell=1}^{N} M_{[1]} \cdots M_{[\ell-1]}\,T_{[\ell]}\,M_{[\ell+1]} \cdots M_{[N]} =: |\partial_j \psi[M]\rangle T^j \quad (4)$$

shorthand: $T := (T_{[1]}, \dots, T_{[N]}) \in \mathbb{M}$ with composite index $j = (\ell, \alpha, \sigma, \beta)$

For a given set of tensors $M \in \mathbb{M}$, specifying a given MPS $|\psi[M]\rangle \in \mathcal{M}_{MPS}$, the space of all states $|\Phi[T]\rangle_M$ with $T \in \mathbb{M}$, is a vector space (since $|\Phi[T]\rangle$ is linear in T). It is called the 'tangent space', $\mathbb{T}^{\perp}_{|\psi[M]\rangle}$, associated with the 'base point' $|\psi(M)\rangle$ in the manifold $\mathcal{M}_{MPS}$.

Note that $\mathbb{T}_{|\psi[M]\rangle} \subset \mathcal{M}_{MPS} \subset \mathbb{H}$.



[Haegeman2014, Fig. 2]

Remark: the gauge freedom available for describing $|\psi[M]\rangle$ implies a related gauge freedom available for constructing its tangent space. We obtain a unique construction via the following criteria:

(i) We pick a representative M along each gauge orbit (fix gauge for $|\psi[M]\rangle$), e.g. by picking one of the canonical forms.

(ii) Changes of M pointing 'along a gauge orbit' amount to gauge transformations and do not change $|\psi[M]\rangle$. To construct tangent space $\mathbb{T}_{|\psi[M]\rangle}$, we consider only T's describing changes of M

(ii) Changes of M pointing along a gauge orbit amount to gauge transformations and do not change $|\psi[M]\rangle$. To construct tangent space $\mathbb{T}_{|\psi[M]\rangle}$, we consider only T's describing changes of M orthogonal to such directions.

(iii) Since time evolution is unitary (norm-preserving), $\langle\psi(t)|\psi(t)\rangle = 1$, we consider only T's describing changes of M producing tangent vectors orthogonal to $|\psi[M]\rangle$ itself.

We denote the vector space of T's satisfying these conditions by $\mathbb{T}_M^\perp$.

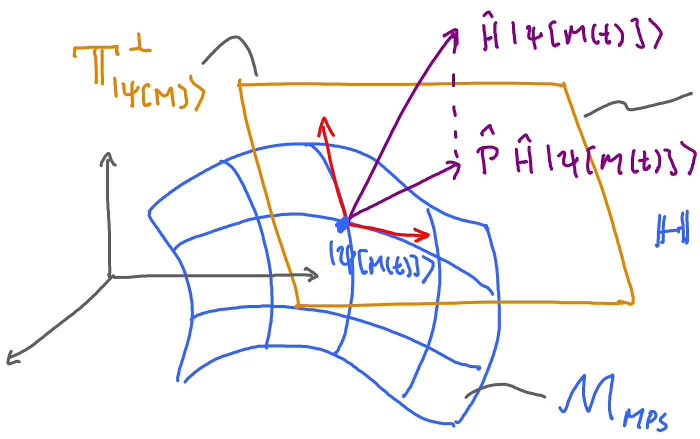
Then each $T \in \mathbb{T}_M^\perp$ uniquely specifies a corresponding tangent vector $|\Phi[T]\rangle_M$ in $\mathbb{T}^\perp_{|\psi[M]\rangle}$, the subset of tangent space orthogonal to $|\psi[M]\rangle$ (w.r.t. scalar product in Hilbert space $\mathbb{H}$):

$$\langle\Phi[T]_M|\Psi[M]\rangle = 0 \qquad \forall\ T \in \mathbb{T}_M^\perp \tag{5}$$

$\mathbb{T}^\perp_{|\psi[M]\rangle}$ contains all states orthogonal to $|\Psi[M]\rangle$ and differing from it by only one M

According to (3) and (iii), left-hand side of Schrödinger equation, $i\frac{d}{dt}|\psi(t)\rangle$, is in $\mathbb{T}^\perp_{|\psi[M]\rangle}$.
However, the right side, $\hat{H}|\psi(t)\rangle$, is not. In fact, action of $\hat{H}$ in general produces MPS with larger bond dimensions. Our decision to solve time evolution within $\mathcal{M}_{MPS}$ of specified dimension thus inevitably involves an approximation. The best we can then do is to project $\hat{H}|\psi(t)\rangle$ into orthogonal tangent space $\mathbb{T}^\perp_{|\psi[M]\rangle}$, using a projector $\hat{P}_{\mathbb{T}^\perp_{|\psi[M(t)]\rangle}}$, and write Schrödinger eq. as

$$i\frac{d}{dt}|\psi[M(t)]\rangle = \boxed{i|\Phi[\dot{M}]\rangle_{M(t)} = \hat{P}_{\mathbb{T}^\perp_{|\psi[M(t)]\rangle}}\hat{H}|\psi[M(t)]\rangle} \tag{6}$$



states orthogonal to $|\Psi[M]\rangle$
and differing from it by only one

why do we want only such states?
because the left side also contains
only such states!

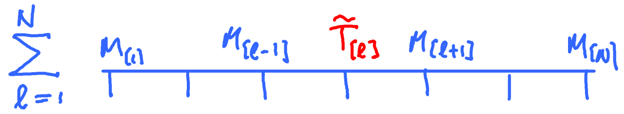
To implement this idea explicitly, we need explicit construction of the projector $\hat{P}$.

Remark: Eq. (6) can also be derived using a 'time-dependent variational principle' (TDVP).
Hence time evolution with tangent space methods is also called TDVP in the literature [Haegeman2011].

3. Tangent space projector

[Haegeman2016], [Vanderstraeten2019, Sec. 3.2] $\boxed{\text{TS.3}}$

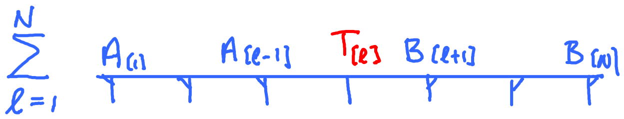
General form of tangent vector:



(1)

Gauge freedom can be used to bring ℓ-th summand into site-canonical form w.r.t. to site ℓ :

$|\Phi[T]\rangle_M =$



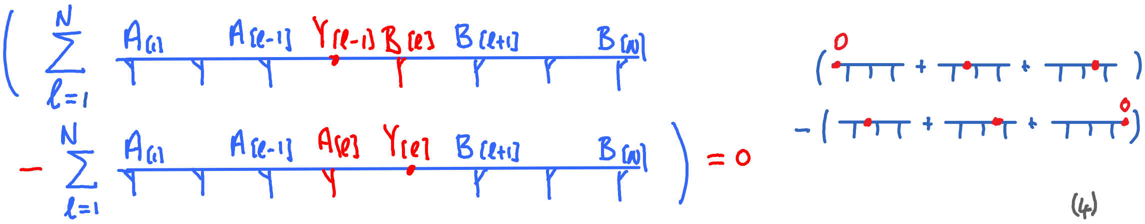
(2)

There is still gauge freedom left: $|\Phi[T]\rangle_M$ does not change under the replacement

$$T_{[\ell]} \longmapsto \tilde{T}_{[\ell]} = T_{[\ell]} + Y_{[\ell-1]} B_{[\ell]} - A_{[\ell]} Y_{[\ell]} \quad \forall \ell , \qquad Y_{[0]} = Y_{[N]} = 0 . \tag{3}$$

with $Y_{[\ell]}$ an arbitrary matrix of dimensions $D_\ell \times D_\ell$

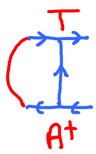
Check: extra terms yield



(4)

This freedom can be exploited to impose the following '<u>left gauge fixing condition</u>' (LGFC) on $T_{[\ell]}$:

$$A^{\dagger}_{[\ell]\sigma} T^{\sigma}_{[\ell]} = 0 \qquad \forall \ell = 1, \dots , N-1$$



$= 0$ (5)

If T does not satisfy LGFC, replace it by $\tilde{T}$ which does:

Impose condition:

$$0 \doteq A^{\dagger}_{[\ell]\sigma} \tilde{T}_{[\ell]\sigma} \overset{(3)}{=} A^{\dagger}_{[\ell]\sigma} \left(T^{\sigma}_{[\ell]} + Y_{[\ell-1]} B^{\sigma}_{[\ell]} - A_{[\ell]} Y^{\sigma}_{[\ell]} \right) \tag{6}$$

solve for Y :

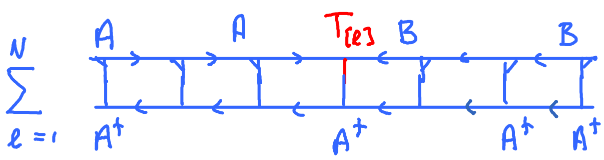
$$Y_{[\ell]} = A^{\dagger}_{[\ell]\sigma} \left(T^{\sigma}_{[\ell]} + Y_{[\ell-1]} B^{\sigma}_{[\ell]} \right) \tag{7}$$

insert back into (3):

$$\tilde{T}^{\sigma}_{[\ell]} = \underbrace{\left(1 - A^{\sigma}_{[\ell]} A^{\dagger}_{[\ell]\sigma} \right)}_{\text{projector onto orthogonal subspace (see below)}} \left(T^{\sigma}_{[\ell]} + Y_{[\ell-1]} B^{\sigma}_{[\ell]} \right) \tag{8}$$

The LGFC has two convenient properties. First, it ensures orthogonality of tangent vector to its base point vector:

$\langle \Psi[M] | \Phi[T] \rangle_M = \sum_{\ell=1}^{N}$



$= 0$ (9)

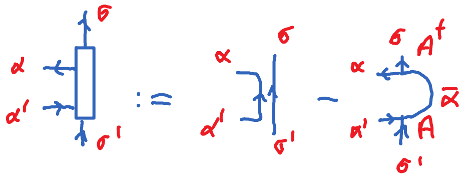
as required by property (iii) of Sec. TS.2. Second, it enables construction of an projector onto tangent space:

Define local 1-site projector:

as required by property (iii) of Sec. 13.2. Second, it enables construction of an projector onto tangent space.

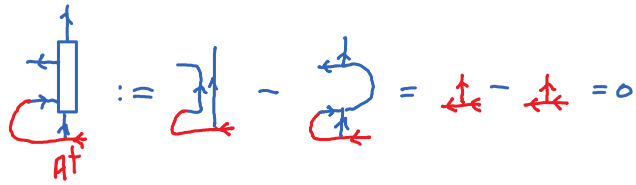
Define local 1-site projector:

$$P_{[\ell]}{}^{\alpha'\sigma'}{}_{\alpha\sigma} := \mathbb{1}^{\alpha'\sigma'}{}_{\alpha\sigma} - A_{[\ell]}{}^{\alpha'\sigma'}{}_{\tilde\alpha}\, A^{\dagger}_{[\ell]}{}^{\tilde\alpha}{}_{\alpha\sigma} \qquad (10)$$



Satisfies:

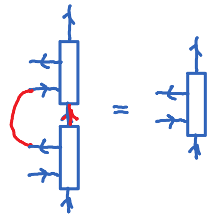
$$A^{\dagger}_{[\ell]\alpha'\sigma'}\, P_{[\ell]}{}^{\alpha'\sigma'}{}_{\alpha\sigma} = A^{\dagger}\big(\mathbb{1} - \underbrace{A A^{\dagger}\big)}_{=\mathbb{1}} = A^{\dagger} - A^{\dagger} = 0 \qquad (11a)$$



$$P_{[\ell]}{}^{\alpha'\sigma'}{}_{\alpha\sigma}\, A^{\alpha\sigma} = \big(\mathbb{1} - A\underbrace{A^{\dagger}\big)A}_{=\mathbb{1}} = A - A = 0 \qquad (11b)$$

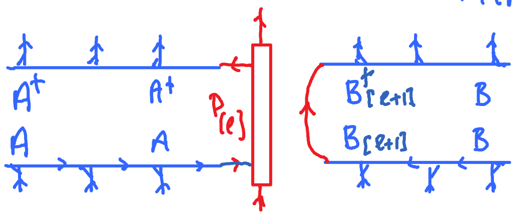
This projects onto the 'orthogonal local space of site ℓ' (orthogonal to space on outgoing leg of $A_{[\ell]}$):

$$P \cdot P \overset{(10)}{=} P \cdot (\mathbb{1} - A A^{\dagger}) \overset{(11b)}{=} P \qquad (12)$$



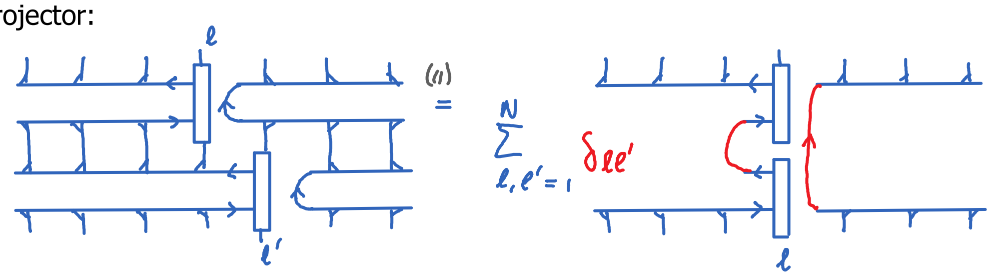
Tangent space projector onto orthogonal tangent space $\Pi^{\perp}_{|\Psi[M]\rangle}$:

$$\hat{P}_{\Pi^{\perp}_{|\Psi[M]\rangle}} = \sum_{\ell=1}^{N} \qquad (13)$$



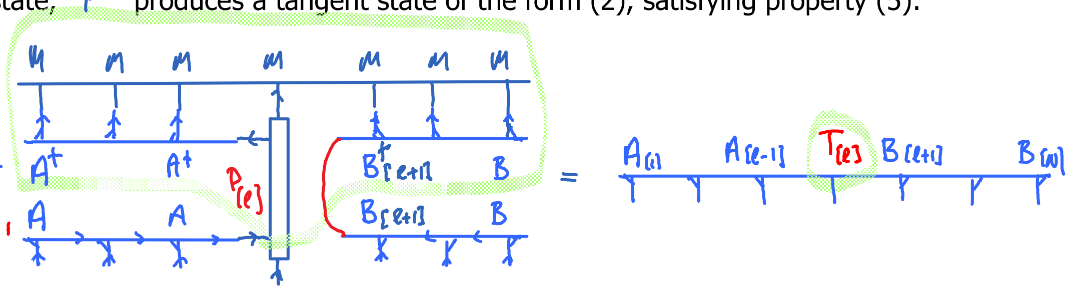
This is indeed a projector:

$$\hat{P} \cdot \hat{P} = \sum_{\ell=1}^{N}\sum_{\ell'=1}^{N} \overset{(11)}{=} \sum_{\ell,\ell'=1}^{N} \delta_{\ell\ell'} \overset{(12)}{=} \hat{P} \qquad (14)$$



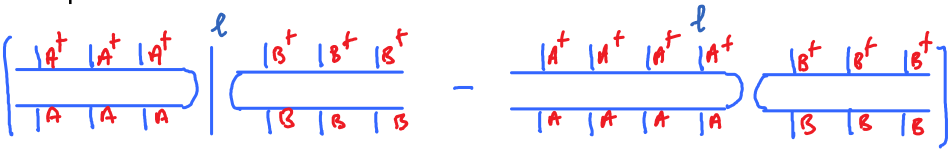
Acting on an arbitrary state, $\hat{P}$ produces a tangent state of the form (2), satisfying property (5):

$$\hat{P}_{\Pi^{\perp}_{|\Psi[M]\rangle}} |\Psi\rangle = \sum_{\ell=1}^{N} \quad = $$



Projector can also be expressed as:

$$\hat{P}_{\Pi^{\perp}_{|\Psi[M]\rangle}} \overset{(10)}{=} \sum_{\ell=1}^{N} \Big[\qquad - \qquad \Big] \qquad (15)$$



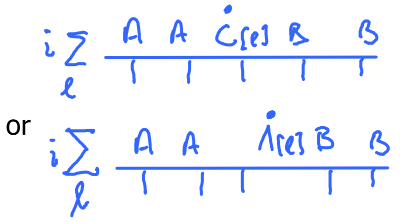
This is our final expression for desired tangent space projector. It is built fully from known tensors!

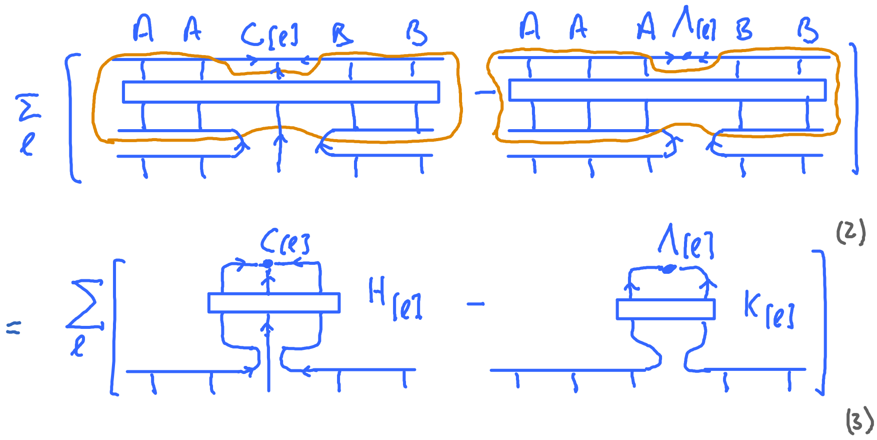
First term: Unit operator in site representation for site ℓ; econd term: subtracts components parallel to $|\Psi[M]\rangle$.

4. Time evolution: 1-site algorithm [Haegeman2016, App. B]

Schrödinger equation, projected onto tangent space, now takes the form

$$i\frac{d}{dt}|\psi[M(t)]\rangle = i|\Phi[\dot M]\rangle_{M(t)} = \hat P_{T_{|\psi[M(t)]\rangle}}\, \hat H\, |\psi[M(t)]\rangle \qquad (1)$$





= usual time evolution, minus that part of time-evolved state orthogonal to initial state

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 site-canonical form, site ℓ involves two terms linear in $C_{[\ell]}$: $\quad i\dot C_{[\ell]}(t) = H_{[\ell]}\, C_{[\ell]}(t)$ (4)

Their contribution can be integrated exactly: replace $C_{[\ell]}(t)$ by $\quad C_{[\ell]}(t+\tau) = e^{-iH_{[\ell]}\tau}\, C_{[\ell]}(t)$ (5)

forward time step

In bond-canonical form, site ℓ involves two terms linear in $\Lambda_{[\ell]}$: $\quad i\dot\Lambda_{[\ell]}(t) = -K_{[\ell]}\,\Lambda_{[\ell]}(t)$ (6)

Their contribution can be integrated exactly: replace $\Lambda_{[\ell]}(t)$ by $\quad \Lambda_{[\ell]}(t-\tau) = e^{-iK_{[\ell]}\tau}\,\Lambda_{[\ell]}(t)$ (7)

backward(!) time step

To successively update entire chains, alternate between site- and bond-canonical form, propagating forward or backward in time with $H_{[\ell]}$ or $K_{[\ell]}$, respectively: (8)

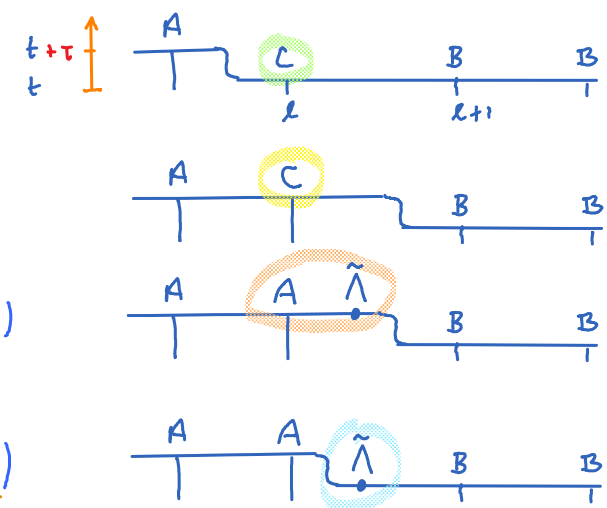
1. Forward sweep, for $\ell = 1, \dots, N-1$, starting from $\underbrace{B_{[1]}(t)}_{C_{[1]}(t) \equiv} B_{[2]}(t) \dots B_{[N]}(t)$: (9)

$$C_{[\ell]}(t)\; B_{[\ell+1]}(t)$$

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

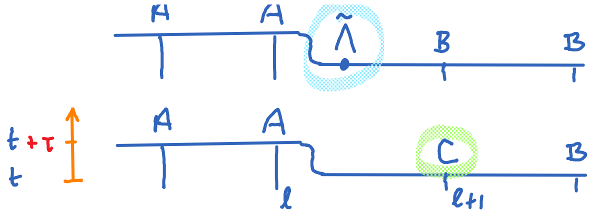
$$= \overbrace{A_{[\ell]}(t+\tau)\;\tilde\Lambda_{[\ell]}(t+\tau)}\; B_{[\ell+1]}(t)$$

$$\xrightarrow[1(c)]{K_{[\ell]}} A_{[\ell]}(t+\tau)\; \underbrace{\tilde\Lambda_{[\ell]}(t)\; B_{[\ell+1]}(t)}_{1(d)}$$



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

$$= A_{[\ell]}(t+\tau)\, C_{[\ell+1]}(t)$$

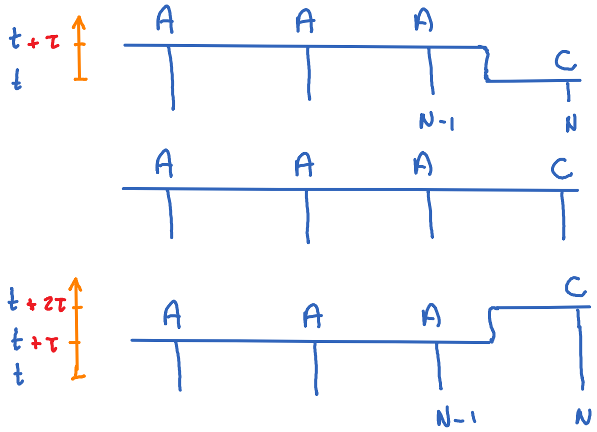


until we reach last site, and MPS described by $A_{[1]}(t+\tau)\dots A_{[N-1]}(t+\tau)\, C_{[N]}(t)$ (10)

2. Turn around: $C_{[N]}(t)$

$$\xrightarrow[2(a)]{H_{[N]}} C_{[N]}(t+\tau)$$

$$\xrightarrow[2(b)]{H_{[N]}} C_{[N]}(t+2\tau)$$



3. Backward sweep, for $\ell = N-1, \dots, 1$, starting from $A_{[1]}(t+\tau)\dots A_{[N-1]}(t+\tau)\, C_{[N]}(t+2\tau)$ (11)

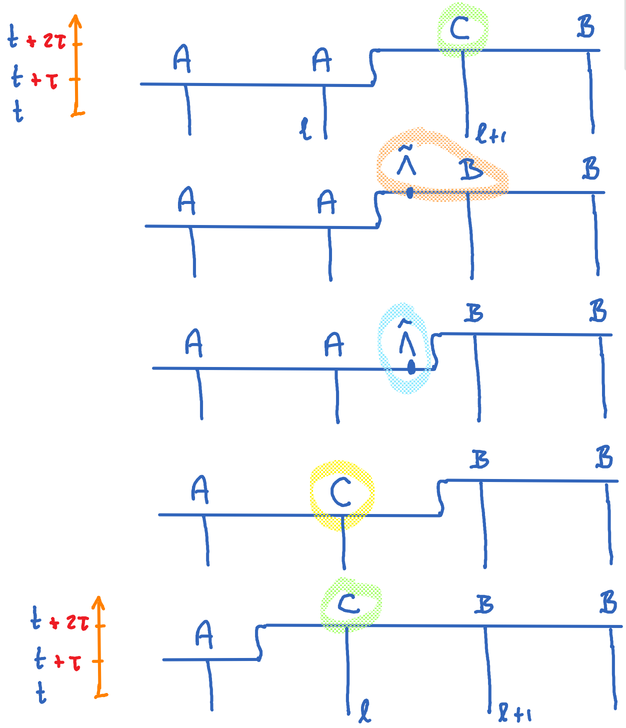
$$A_{[\ell]}(t+\tau)\, C_{[\ell+1]}(t+2\tau)$$

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

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

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

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



until we reach first site, and MPS described by $C_{[1]}(t+2\tau)\, B_{[2]}(t+2\tau)\dots B_{[N]}(t+2\tau)$ (12)

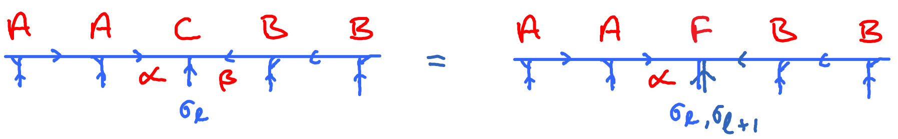
The scheme described above involves 'one-site updates'. This has the drawback (as in one-site DMRG), that it is not possible to dynamically exploring different symmetry sectors. To overcome this drawback, a 'two-site update' version of tangent space methods can be set up [Haegemann2016, App. C].

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!

5. Time evolution: 2-site algorithm (optional) [Haegeman2016, Sec. V & App. C]

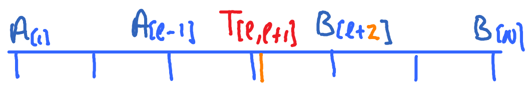
2-site tangent space methods are analogous to 1-site methods, but use a 2-site projector. There is a conceptual difference, though: the main reason for using 2-site schemes is that they allow sectors with new quantum numbers to be introduced if the action of H requires this. However, states with different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

We now work with states in 1-site or 2-site canonical form, related by

$|\psi[M]\rangle =$  (1)

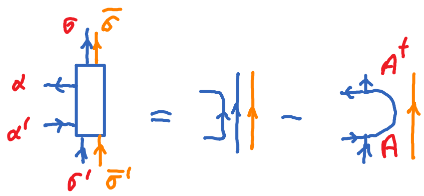
$$F_{[\ell,\ell+1]} = C_{[\ell]} B_{[\ell+1]} = A_{[\ell]} C_{[\ell+1]} \tag{2}$$

We consider tangent space of 2-site (neighbor) variations:

$|\Phi[T]\rangle_M = \sum_{\ell=1}^{N}$  $\in \mathbb{T}^{2,\perp}_{|\psi[M]\rangle}$ (3)

We need a global projector onto this space. First define a local 2-site projector (compare TS-3.10):

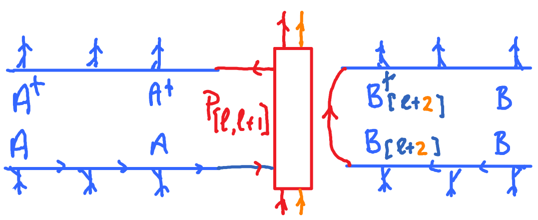
$$P_{[\ell]}{}^{\alpha'\sigma'\bar\sigma'}_{\alpha\sigma\bar\sigma} := \mathbb{1}^{\alpha'\sigma'\bar\sigma'}_{\alpha\sigma\bar\sigma} - A_{[\ell]}^{\alpha'\sigma'} A^\dagger_{[\ell]\alpha\sigma} \mathbb{1}^{\bar\sigma'}_{\bar\sigma}$$

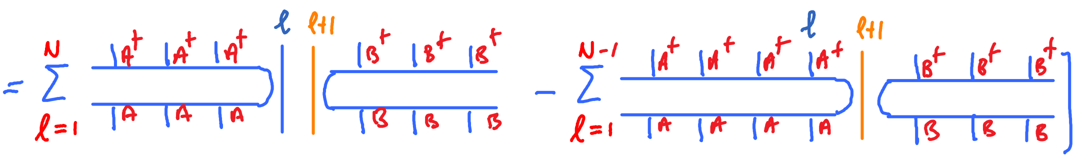
 (4)

As for local 1-site projector, we have $A^\dagger P = 0, \quad P A = 0, \quad P \cdot P = P$ (5)

This projects onto the 'orthogonal local space of sites $\ell, \ell+1$ ' (orthogonal to space on outgoing leg of $F_{[\ell,\ell+1]}$):

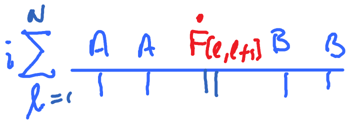
Global projector onto 2-site tangent space:

$\hat{P}_{\mathbb{T}^{\perp}_{|\psi[M]\rangle}} = \sum_{\ell=1}^{N}$  (6)

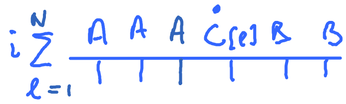
 (7)

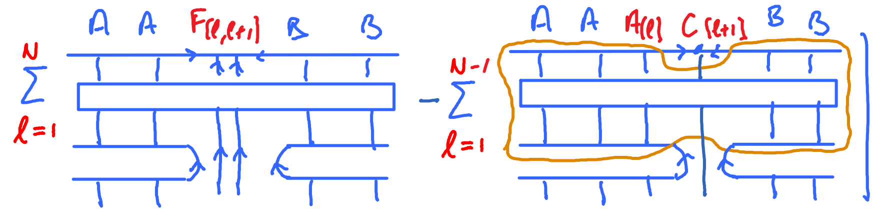
Schrödinger equation, projected onto 2-site tangent space, now takes the form

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



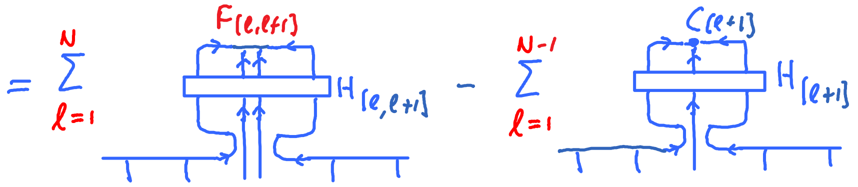
or





(8)

= usual time evolution, minus
that part of time-evolved state
orthogonal to initial state



(9)

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 ℓ involves two terms linear in $F_{[\ell,\ell+1]}$: $\quad i \dot{F}_{[\ell,\ell+1]}(t) = H_{[\ell,\ell+1]} F_{[\ell,\ell+1]}(t)$ (10)

Their contribution can be integrated exactly: replace $F_{[\ell,\ell+1]}(t)$ by $F_{[\ell,\ell+1]}(t+\tau) = e^{-iH_{[\ell,\ell+1]}\tau} F_{[\ell,\ell+1]}(t)$ (11)

forward time step

In 1-site-canonical form, site $\ell+1$ involves two terms linear in $C_{[\ell+1]}$: $\quad i \dot{C}_{[\ell+1]}(t) = -H_{[\ell+1]} C_{[\ell+1]}(t)$ (12)

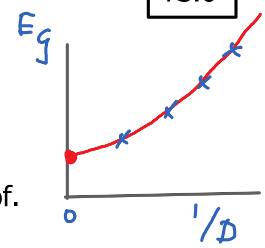
Their contribution can be integrated exactly: replace $C_{[\ell]}(t)$ by $\quad C_{[\ell]}(t-\tau) = e^{-iH_{[\ell+1]}\tau} C_{[\ell+1]}(t)$ (13)

backward(!) time step

To successively update entire chains, alternate between 2-site- and 1-site-canonical form,
propagating forward or backward in time with $H_{[\ell,\ell+1]}$ or $H_{[\ell]}$, 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!

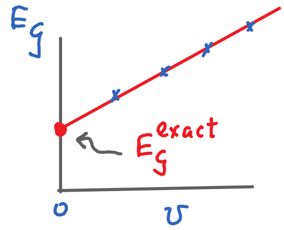
6. Error estimates [Hubig2018]



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,

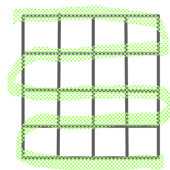


$$v := \langle\psi|(\hat{H} - E)^2|\psi\rangle \quad \text{(= zero for an exact eigenstate)} \qquad (1)$$

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

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

If quantity of interest is energy, then extrapolation is linear, $E_g(v) = E_g^{exact} + a \cdot v$ (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 v 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: define projectors $\hat{P}_i$ onto tangent spaces $\mathbb{T}^i_{|\psi(M)\rangle}$ for 'variations of length i' of $|\psi\rangle$,

where $\mathbb{T}^i_{|\psi(M)\rangle}$ = space of all states differing from $|\psi(M)\rangle$ by i contiguous M's.

(in Sec. TS.3 we defined $\mathbb{T}^1_{|\psi(M)\rangle} = \mathbb{T}^\perp_{|\psi(M)\rangle}$)

By definition, such projectors satisfy

$$\hat{P}_0 = |\psi\rangle\langle\psi|, \quad (4a) \qquad \hat{P}_i \hat{P}_j = \delta_{ij} \hat{P}_i, \quad (4b) \qquad \mathbb{1} = \sum_{i=0}^{N} \hat{P}_i \quad (4c)$$

target state — orthogonality — completeness in space of MPS with specified dimensions

Insert completeness into definition of variance:

$$v \overset{(4c)}{=} \langle\psi|(\hat{H} - E) \sum_{i=0}^{N} \hat{P}_i (\hat{H} - E)|\psi\rangle =: \sum_{i=0}^{N} v_i \qquad (5)$$

Now two crucial simplifications occur:

$$v_0 = \langle\psi|(\hat{H} - E)\underbrace{|\psi\rangle\langle\psi|}_{(4a)\ \hat{P}_0}(\hat{H} - E)|\psi\rangle = (E - E)(E - E) = 0 \qquad (6)$$

largest contribution to variance cancels by construction!

$$v_{i\neq 0} = \langle\psi|(\hat{H} - E)\hat{P}_i(\hat{H} - E)|\psi\rangle = \langle\psi|\hat{H}\hat{P}_i\hat{H}|\psi\rangle, \quad \text{since} \quad \hat{P}_i|\psi\rangle \overset{(4a,b)}{=} 0 \qquad (7)$$

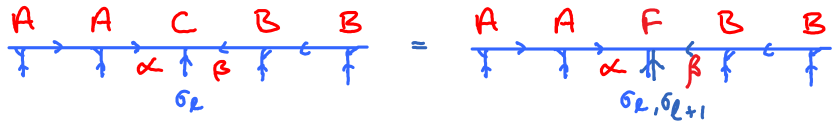
In practice, use approximation $\quad \mathcal{V} \simeq \mathcal{V}_1 + \mathcal{V}_2 = \boxed{\langle\psi|\hat{H}\hat{\mathcal{P}}_1\hat{H}|\psi\rangle + \langle\psi|\hat{H}\hat{\mathcal{P}}_2\hat{H}|\psi\rangle}$ (8)

(8) is exact if longest-range terms in $\hat{H}$ are nearest-neighbor, because then $\hat{\mathcal{P}}_{i\geq 3}\hat{H}|\psi\rangle = 0$ (9)

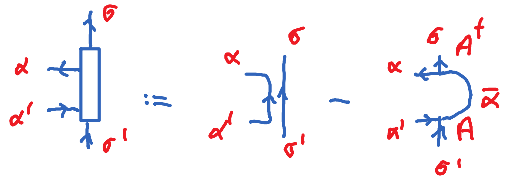
<u>Construction of projectors</u>

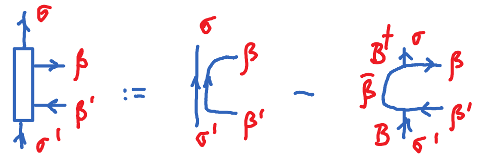
$\hat{\mathcal{P}}_1$ is already known from Sec. TS.3. $\hat{\mathcal{P}}_2$ is straightforward generalization.

When evaluating action of $\hat{H}$, adopt 1- or 2-site canonical form [see (TS.1.7-8)]

$|\psi[n]\rangle =$  (10)

Define local 1-site projectors [cf. (TS.3.10)]:

$$P_{[\ell]}{}^{\alpha'\sigma'}{}_{\alpha\sigma} := \mathbb{1}^{\alpha'\sigma'}{}_{\alpha\sigma} - A_{[\ell]}{}^{\alpha'\sigma'}{}_{\bar{\alpha}}\, A^{\dagger\,\bar{\alpha}}_{[\ell]\,\alpha\sigma}$$  (11 a)

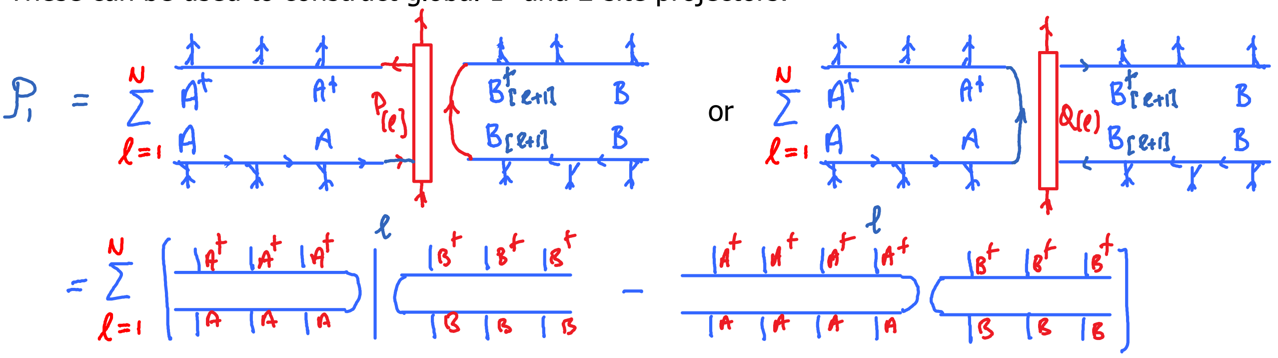
$$Q_{[\ell]}{}_{\beta\sigma}{}^{\sigma'\beta'} := \mathbb{1}_{\beta\sigma}{}^{\sigma'\beta'} - B^{\dagger}_{[\ell]\,\beta\sigma}{}^{\bar{\beta}}\, B_{[\ell]\,\bar{\beta}}{}^{\sigma'\beta'}$$  (11 b)

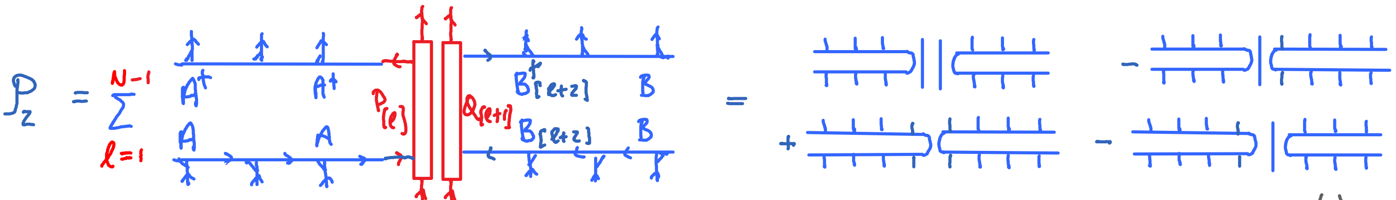
For each ℓ, these satisfy:
[cf. (TS.3.11,12)]

$$A^\dagger P = PA = 0, \qquad P^2 = P, \qquad (12\,a)$$

$$BQ = QB^\dagger = 0, \qquad Q^2 = Q. \qquad (12\,b)$$

These can be used to construct global 1- and 2-site projectors:

 (13)

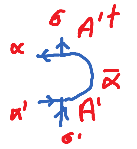
 (14)

Using (13,14), the variance $\mathcal{V} \overset{(8)}{\simeq} \mathcal{V}_1 + \mathcal{V}_2$ can be straightforwardly evaluated via contractions.
For remarks on the optimal order of contractions, see [Hubig2018, end of Sec. IV]

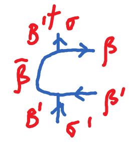
Alternative construction of 1-site projectors (optional)

The 1-site projectors of (11) can also be expressed as (whether (11) or (13) is more convenient depends on context)

$$P_{[\ell]}{}^{\alpha'\sigma'}{}_{\alpha\sigma} := A'_{[\ell]}{}^{\alpha'\sigma'}{}_{\bar\alpha}\; A'^{\dagger}_{[\ell]}{}^{\bar\alpha}{}_{\alpha\sigma} \, ,$$



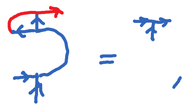
$$Q_{[\ell]\beta\sigma}{}^{\sigma'\beta'} := B'^{\dagger}_{[\ell]\beta\sigma}{}^{\bar\beta}\; B'_{[\ell]\bar\beta}{}^{\sigma'\beta'}$$



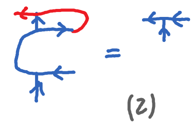
(1)

where A' and $B'^\dagger$ the 'orthogonal complements' of A and $B^\dagger$, are projector eigenvectors:

$$P_{[\ell]}{}^{\alpha'\sigma'}{}_{\bar\alpha\bar\sigma}\; A'_{[\ell]}{}^{\bar\alpha\bar\sigma}{}_{\alpha} = A'_{[\ell]}{}^{\alpha'\sigma'}{}_{\alpha} \, ,$$



$$B'_{[\ell]\beta}{}^{\bar\sigma\bar\beta}\; Q_{[\ell]\bar\beta\bar\sigma}{}^{\sigma'\beta'} = B'_{[\ell]\beta}{}^{\sigma'\beta'}$$



(2)

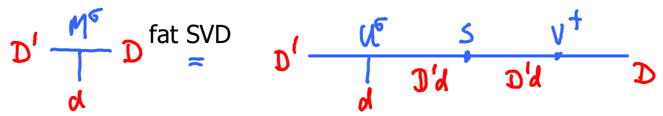
By construction, the following normalization and orthogonality conditions hold:

$$A^\dagger A = \mathbb{1}, \qquad A'^\dagger A' = \mathbb{1}, \qquad B B^\dagger = \mathbb{1}, \qquad B' B'^\dagger = \mathbb{1}, \qquad (3)$$

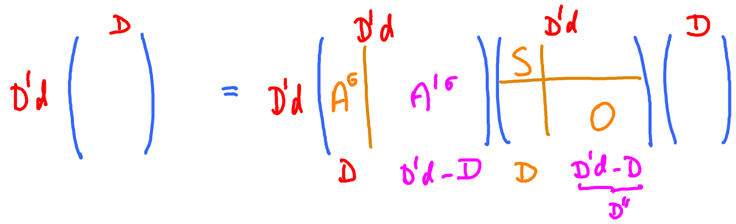
$$A'^\dagger A = 0, \qquad A^\dagger A' = 0, \qquad B' B^\dagger = 0, \qquad B B'^\dagger = 0 . \qquad (4)$$

A', B' can be computed either from A, B, by solving the eigenvector relations (2);
or by using 'fat SVD' (rather than the usual 'thin SVD') when computing A and B :

Recall that each $A^\sigma_{[\ell]}$ was obtained by 'thin' SVD of some $M^\sigma_{[\ell]}$. Let us consider corresponding 'fat' SVD:

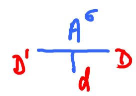


(5)



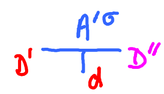
(6)

A^σ is built from the first D columns of the $D'd \times D'd$ unitary matrix U^σ :



(7)

Let A'^σ be similarly built from its remaining $D'' = D'd - D$ columns:

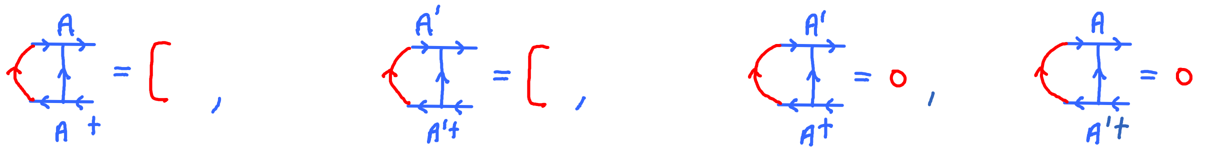


(8)

Since U is unitary, the columns of A and A' form orthonormal bases of <u>mutually orthogonal</u> subspaces:
(A and A' are orthogonal isometries)

$$U_\sigma^\dagger U^\sigma = \mathbb{1}^{dD'\times dD'} \Longrightarrow \begin{array}{c} \\ D \\ D'' \end{array}\!\! \begin{bmatrix} A_\sigma^\dagger \\ A'^\dagger_\sigma \end{bmatrix} \begin{bmatrix} A^\sigma & A'^\sigma \end{bmatrix} = \begin{array}{c} \begin{array}{cc} D & D'' \end{array} \\ \begin{bmatrix} \mathbb{1} & \\ & \mathbb{1} \end{bmatrix} \end{array} : \qquad (9)$$

$$A_\sigma^\dagger A^\sigma = \mathbb{1}^{D\times D}, \qquad A'^\dagger_\sigma A'^\sigma = \mathbb{1}^{D''\times D''}, \qquad A_\sigma^\dagger A'^\sigma = 0 , \qquad A'^\dagger_\sigma A^\sigma = 0 \qquad (10a)$$



(10b)