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]

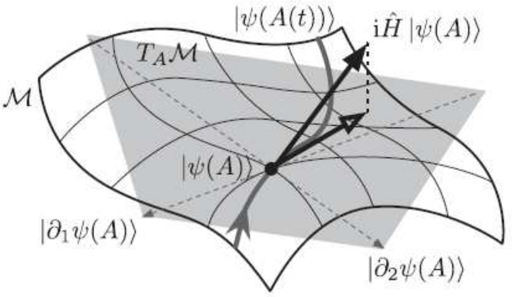


FIG. 1. A sketch of the manifold $\mathcal{M} = \mathcal{M}_{\text{uMPS}}$ (wire frame) embedded in state space. The tangent plane $T_A\mathcal{M}$ to $\mathcal{M}$ (rotated gray square) in a uMPS $|\psi(A)\rangle$ (black dot) is spanned by generally nonorthogonal coordinate axes $|\partial_1\psi(A)\rangle$ and $|\partial_2(A)\rangle$ (dotted lines). The direction $i\hat{H}|\psi(A)\rangle$ of time evolution (arrow with solid head) is best approximated by its orthogonal projection into the tangent plane (arrow with open head). The optimal path $|\psi(A(t))\rangle$ (gray curve) follows the vector field generated by these orthogonally projected vectors throughout $\mathcal{M}$.

This very fundamental and general idea 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).

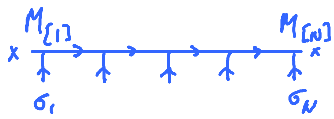
[Vanderstraeten2019] Review-style lecture notes on tangent space methods for uniform MPS.

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:

$$|\psi[M]\rangle = |\vec{\sigma}_N\rangle\, M^{\sigma_1}_{[1]} M^{\sigma_2}_{[2]} \cdots M^{\sigma_N}_{[N]} \qquad (1)$$



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: $\mathsf{M} \equiv (M_{[1]}, \ldots, M_{[N]}) \in \mathbb{M}$ space of tensors with specified dimensions

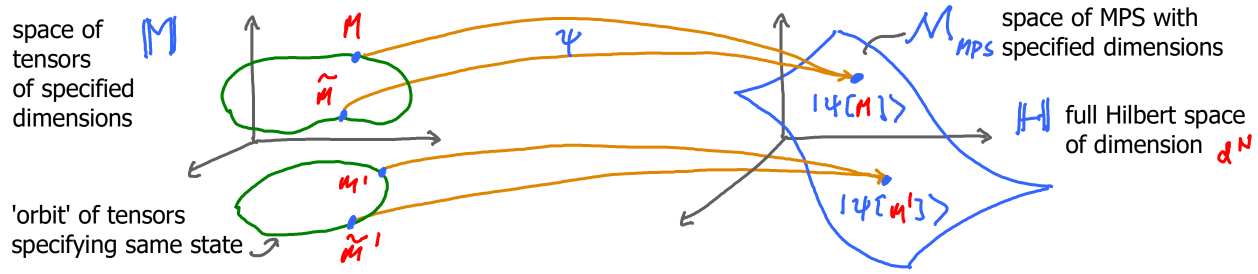
Gauge freedom: $|\psi[M]\rangle$ is unchanged under 'gauge transformation' on bond indices:

(2)

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

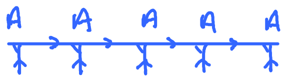
with $G_{[\ell]} \in GL(D_\ell, \mathbb{C})$ group of general complex linear transformation in D_ℓ dimensions

space of ... space of MPS with

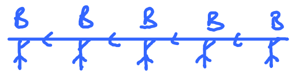
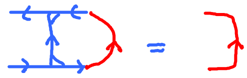


Note: $\mathbb{H}$ and $\mathbb{M}$ are vector spaces, but $\mathcal{M}_{MPS}$ is not, since sum of two MPS with same bond dimensions in general is an MPS with larger bond dimensions. $\mathcal{M}_{MPS}$ is a differential manifold, since it depends smoothly on the tensors in $\mathbb{M}$.

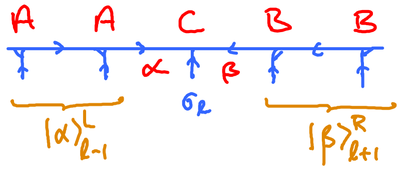
Gauge freedom can be exploited to bring MPS into left-, right-, bond- or site-canonical form:

<u>Left-canonical:</u> $|\psi[M]\rangle =$  with  (4)

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

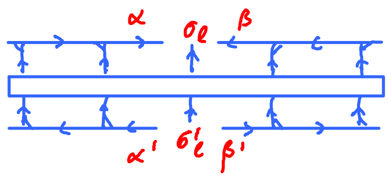
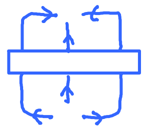
<u>Right-canoncial:</u> $|\psi[M]\rangle =$  with  (5)

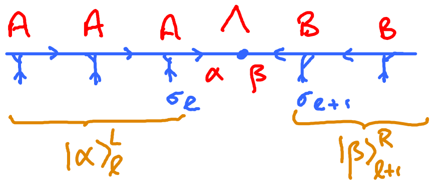
Gauge can be fixed uniquely by requiring $B^\sigma B_\sigma^\dagger = \mathbb{1}$ and $B^\dagger_\sigma B^\sigma =$ diagonal $\forall B_{[\ell]}$

<u>Site-canonical:</u> $|\psi[M]\rangle =$  $= |\beta\rangle^R_{\ell+1} |\sigma_\ell\rangle |\alpha\rangle^L_{\ell-1} C^{\alpha\sigma_\ell\beta}_{[\ell]}$ (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.

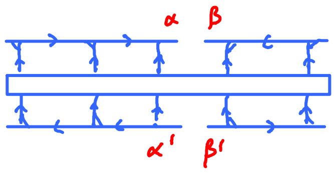
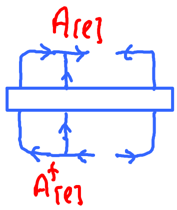
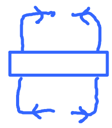
Hamiltonian matrix elements:

$${}^L_{\ell-1}\langle\alpha'| \langle\sigma'_\ell| {}^R_{\ell+1}\langle\beta'| \hat{H} |\beta\rangle^R_{\ell+1} |\sigma_\ell\rangle |\alpha\rangle^L_{\ell-1} =$$  $=$  $H_{[\ell]}$ (7)

<u>Bond-canonical:</u> $|\psi[M]\rangle =$  $= |\beta\rangle^R_{\ell+1} |\alpha\rangle^L_\ell \Lambda^{\alpha\beta}_{[\ell]}$

related to site-canonical form by $C_{[\ell]} = A_{[\ell]} \Lambda_{[\ell]} = \Lambda_{[\ell-1]} B_{[\ell]}$

Hamiltonian matrix elements:

$${}^L_\ell\langle\alpha'| {}^R_{\ell+1}\langle\beta'| \hat{H} |\beta\rangle^R_{\ell+1} |\alpha\rangle^L_\ell =$$  $=$  $H_{[\ell]} \equiv$  $K_{[\ell]}$ (12)

2. Tangent space

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

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 <u>specified</u> dimensions:

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

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

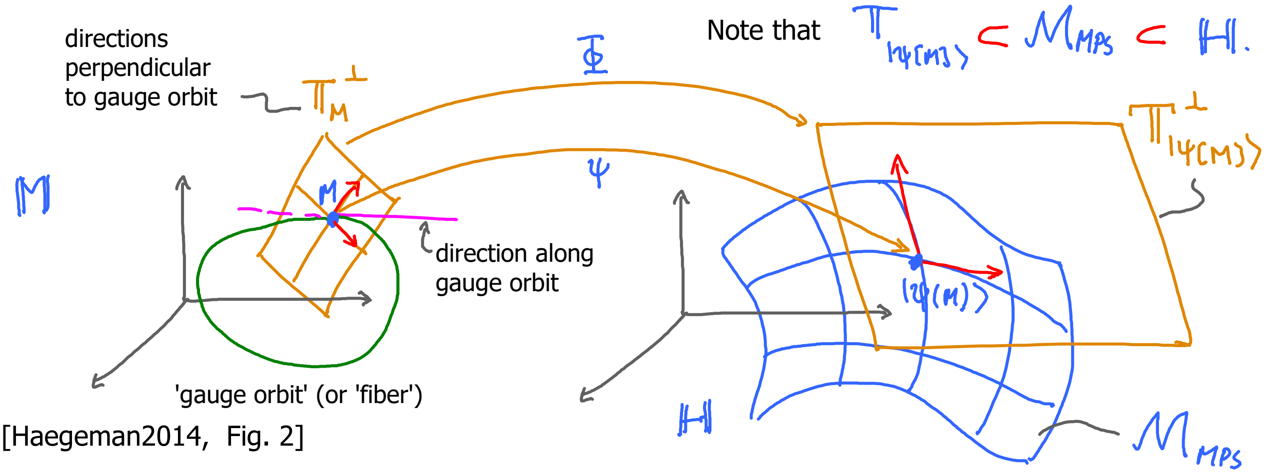
Here we have introduced the general notation

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

shorthand: $T \equiv (T_{[1]}, \dots, T_{[N]}) \in \mathbb{M}$ 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 <u>vector space</u> (since $|\Phi[T]\rangle$ is linear in T). It is called the 'tangent space', $\mathbb{T}_{|\psi[M]\rangle}$, 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 $\mathbb{T}_M^{\perp}$.

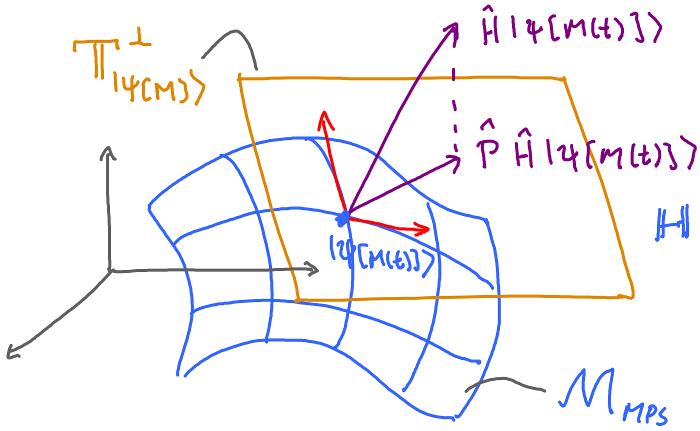
Then each $T \in \mathbb{T}_M^{\perp}$ uniquely specifies a corresponding tangent vector $|\Phi[T]\rangle_M$ in $\mathbb{T}^{\perp}_{|\psi[M]\rangle}$, the subset of tangent space orthogonal to $|\psi[M]\rangle$ (w.r.t. scalar product in Hilbert space $\mathbb{H}$):

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

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

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



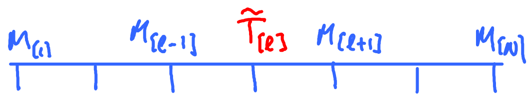
To implement this idea explicitly, we need explicit construction of the projector $\hat{P}$.

Remark: Eq. (6) can also be derived using a 'time-dependent variational principle' (TDVP).

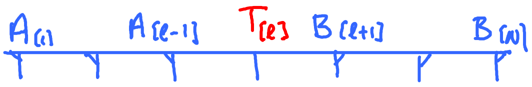
Hence time evolution with tangent space methods is also called TDVP in the literature [Haegeman2011].

3. Tangent space projector

[Haegeman2016], [Vanderstraeten2019, Sec. 3.2] TS.3

General form of tangent vector: $\sum_{\ell=1}^{N}$  (1)

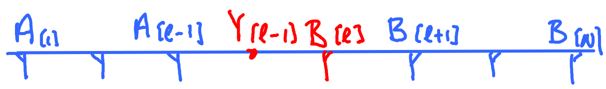
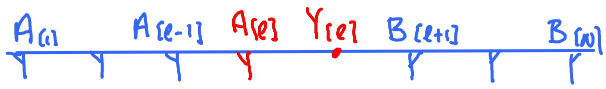
Gauge freedom can be used to bring ℓ-th summand into site-canonical form w.r.t. to site ℓ :

$$|\Phi[T]\rangle_M = \sum_{\ell=1}^{N}$$  (2)

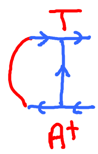
There is still gauge freedom left: $|\Phi[T]\rangle_M$ does not change under the replacement

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

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

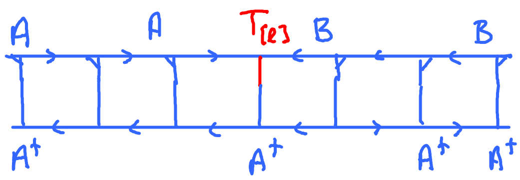
Check: extra terms yield $\Big(\sum_{\ell=2}^{N}$  $- \sum_{\ell=1}^{N-1}$  $\Big) = 0$ (4)

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 satify LGFC, replace it by $\tilde{T}$, with Y chosen such that $\tilde{T}$ does satisfy LGFC.]

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

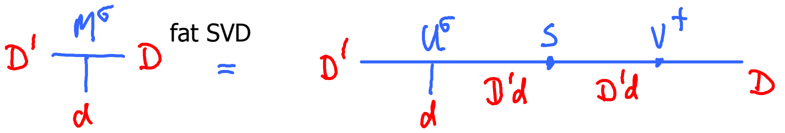
$$\langle \psi[M] | \Phi[T] \rangle_M = \sum_{\ell=1}^{N}$$  $= 0$ (6)

as required by property (iii) of Sec. TS.2. Second, it enables construction of an orthonormal basis for the orthogonal tangent space $\mathbb{T}^{\perp}_{|\psi[M]\rangle}$. To this end, we adopt a more convenient parameterization of $T_{[\ell]}$.

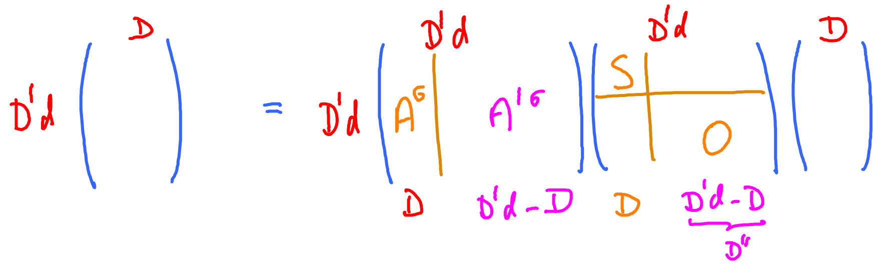
<u>Parametrization of $T_{[\ell]}$:</u> [Vanderstraeten2019, Sec. 3.2]

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

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

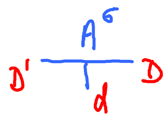


(7)



(8)

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

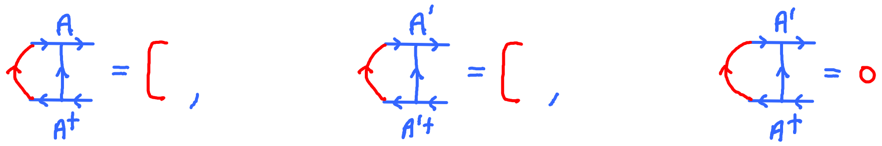


Let A'^{σ} be similarly built from its remaining $D'' = D'd - D$ columns:

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

$$U^{\dagger}_{\sigma} U^{\sigma} = \underset{dD' \times dD'}{\mathbb{1}} \quad \Rightarrow \quad \begin{array}{c} D \\ D'' \end{array} \begin{bmatrix} A^{\dagger}_{\sigma} \\ \hline A'^{\dagger}_{\sigma} \end{bmatrix} \left[A^{\sigma} \middle| A'^{\sigma} \right] = \begin{array}{cc} D & D'' \\ \multicolumn{2}{c}{\left[\begin{array}{c|c} \mathbb{1} & \\ \hline & \mathbb{1} \end{array}\right]} \end{array} : \qquad (9)$$

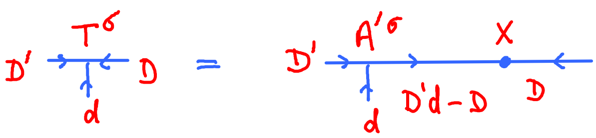
$$A^{\dagger}_{\sigma} A^{\sigma} = \underset{D \times D}{\mathbb{1}}, \qquad A'^{\dagger}_{\sigma} A'^{\sigma} = \underset{D'' \times D''}{\mathbb{1}}, \qquad A^{\dagger}_{\sigma} A'^{\sigma} = 0 \qquad (10a)$$



(10b)

Exploiting orthogonality of A and A', we can parametrize T in following factorized form

$$T^{\sigma}_{[\ell]} = A'^{\sigma_\ell}_{[\ell]} X_{[\ell]} ,$$

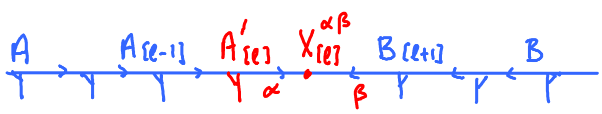


(11)

where $X_{[\ell]}$ is an arbitrary $(D'd - D) \times D$ matrix, and (9,far right) ensures that LGFC (5) holds.

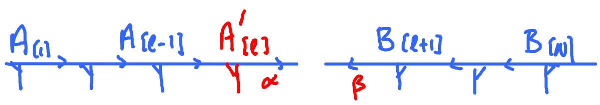
After left-gauge-fixing, tangent vectors have the following general form, parametrized by X :

$$|\Phi[X]\rangle_M \overset{(1),(11)}{=} \sum_{\ell=1}^{N}$$



$$\equiv \sum_{\ell=1}^{N} X^{\alpha\beta}_{[\ell]} |\Phi_{\ell,\alpha\beta}\rangle_M \qquad (12)$$

Here the set of states $|\Phi_{\ell,\alpha\beta}\rangle_M \equiv$



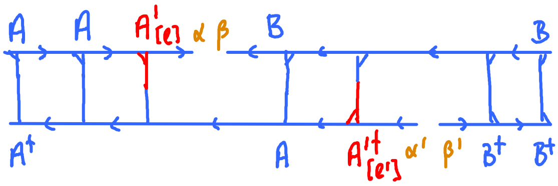
(13)

form an orthonormal basis for the orthogonal tangent space $\mathbb{T}^{\perp}$ since

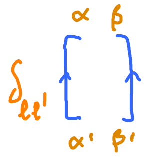
$|\Phi_{\ell,\alpha\beta}\rangle_M$

form an orthonormal basis for the orthogonal tangent space $\mathbb{T}^{\perp}_{|\Psi[M]\rangle}$, since

$${}_M\langle \Phi_{\ell',\alpha'\beta'} | \Phi_{\ell,\alpha\beta}\rangle_M =$$



$$= \delta_{\ell\ell'}$$



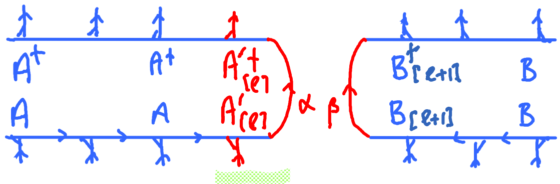
$$= \delta_{\ell\ell'} \, \mathbb{1}^{\alpha}{}_{\alpha'} \, \mathbb{1}^{\beta}{}_{\beta'} \qquad (14)$$

[(9) ensures that terms with $\ell' \neq \ell$ vanish, and for the $\ell' = \ell$ terms, we can close zipper from left and right.]

Tangent space projector

Tangent space basis yields desired projector onto orthogonal tangent space $\mathbb{T}^{\perp}_{|\Psi[M]\rangle}$:

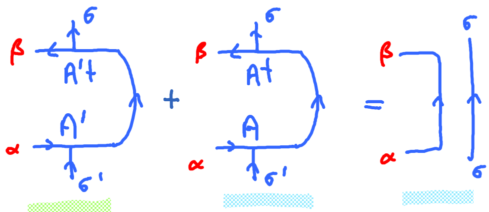
$$\hat{P}_{\mathbb{T}^{\perp}_{|\Psi[M]\rangle}} = \sum_{\ell\alpha\beta} |\Phi_{\ell,\alpha\beta}\rangle\langle\Phi_{\ell,\alpha\beta}| = \sum_{\ell=1}^{N}$$



$$(15)$$

It is convenient to 'eliminate' dependence on A' . Completeness of column-vectors of U in (7) ensures:

$$\big(\underset{D'\times D'}{A'^{\sigma'} A'^{\dagger}_{\sigma}} + \underset{d\times d}{A^{\sigma'} A^{\dagger}_{\sigma}}\big)^{\alpha}{}_{\beta} = \mathbb{1}^{\alpha}{}_{\beta} \, \mathbb{1}^{\sigma'}{}_{\sigma} \, ,$$

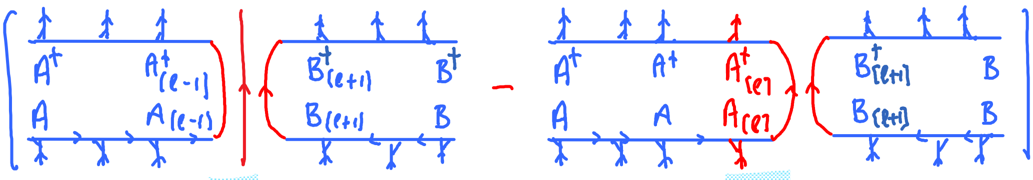


$$(16)$$

[Check: $A'^{\dagger}_{\sigma'}$ (16): $\quad \underbrace{A'^{\dagger}_{\sigma'} \big(A'^{\sigma'}}_{(10)\,=\,\mathbb{1}} A'^{\dagger}_{\sigma} + \overbrace{A^{\sigma'} A^{\dagger}_{\sigma}\big)}^{(10)\,=\,0} = A'^{\dagger}_{\sigma}$ ✓] (17)

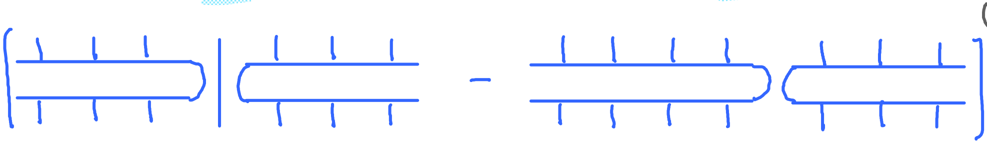
Then

$$\hat{P}_{\mathbb{T}^{\perp}_{|\Psi[M]\rangle}} \overset{(16)}{=} \sum_{\ell=1}^{N}$$



$$(18)$$

$$= \sum_{\ell=1}^{N}$$



$$(19)$$

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

First term: Unit operator in site reprensentation for site ℓ ;

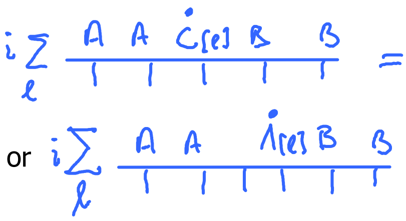
Second term: subtracts components parallel to $|\Psi[M]\rangle$.

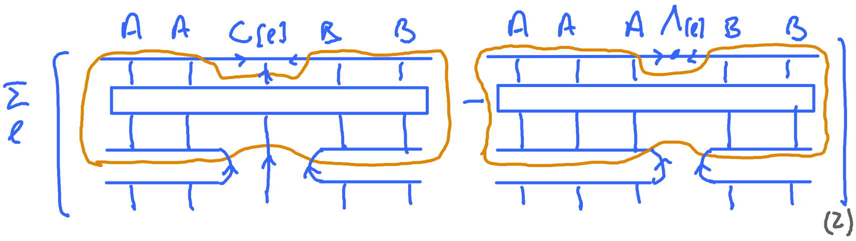
4. Time evolution

[Haegeman2016, App. B]

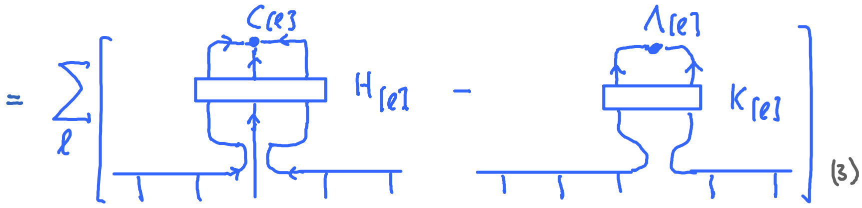
Schrödinger equation, projected onto tangent space, now takes the form

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





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



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 $\quad C_{[\ell]}(t+\tau) = e^{-iH_{[\ell]}\tau} C_{[\ell]}(t)$

forward time step (5)

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 $\quad \Lambda_{[\ell]}(t-\tau) = e^{-iK_{[\ell]}\tau} \Lambda_{[\ell]}(t)$

backward(!) time step (7)

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)

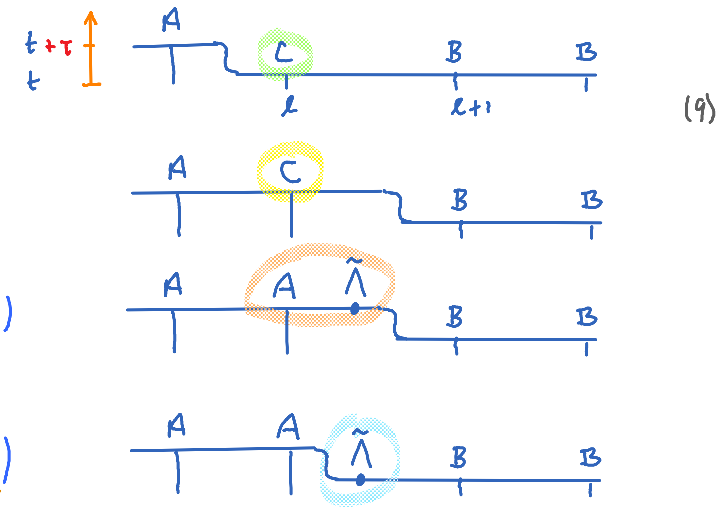
1. Forward sweep, for $\ell = 1, \dots, N-1$, starting from $\underbrace{B_{[1]}(t) B_{[2]}(t) \dots B_{[N]}(t)}_{}$ $C_{[1]}(t) \equiv$:

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

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

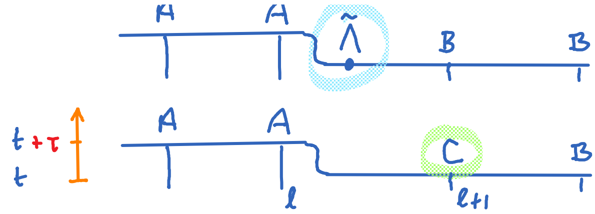
$$= \overbrace{A_{[\ell]}(t+\tau)\, \tilde{\Lambda}_{[\ell]}(t+\tau)}\, B_{[\ell+1]}(t)$$

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



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

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

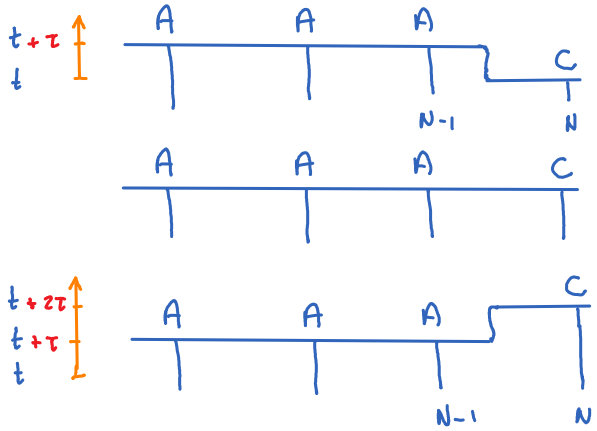


until we reach last site, and MPS described by $A_{[1]}(t+\tau)\dots A_{[N-1]}(t+\tau)\,C_{[N]}(t)$ (14)

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

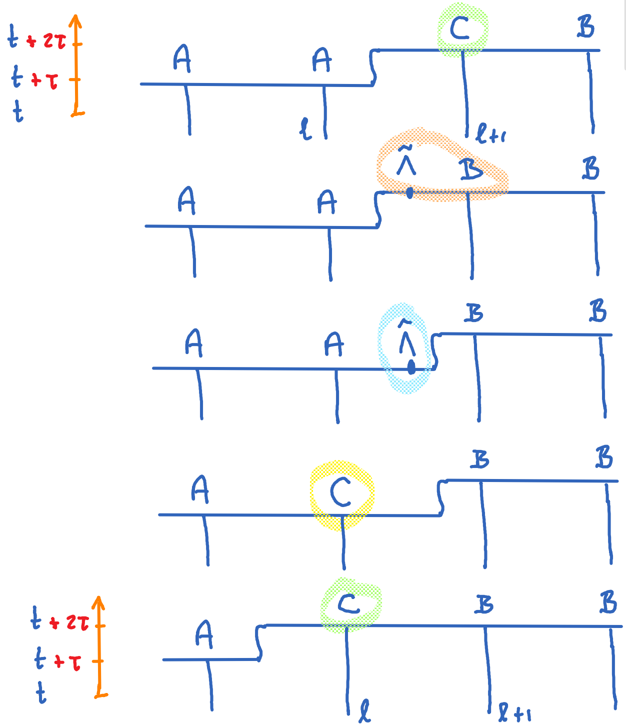
$$A_{[\ell]}(t+\tau)\,C_{[\ell+1]}(t+2\tau)$$

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

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

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

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



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

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!