Introduction to TDVP

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References:
Haegeman et al arXiv:1103.0936
Haegeman et al arXiv:1408.5056 (follow here)
Vanderstraeten et al arXiv:1810.07006
Paeckel et al arXiv:1901.05824

goal: evolution with Schrödinger equation $i\hbar\,\partial_t |\psi\rangle = H|\psi\rangle$

issue: solution is not a (finite-bond dimension) MPS

Time dependent variational principle (TDVP):

parametrize $|\psi(M^i(t))\rangle$ and derive equations for $\frac{d}{dt} M^i \equiv \dot{M}^i$

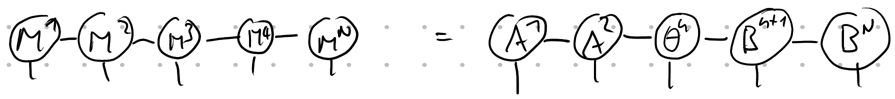
minimize

$$\Big\| \underbrace{\dot{M}^i(t)\, |\partial_i \psi(M^i)\rangle}_{\text{in tangent space}} - \underbrace{\left(-\tfrac{i}{\hbar}\right) H\, |\psi(M^i(t))\rangle}_{|\varphi\rangle \text{ not in tangent space}} \Big\|$$

$$\rightsquigarrow \quad \boxed{\frac{d}{dt}|\psi(M^i(t))\rangle = \left(-\frac{i}{\hbar}\right) P_T\, H\, |\psi(M^i(t))\rangle}$$

MPS manifold

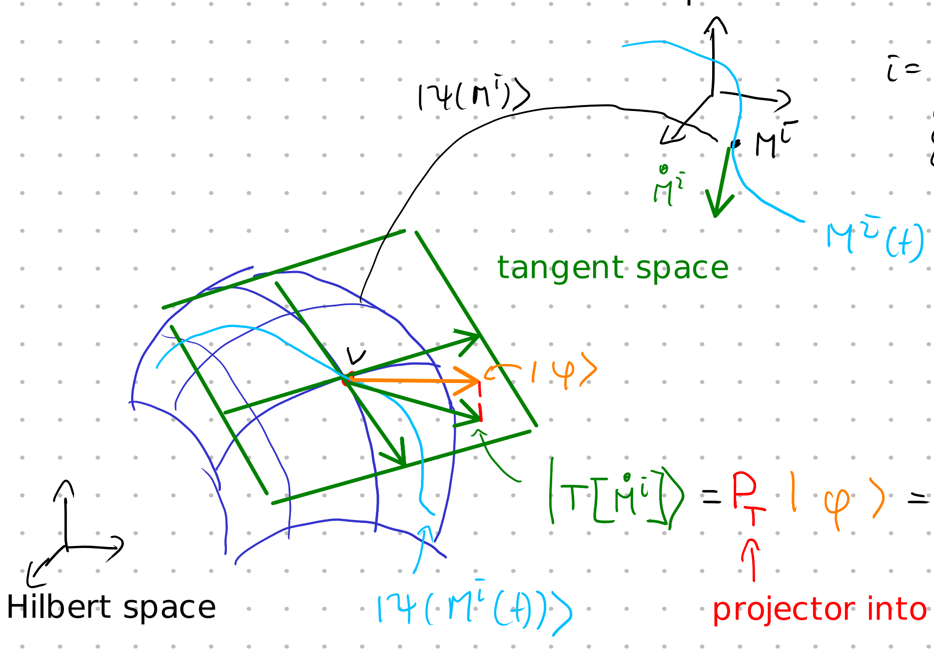
MPS with fixed bond dimension (and non-zero singular values)...

$|\psi(M^i)\rangle =$ 

... form a manifold

space of MPS tensor entries M^i

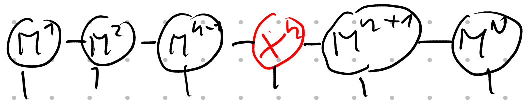
$i =$ superindex $\{(\alpha^n, j^n, \alpha^{n+1}, n)\}_{\forall n}$



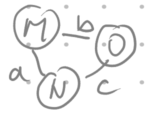
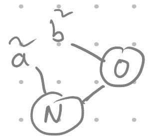
$|T[\dot{M}^i]\rangle = P_T\, |\varphi\rangle = P_T \left(-\frac{i}{\hbar}\right) H\, |\psi(M^i)\rangle$

projector into tangent space

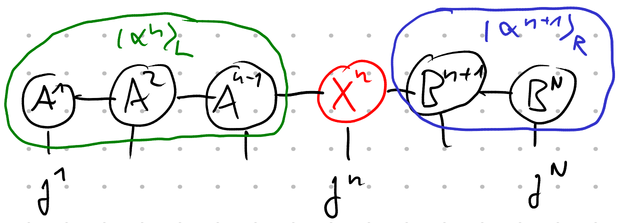
Tangent vector of general MPS

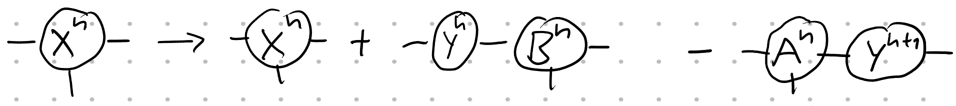
$X^{i} \, |\partial_{M^{i}} \psi(M^{i})\rangle = \sum_{n=1}^{N} \sum_{\{j^n\}}$  $|j^1 \dots j^N\rangle$

partial derivative = leave tensor out

$\partial_{M^{\tilde a \tilde b}}$  $= \sum_{abc} \underbrace{\frac{\partial M^{ab}}{\partial M^{\tilde a \tilde b}}}_{\delta_{a\tilde a}\,\delta_{b \tilde b}} N^{bc} O^{ca} =$ 

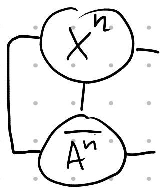
Tangent vector in mixed canonical form

$|T[X^{i}]\rangle = \sum_{n=1}^{N} \sum_{\{j^n\}}$  $|j^1 \dots j^N\rangle$

overcomplete: 

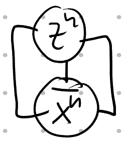
$(Y^1 = Y^{N+1} = 0)$

for some tensors Y describes same tangent vector

$\rightsquigarrow$ demand left gauge fixing  $= 0$ for all n < N

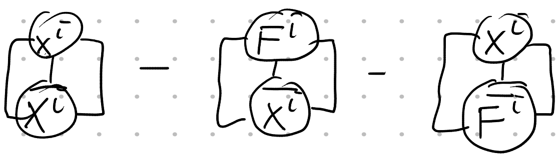
(convention)

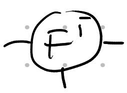
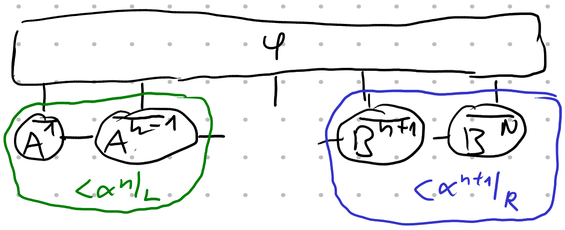
$\rightsquigarrow$ simplifies overlaps of tangent vectors:

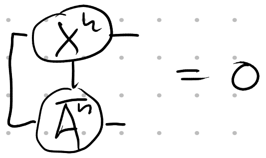
$\langle T[X^{i}] \,|\, T[Z^{i}]\rangle = \sum_n$ 

Tangent space projector P_T

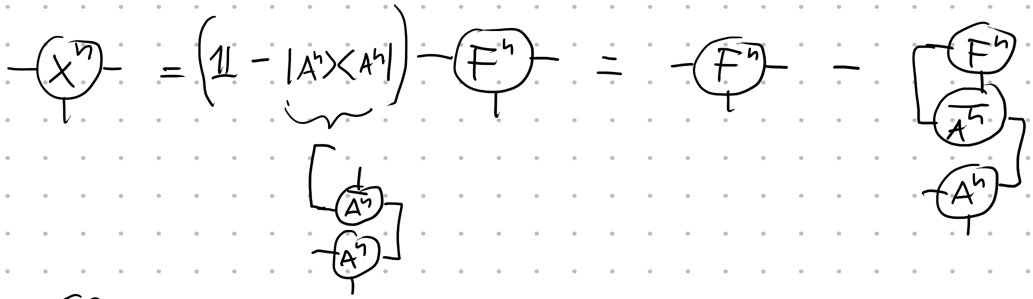
given $|\varphi\rangle$ we need to find $\min_{X^{i}} \| \, |T[X^{i}]\rangle - |\varphi\rangle \, \|^2 =$

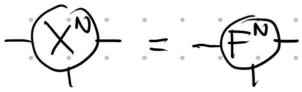
$= \min \Big| \sum_n$  $+ \langle \varphi | \varphi \rangle \Big|$

with  $=$ 

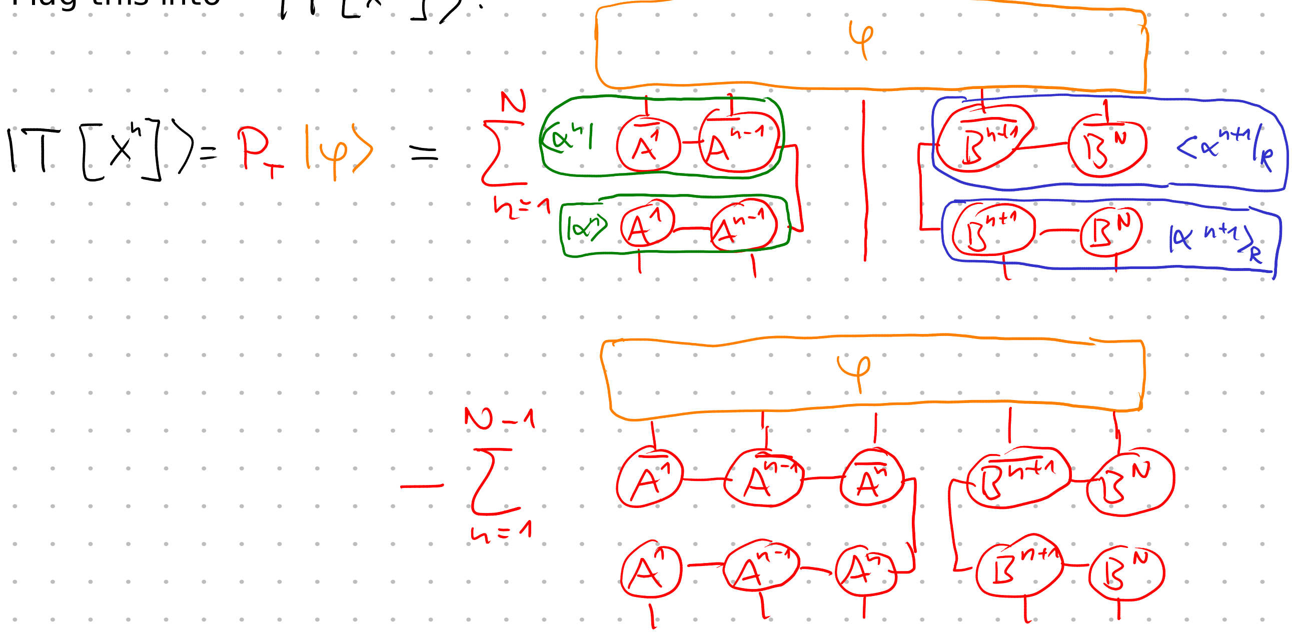
under the constraint  for $n < N$

minimal for

$n < N$: 

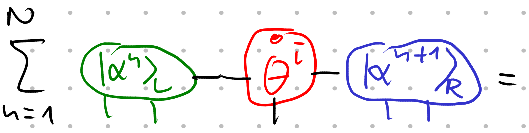
$n = N$: 

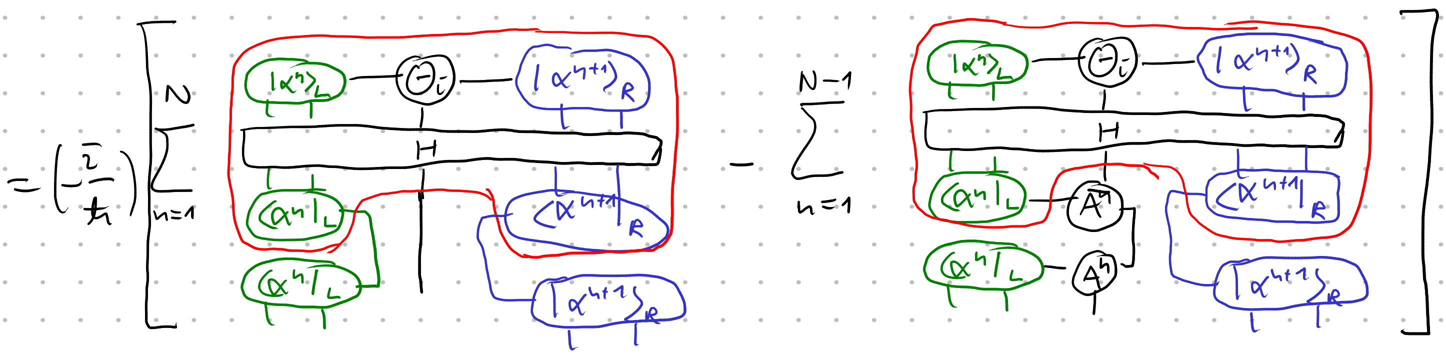
Plug this into $|T[X^n]\rangle$:



$$P_T = \sum_{n=1}^{N} |\alpha^n\rangle_L \langle\alpha^n|_L \otimes \mathbb{1}_n \otimes |\alpha^{n+1}\rangle_R \langle\alpha^{n+1}|_R - \sum_{n=1}^{N-1} |\alpha^{n+1}\rangle_L \langle\alpha^{n+1}|_L \otimes |\alpha^{n+1}\rangle_R \langle\alpha^{n+1}|_R$$

Plugging this into the $\boxed{\text{TDVP}}$ equation yields

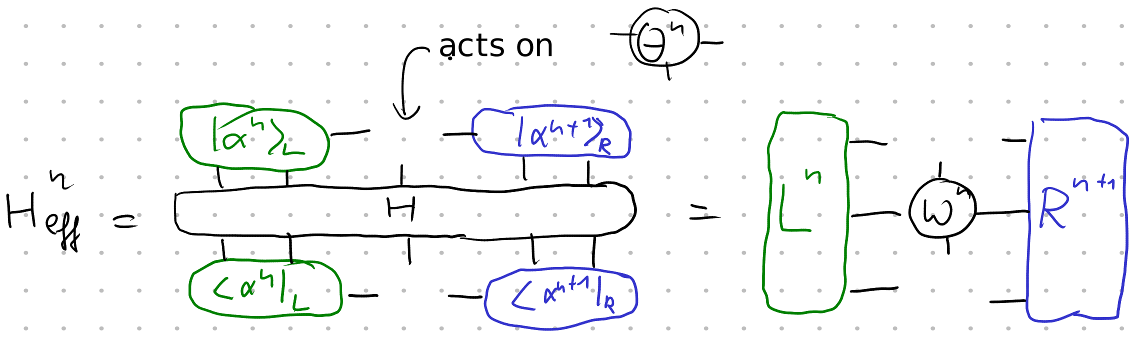
 $= |T[\dot{\Theta}^i]\rangle = \left(-\frac{i}{\hbar}\right) P_T H |\psi\rangle =$



We don't know how to integrate all terms at once,
but we can integrate each term individually!

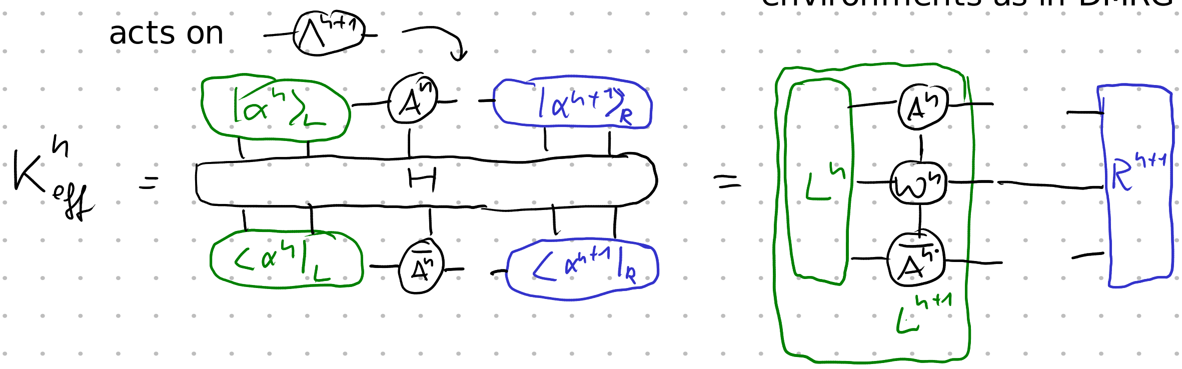
Doing so yields the TDVP algorithm on the next page.

Define one-site



environments as in DMRG

zero-site



TDVP algorithm for MPS

Start with MPS in right canonical form

for n in {1, 2, ..., N-1}: sweep left to right

evolve Θ^n with H^n_{eff} forward by $+\frac{dt}{2}$

split $\Theta^n \overset{SVD}{\underset{QR}{=}} A^n \Lambda^{n+1}$

calculate L^{n+1}, K^n_{eff}

evolve Λ^{n+1} with K^n_{eff} backward by $-\frac{dt}{2}$

evolve Θ^N forward by dt

for n in {N-1, ..., 2, 1} sweep right to left

split $\Theta^{n+1} \overset{SVD}{\underset{QR}{=}} \Lambda^{n+1} B^{n+1}$

calculate R^n, K^n_{eff}

evolve Λ^n with K^n_{eff} backward by $-\frac{dt}{2}$

evolve Θ^n with H^n_{eff} forward by $+\frac{dt}{2}$

Properties:

very similar to DMRG:
recover (finite) DMRG for imaginary evolution with $dt \to \infty$

symmetric under inverse evolution,
hence correct to second order in dt

no truncation necessary,
always stay in manifold of MPS with fixed bond dimension
->can use two-site scheme to expand the bond dimension

symplectic, preserves the energy