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

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goal: evoluton with Schroedinger equation $i\hbar \partial_t |\Psi\rangle = H |\Psi\rangle$

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

Time dependent variation principle (TDVP)

parametrize $|\Psi(M^i(t))\rangle$ and derive equation for $\frac{d}{dt} M^i = \dot{M}^i$

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

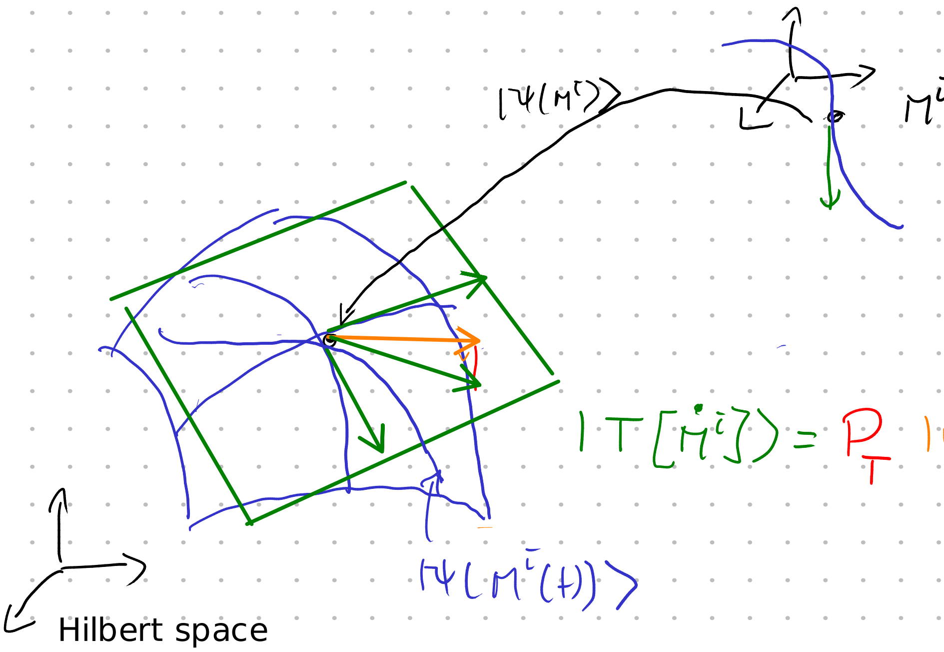
$$\rightsquigarrow \quad \boxed{\frac{d}{dt} |\Psi(M^i(t))\rangle = \left(-\tfrac{i}{\hbar}\right) P_T\, H\, |\Psi(M^i(t))\rangle}$$

MPS manifold

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

$$|\Psi(M^i)\rangle = M^1 - M^2 - M^3 - M^4 - M^N = A^1 - A^2 - \Theta^n - B^{n+1} - B^N$$

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

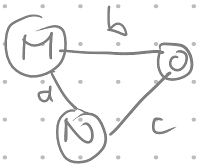
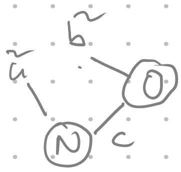


$$|T[\dot{M}^i]\rangle = P_T\, |\varphi\rangle = P_T \left(-\tfrac{i}{\hbar}\right) H\, |\Psi(M^i)\rangle$$

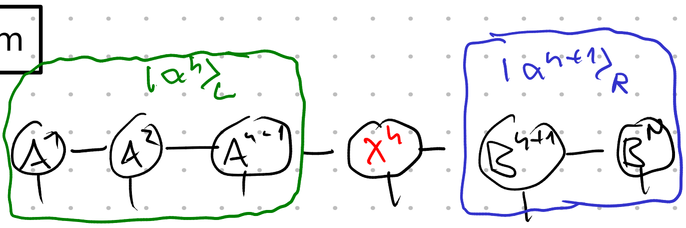
Tangent vector of general MPS

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

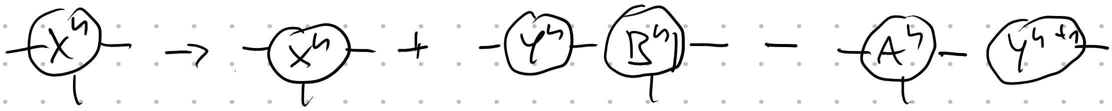
partial derivate = leave tensor out

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

Tangent vector in mixed canonical form

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

overcomplete:



for some  describes the same tangent vector $(Y^1 = Y^{N+1} = 0)$

$$|T[X^i]\rangle = |T[X^i + Y^n B^n - A^n Y^{n+1}]\rangle$$

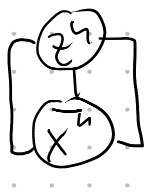
demand left gauge fixing

$\uparrow$

convention

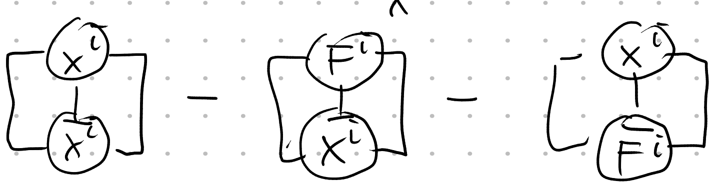
 $= 0$ for all n < N

$\leadsto$ simplifies overlaps of tangent vectors:

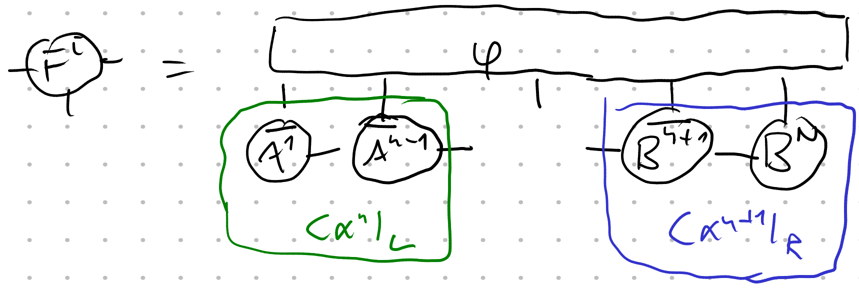
$$\langle T[X^i] | T[Z^i]\rangle = \sum_n$$ 

Tangent space projector P_T

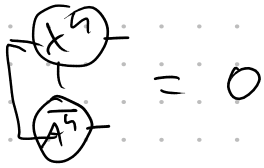
given $|\varphi\rangle$ we need to find $\min\limits_{X^i} \| \, |T[X^i]\rangle - |\varphi\rangle \|^2$

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

with



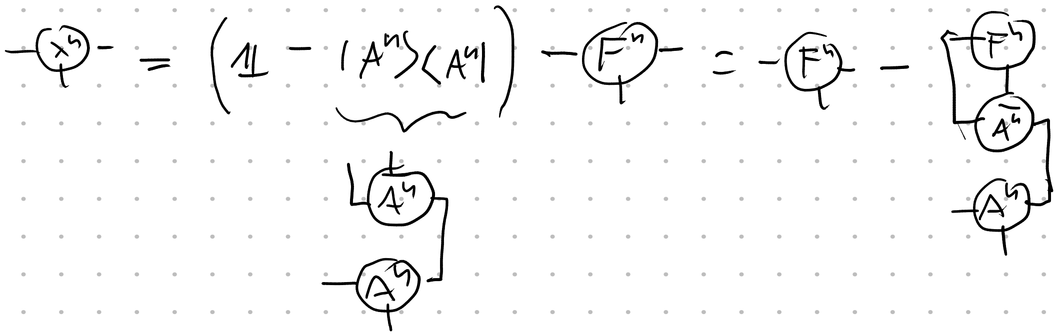
under the constraint



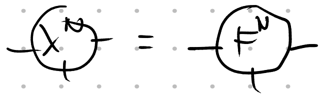
for n < N

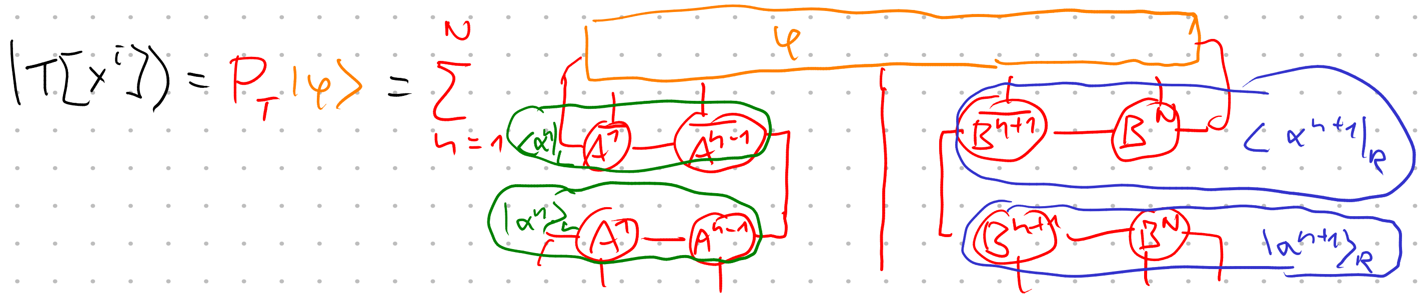
minmal for

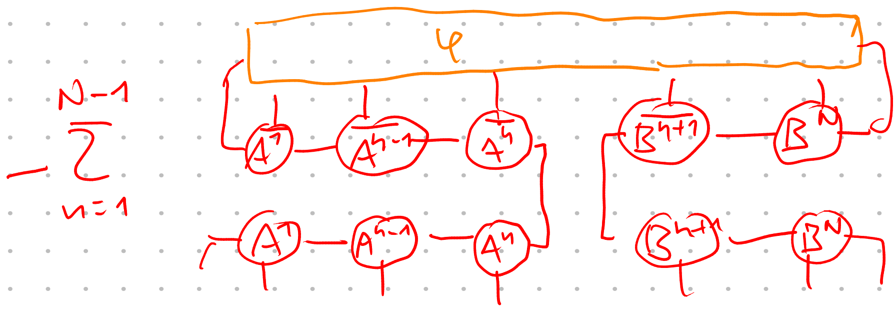
for n < N



for n = N

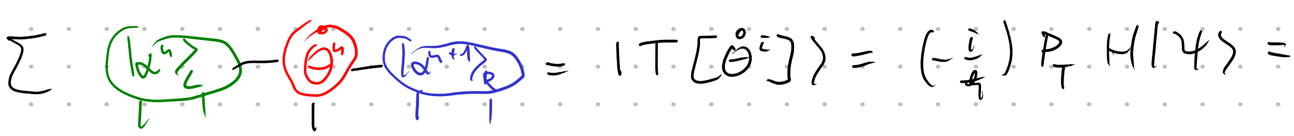


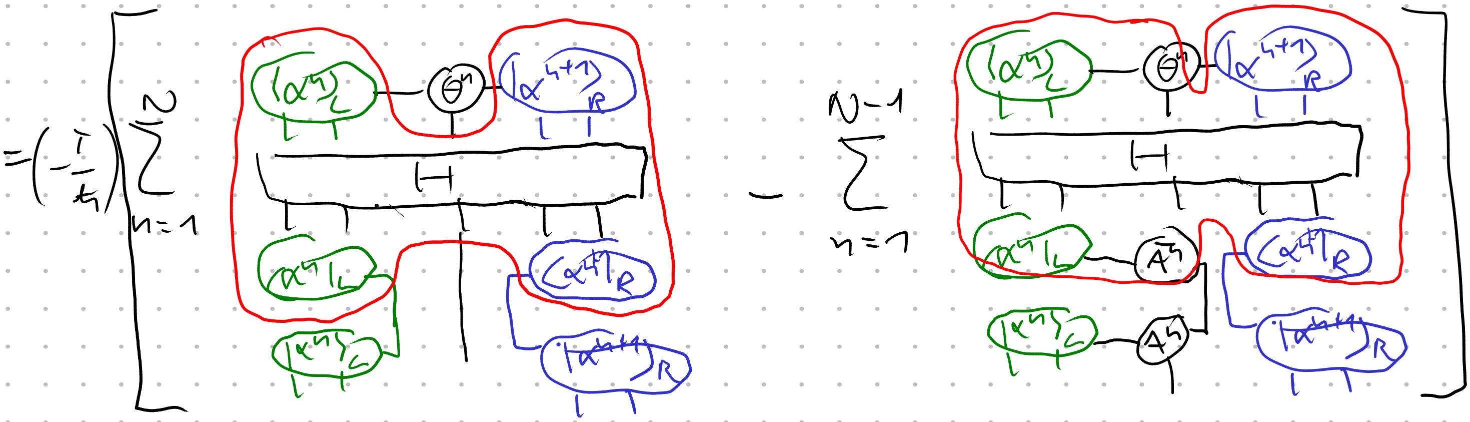




$$P_T = \sum_{n=1}^{N} |\alpha^n\rangle_L \langle \alpha^n|_L \otimes \mathbb{1}_n \otimes |\alpha^{n+1}\rangle_R \langle \alpha^{n+1}|_R$$
$$- \sum_{n=1}^{N-1} |\alpha^{n+1}\rangle_L \langle \alpha^{n+1}|_L \otimes |\alpha^{n+1}\rangle_R \langle \alpha^{n+1}|_R$$

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



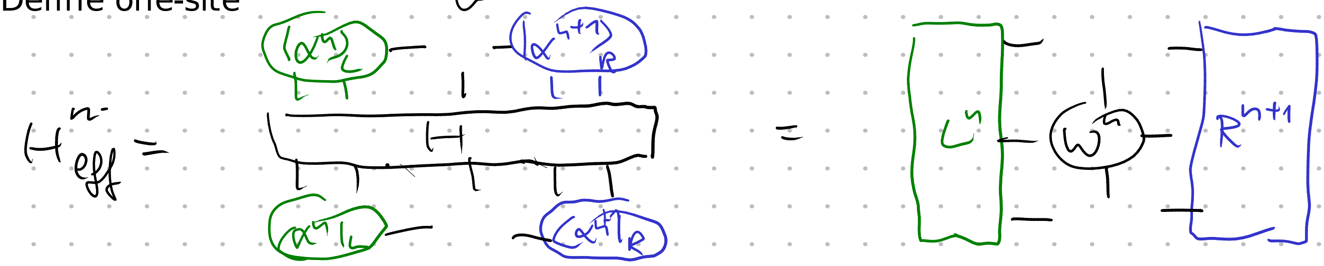


We don't know hot to integrate all terms at once,
but we can integrate each n term individually!

Doing this integration yields the TDVP algorithm for MPS (below)

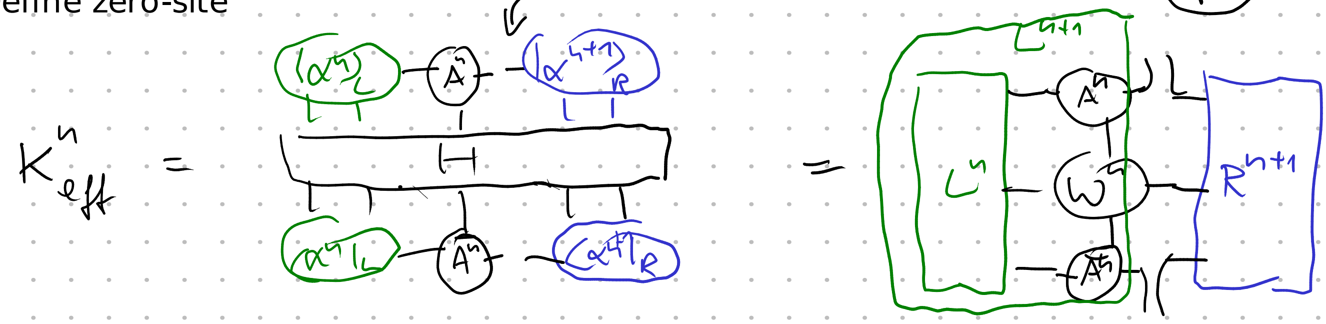
Define one-site

acts on just one site



Define zero-site

acts on "zero-site" wave function Λ^{n-1}



TDVP algoritm for finite MPS

Start with MPS in right-canonical form

for n in {1, 2, ... N-1}:

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

split $\Theta^n = A^n \Lambda^{n+1}$

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

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

evolve Θ^N forward with H^N_{eff} by dt

for n in {N-1, ..., 1}

split $\Theta^{n+1} = \Lambda^{n+1} B^{n+1}$

calculate R^n, K^n_{eff}

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

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

Properties:

similar to DMRG,
recover DMRG when doing imaginary time evolution with dt-> inf

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

no truncation necessary, always stay in the manifold of fixed bond dim MPS

-> one can use a similar two-site scheme to expand the bond dim.

symplectic, preserves the energy exactly