

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

minimize $\| \underbrace{\dot{M}^{\bar{i}}(t) |\partial_{\bar{i}} \psi(M^{\bar{i}})\rangle}_{\text{in the tangent space}} - \underbrace{\left(\frac{i}{\hbar}\right) H |\psi(M^{\bar{i}})\rangle}_{\text{not in the tangent space}} \|$

$$\Rightarrow \frac{d}{dt} |\psi(M^{\bar{i}}(t))\rangle = \left(\frac{-i}{\hbar}\right) P_T H |\psi(M^{\bar{i}}(t))\rangle$$

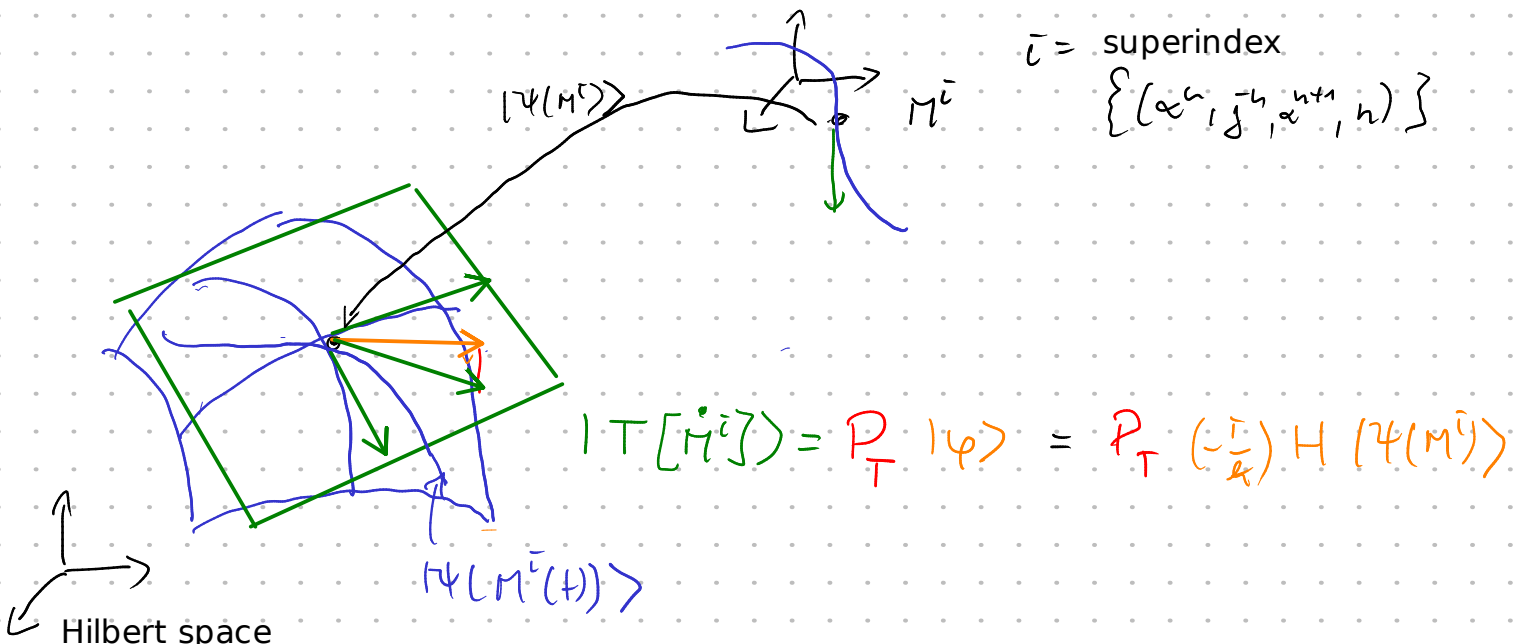
MPS manifold

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

$$|\psi(M^{\bar{i}})\rangle = \begin{matrix} \textcircled{M^1} & \textcircled{M^2} & \textcircled{M^3} & \textcircled{H} & \textcircled{M^N} \end{matrix} = \begin{matrix} \textcircled{A^1} & \textcircled{A^2} & \textcircled{G^3} & \textcircled{B^{N+1}} & \textcircled{B^N} \end{matrix}$$

space of MPS tensor entries

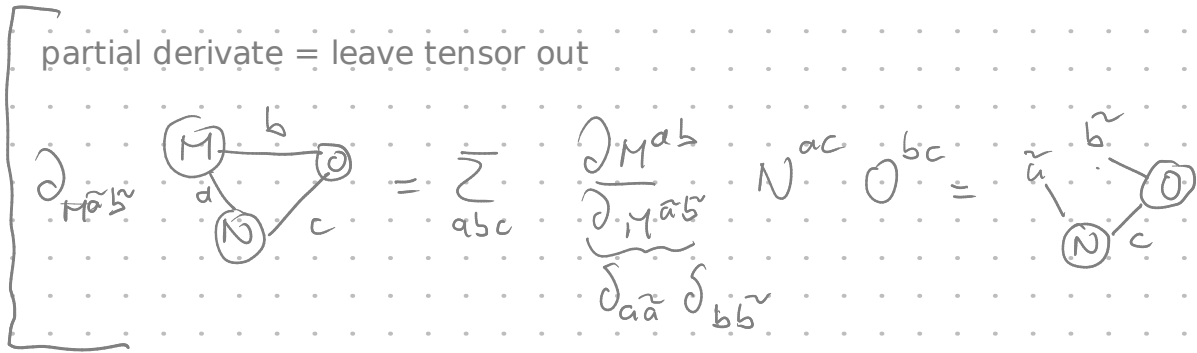
$\bar{i} = \text{superindex}$
 $\{(\alpha^{\bar{i}}, \beta^{\bar{i}}, \alpha^{\bar{i}+1}, \eta)\}$



Tangent vector of general MPS

$$X^i |\partial_{M^i} \Psi(M^i)\rangle = \sum_{n=1}^N \sum_{\{j^n\}} (M^1) \cdots (M^{n-1}) \textcircled{X^n} (M^{n+1}) \cdots (M^N) |\delta^1 \dots \delta^N\rangle$$

partial derivate = leave tensor out



Tangent vector in mixed canonical form

$$|T[X^i]\rangle = \sum_{n=1}^N \sum_{\{j^n\}} \left[\underbrace{(A^1) \cdots (A^{n-1})}_{\text{left}} \textcircled{X^n} \underbrace{(B^{n+1}) \cdots (B^N)}_{\text{right}} \right] |\delta^1 \dots \delta^N\rangle$$

overcomplete:

$$\textcircled{X^n} \rightarrow \textcircled{X^n} + \textcircled{Y^n} \textcircled{B^n} - \textcircled{A^n} \textcircled{Y^{n+1}}$$

for some $\textcircled{Y^n}$ describes the same tangent vector

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

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

demand left gauge fixing

↑
convention

$$\left[\begin{array}{c} \textcircled{X^n} \\ \textcircled{A^n} \end{array} \right] = 0 \quad \text{for all } n < N$$

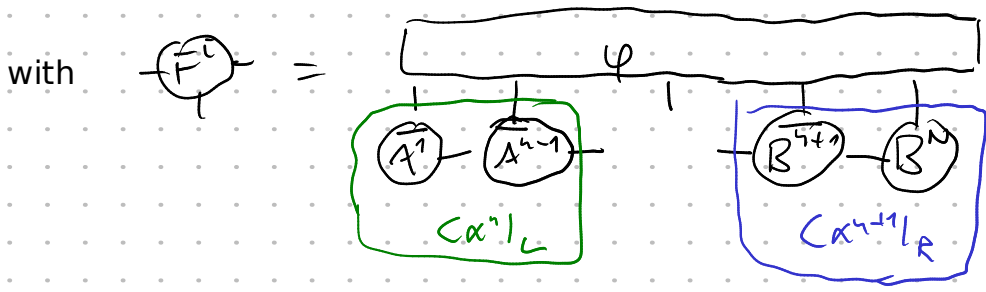
∴ simplifies overlaps of tangent vectors:

$$\langle T[X^i] | T[Z^i] \rangle = \sum_n \left[\begin{array}{c} \textcircled{Z^n} \\ \textcircled{X^n} \end{array} \right]$$

Tangent space projector P_T

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

$$= \min \left| \sum_n \left[\begin{array}{c} \textcircled{X^n} \\ \textcircled{X^n} \end{array} \right] - \left[\begin{array}{c} \textcircled{F^n} \\ \textcircled{X^n} \end{array} \right] - \left[\begin{array}{c} \textcircled{X^n} \\ \textcircled{F^n} \end{array} \right] + \langle \psi | \psi \rangle \right|$$



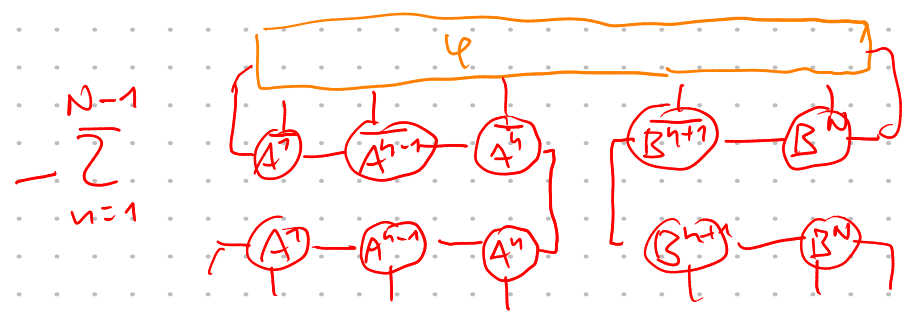
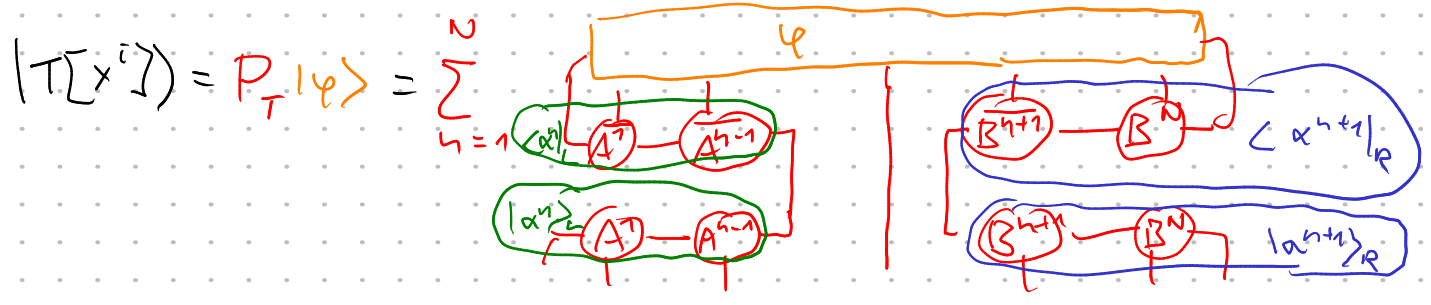
under the constraint

$$\begin{matrix} \textcircled{X^n} \\ | \\ \textcircled{A^n} \end{matrix} = 0 \quad \text{for } n < N$$

minimal for

for $n < N$
$$\textcircled{X^n} = \left(\mathbb{1} - \underbrace{|A^n\rangle\langle A^n|}_{\begin{matrix} \downarrow \\ \textcircled{A^n} \\ \downarrow \\ \textcircled{A^n} \end{matrix}} \right) \textcircled{F^n} = \textcircled{F^n} - \begin{matrix} \textcircled{F^n} \\ | \\ \textcircled{A^n} \\ | \\ \textcircled{A^n} \end{matrix}$$

for $n = N$
$$\textcircled{X^N} = \textcircled{F^N}$$



$$P_T = \sum_{n=1}^N |\alpha^n\rangle_L \langle \alpha^n|_L \otimes \mathbb{1}_L \otimes |\alpha^{n+1}\rangle_R \langle \alpha^{n+1}|_R - \sum_{n=1}^{N-1} |\alpha^{n+1}\rangle_L \langle \alpha^{n+1}|_L \otimes |A^{n+2}\rangle_R \langle A^{n+2}|_R$$

Plugging this into the TDVP equation yields

$$\sum \begin{matrix} \textcircled{|\alpha^n\rangle_L} \\ | \\ \textcircled{\Theta^n} \\ | \\ \textcircled{|\alpha^{n+1}\rangle_R} \end{matrix} = |T[\Theta^i]\rangle = \left(-\frac{i}{\beta}\right) P_T H |\psi\rangle =$$

$$= \left(-\frac{1}{\lambda_n} \right) \sum_{n=1}^N \left[\begin{array}{c} \text{Diagram 1: } \alpha_L^{(n)} \text{ and } \alpha_R^{(n+1)} \text{ are circled in green and blue respectively. A gate } \Theta^n \text{ acts on } \alpha_L^{(n)} \text{ and } \alpha_R^{(n+1)}. \text{ The rest of the MPS is shown below.} \\ \text{Diagram 2: } \alpha_L^{(n)} \text{ and } \alpha_R^{(n+1)} \text{ are circled in green and blue respectively. A gate } \Theta^n \text{ acts on } \alpha_L^{(n)} \text{ and } \alpha_R^{(n+1)}. \text{ Below, } \alpha_L^{(n)} \text{ and } \alpha_R^{(n+1)} \text{ are connected to } A^n \text{ gates, which then connect to } \alpha_L^{(n+1)} \text{ and } \alpha_R^{(n+2)} \text{ respectively.} \end{array} \right]$$

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

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

Define one-site acts on just one site

$$H_{\text{eff}}^n = \begin{array}{c} \alpha_L^{(n)} \text{ --- } \alpha_R^{(n+1)} \\ | \qquad \qquad | \\ \text{---} H \text{---} \\ | \qquad \qquad | \\ \alpha_L^{(n+1)} \text{ --- } \alpha_R^{(n+2)} \end{array} = \begin{array}{c} \boxed{L^n} \text{ --- } \Theta^n \text{ --- } \boxed{R^{n+1}} \end{array}$$

Define zero-site acts on "zero-site" wave function

$$K_{\text{eff}}^n = \begin{array}{c} \alpha_L^{(n)} \text{ --- } A^n \text{ --- } \alpha_R^{(n+1)} \\ | \qquad \qquad | \\ \text{---} H \text{---} \\ | \qquad \qquad | \\ \alpha_L^{(n+1)} \text{ --- } A^n \text{ --- } \alpha_R^{(n+2)} \end{array} = \begin{array}{c} \Lambda^{n+1} \\ | \\ \boxed{L^n} \text{ --- } \begin{array}{c} A^n \\ | \\ \Theta^n \\ | \\ A^n \end{array} \text{ --- } \boxed{R^{n+1}} \end{array}$$

TDVP algorithm for finite MPS

Start with MPS in right-canonical form

for n in $\{1, 2, \dots, N-1\}$:

evolve $\textcircled{\Theta^n}$ with H_{eff}^n forward by $\frac{dt}{2}$

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

calculate $L^{n+1}, K_{\text{eff}}^n$

evolve $\textcircled{\Lambda^{n+1}}$ with K_{eff}^n backwards by $= \frac{dt}{2}$

evolve $\textcircled{\Theta^N}$ forward with H_{eff}^N by dt

for n in $\{N-1, \dots, 1\}$

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

calculate R^n, K_{eff}^n

evolve $\textcircled{\Lambda^{n+1}}$ with K_{eff}^n backwards by $= \frac{dt}{2}$

evolve $\textcircled{\Theta^n}$ with H_{eff}^n forward by $\frac{dt}{2}$

Properties:

similar to DMRG,
recover DMRG when doing imaginary time evolution with $dt \rightarrow \text{inf}$

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

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

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

symplectic, preserves the energy exactly