

The Problem: Calculation of Time Evolution

1. The time evolution of a closed quantum system is governed by the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle$$

$\hbar \rightarrow$ Planck's constant (set to 1)
 $H \rightarrow$ Hamiltonian

Assuming that the Hamiltonian is time independent:

$$|\Psi(t)\rangle = e^{-iHt} |\Psi(0)\rangle \quad |\Psi(0)\rangle \rightarrow \text{Initial state}$$

2. The time evolution of an open quantum system is governed (under certain conditions) Lindblad master equation:

$$\frac{\partial}{\partial t} \rho(t) = \mathcal{L} \rho(t)$$

$\rho \rightarrow$ Density matrix
 $\mathcal{L} \rightarrow$ Liouvillian superoperator

Assuming that the Liouvillian is time independent:

$$\rho(t) = e^{\mathcal{L}t} \rho(0)$$

Zwolak and Vidal, PRL 2004; Verstraete et al., PRL 2004

3. A thermal state of a system at a temperature T can be calculated through **imaginary time evolution**, with time $\beta = 1/T$ (Boltzmann constant set to 1)

$$\rho(T) = \frac{e^{-\beta H}}{\mathcal{Z}(\beta)} \quad \text{with} \quad \mathcal{Z}(\beta) = \text{Tr}(e^{-\beta H}) \quad \begin{matrix} \text{Zwolak and Vidal, PRL 2004;} \\ \text{Verstraete et al. PRL 2004} \end{matrix}$$

the partition function

4. An alternative way to calculate the ground state of a Hamiltonian is to perform imaginary time evolution on an initial state with a finite overlap with the ground state:

$$|\Psi_{\text{ground}}\rangle = \lim_{\tau \rightarrow \infty} \frac{e^{-H\tau} |\Psi_0\rangle}{\|e^{-H\tau} |\Psi_0\rangle\|} \quad \begin{matrix} \text{Vidal, PRL 2004; Vidal, PRL 2007} \\ \text{with} \quad \langle \Psi_0 | \Psi_{\text{ground}} \rangle \neq 0 \end{matrix}$$

5. The solutions of some partial differential equation have similar forms. They can also be recast as imaginary time evolution of a quantum system that encodes the function:

$$\frac{\partial}{\partial t} F(t) = H F(t) \quad \rightarrow \quad F(t) = e^{Ht} F(0)$$

MPS algorithms have been developed
for solving all of these problems:

- Time evolving block decimation (TEBD)
- Time-dependent variational principle (TDVP)

Time Evolving Block Decimation (TEBD)

The method approximates the exponential of the Hamiltonian and applies it to the MPS

$$|\Psi(t)\rangle = e^{-iHt} |\Psi(0)\rangle$$

We assume that the Hamiltonian involves single-site and two-site nearest-neighbor terms:

$$H = \sum_j h_{j,j+1}$$

$h_{j,j+1} \rightarrow$ Local Hamiltonian

Exactly calculating the full exponential of the Hamiltonian (i.e., the time evolution operator) is infeasible. Instead, we approximate the exponential at each time step δt :

$$e^{-iHT} \approx [e^{-iH\delta t}]^{T/\delta t} = \prod_{k=1}^{T/\delta t} e^{-iH\delta t}$$

We will perform the time evolution step by step. This is valid as long as the time step δt is much smaller than the characteristic time scale of the fastest process.

If the Hamiltonian is time dependent ($H(t)$), the method is also valid as long as the time step δt is very small, so the Hamiltonian is almost constant at every time.

Now we consider the evolution operator of a single time step

$$e^{-iH\delta t} = e^{-i\delta t \sum_j h_{j,j+1}} \neq \prod_j e^{-i\delta t h_{j,j+1}}$$

We can see this from several expansions. For example, from the Baker-Campbell-Hausdorff formula

$$e^A e^B = e^C \quad C = A + B + \frac{1}{2} [A, B] + \dots \quad \text{and} \quad [a, b] = ab - ba$$

If we restrict to the simplest expansion

$$\begin{aligned} e^{\delta t A} e^{\delta t B} &\approx e^{\delta t (A+B) + \frac{\delta t^2}{2} [A, B]} \approx e^{\delta t (A+B)} \left(1 + \frac{\delta t^2}{2} [A, B]\right) \\ \rightarrow e^{\delta t (A+B)} &\approx e^{\delta t A} e^{\delta t B} + O(\delta t^2) \end{aligned}$$

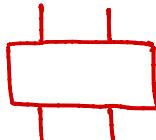
This approximation is not used in MPS time evolution. It is used for quantum computation purposes due to low number of operations.

For higher order, it is common to use a Suzuki-Trotter expansion

$$e^{-iH\delta t} = \left(\prod_{j=1}^{N-1} e^{-ih_{j,j+1}\delta t/2} \right) \left(\prod_{j=N-1}^1 e^{-ih_{j,j+1}\delta t/2} \right) + O(\delta t^3)$$

$$= [e^{-ih_{1,2}\delta t/2} \ e^{-ih_{2,3}\delta t/2} \ e^{-ih_{3,4}\delta t/2} \dots \ e^{-ih_{N-1,N}\delta t/2}]$$

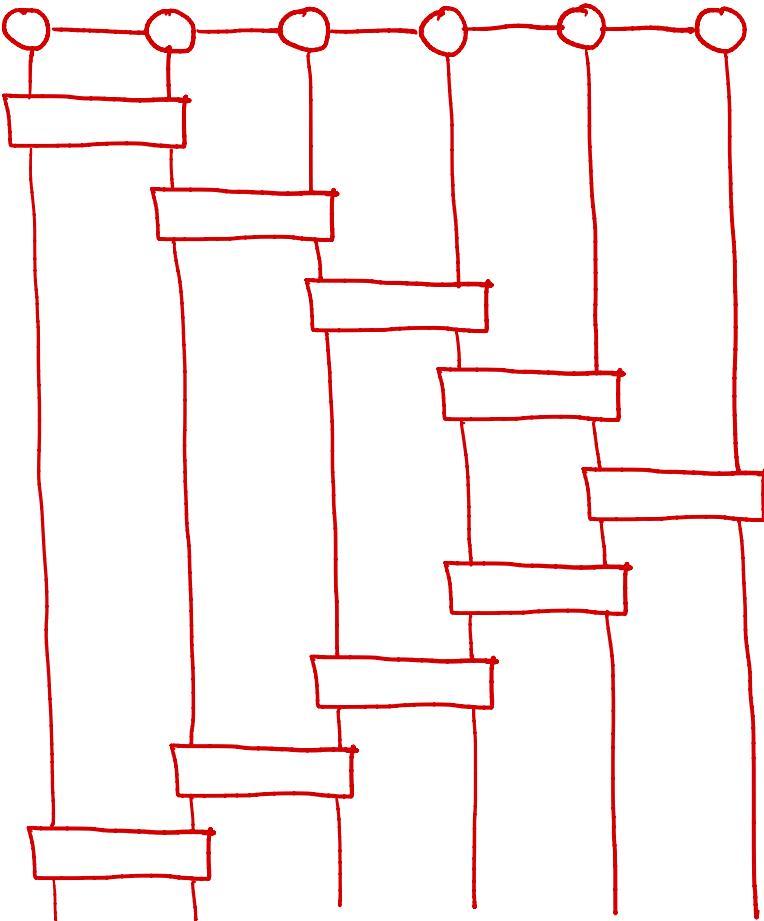
$$[e^{-ih_{N-1,N}\delta t/2} \dots \ e^{-ih_{3,4}\delta t/2} \ e^{-ih_{2,3}\delta t/2} \ e^{-ih_{1,2}\delta t/2}] + O(\delta t^3)$$



Each exponential is a four-site tensor

This is the standard time evolution approximation. Higher order are possible, but very rarely used.

Diagrammatic representation



After each two-site gate, MPS recovered through SVD. Each gate increases bond dimension. Truncation has to be performed to prevent an uncontrolled growth of the bond dimension. Orthogonality center moves with each gate.

Sources of error:

- Trotter error: For second order expansion

$$\mathcal{O}(\delta t^3) \quad \text{Per time step}$$

$$\frac{\mathcal{O}(\delta t^3)T}{\delta t} = \mathcal{O}(\delta t^2) \quad \text{Up to time } T$$

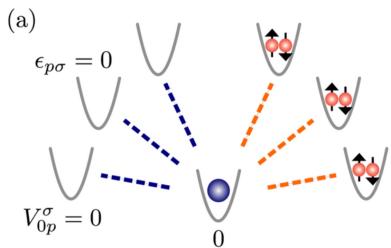
Controllable with smaller δt . Higher order expansions might be more demanding.

- Truncation error: Measured from discarded singular values. Controllable with higher truncation parameter χ .

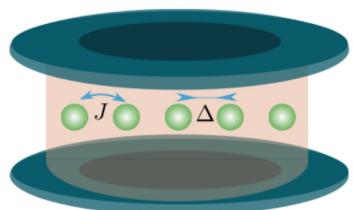
Both errors must be balanced. Reducing δt

More gates and more truncation

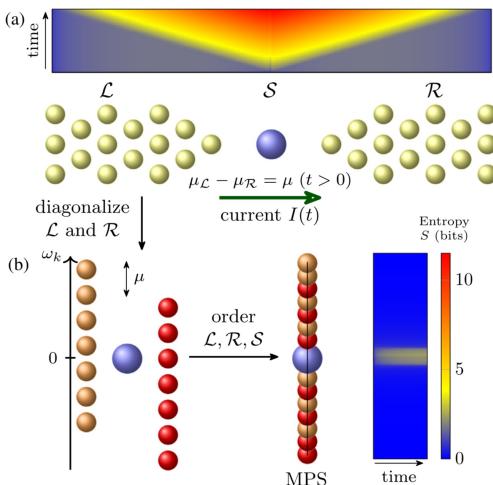
Systems with long -range interactions



Impurity models



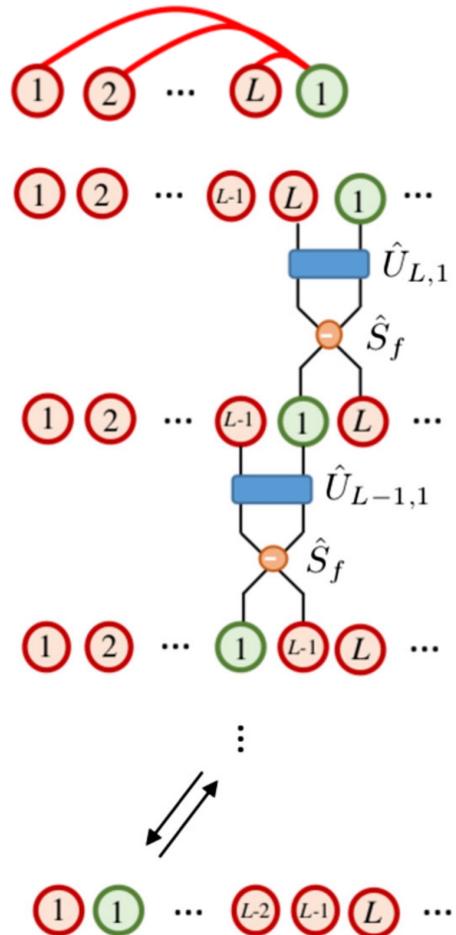
Quantum transport



Rams and Zwolak, PRL 2020

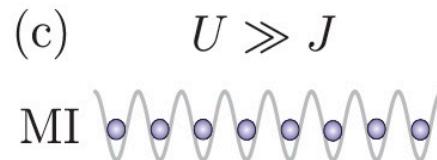
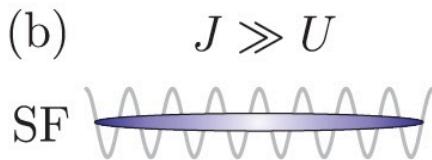
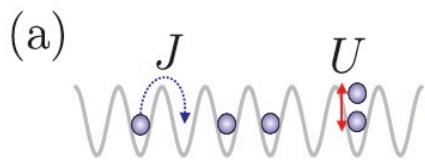
Not used much with MPS as it is usually expected that entanglement will grow very fast. Mostly recent works show that this is not necessarily the case.

Long-range interactions simulated through swap gates.



Example of Application: Bose-Hubbard Model

$$H = -J \sum_{j=1}^{N-1} (\alpha_j \alpha_{j+1}^+ + \alpha_{j+1} \alpha_j^+) + \frac{U}{2} \sum_{j=1}^N n_j (n_j - 1) \quad n_j = \alpha_j^+ \alpha_j$$



Superfluid

Mott insulator

$$H = \sum_{j=1}^{N-1} h_{j,j+1}$$

Initial state

$$\begin{aligned} h_{j,j+1} &= \alpha_j \alpha_{j+1}^+ + \alpha_{j+1} \alpha_j^+ \\ &+ \frac{1}{2} \frac{U}{2} [n_j(n_j - 1)(\delta_{j,1} + 1) \\ &+ n_{j+1}(n_{j+1} - 1)(\delta_{j+1,N} + 1)] \end{aligned}$$

$|010101\rangle$

Operators

$$\gamma_j = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 2 & \\ & & & 3 \\ & & & \ddots \end{pmatrix}$$

$$\gamma_j^2 = \begin{pmatrix} 0 & & & \\ & 1 & & \\ & & 4 & \\ & & & 9 \\ & & & \ddots \end{pmatrix}$$

$$a_j = \begin{pmatrix} 0\sqrt{1} & & & \\ 0\sqrt{2} & & & \\ 0\sqrt{3} & & & \\ 0\sqrt{4} & & & \\ & \ddots & & \end{pmatrix}$$

$$a_j^+ = \begin{pmatrix} 0 & & & \\ \sqrt{1} & 0 & & \\ & \sqrt{2} & 0 & \\ & & \sqrt{3} & 0 \\ & & & \sqrt{4} \\ & & & \ddots \end{pmatrix}$$

Implemented on site type “Qudit” in ITensor. Also implemented my own!

Krylov Time Evolution Methods

General method of time evolution, not only for tensor networks. Not as used as TEBD or TDVP.

For Hamiltonian H and initial state $|\Psi\rangle$, the Krylov subspace K_N is the span of vectors

$$\{|\Psi\rangle, H|\Psi\rangle, H^2|\Psi\rangle, \dots, H^{N-1}|\Psi\rangle\}$$

$$\rightarrow |v_0\rangle = \frac{|\Psi\rangle}{\| |\Psi\rangle \|} \quad |v_1\rangle \quad \text{Built from normalized } H|v_0\rangle \text{ and orthonormal to } |v_0\rangle$$

$$\dots |v_j\rangle \quad \text{Built from normalized } H|v_{j-1}\rangle \text{ and orthonormal to all previous } |v_i\rangle$$

The Krylov subspace is $\{|v_0\rangle, |v_1\rangle, \dots, |v_{N-1}\rangle\}$

The method searches the element within the Krylov subspace that approximates most closely the time evolution at each time step

$$|\Psi(t + \Delta t)\rangle \equiv \arg \min_{|\psi\rangle \in K_N} \| |\psi\rangle - e^{-iH\Delta t} |\Psi(t)\rangle \|$$

For the moment suppose that $N = \dim(H)$ (full size of Hilbert space)

We define the projector

$$P_N = \sum_{i=0}^{N-1} |v_i\rangle \langle v_i| = \left(\begin{array}{c} |v_0\rangle \\ |v_1\rangle \\ \vdots \\ |v_{N-1}\rangle \end{array} \right) \left(\begin{array}{c} \langle v_0| \\ \langle v_1| \\ \vdots \\ \langle v_{N-1}| \end{array} \right)$$

$$= V_N^+ V_N = I \text{ if } N = \dim(H)$$

The solution to the minimization problem is

$$|\Psi(t+\Delta t)\rangle = P_N^+ e^{-iH\Delta t} P_N |\Psi(t)\rangle = V_N^+ V_N \sum_{n=0}^{\infty} \frac{(-i\Delta t)^n}{n!} H^n V_N^+ V_N |\Psi(t)\rangle$$

Under the assumption $V_N H^n V_N^+ = V_N H \underbrace{V_N^+ V_N}_{I} H \underbrace{V_N^+ V_N}_{I} \cdots H V_N^+ \equiv T_N^n$

The elements of the “rotated” Hamiltonian T are

$$(T_N)_{i,i'} = \langle v_i | H | v_{i'} \rangle$$

The evolved state would be $|\Psi(t + \Delta t)\rangle = V_N^+ e^{-i\Delta t T_N} V_N |\Psi(t)\rangle$

The point of the Krylov method is to do a similar process, but with $N \ll \dim(H)$

The Krylov basis is no longer complete: $V_N^+ V_N \neq I$

Then we have the approximation $|\Psi(t + \Delta t)\rangle \approx V_N^+ e^{-i\Delta t T_N} V_N |\Psi(t)\rangle$

We do not have a correct representation of elements $\sim H^N \rightarrow$ Error $O(\Delta t^N / N!)$

Since T_N is small, it can be exponentiated with standard LAPACK routines

For application of Krylov method to MPS, see review of Paeckl *et al.* (Ann. Phys. 2019)

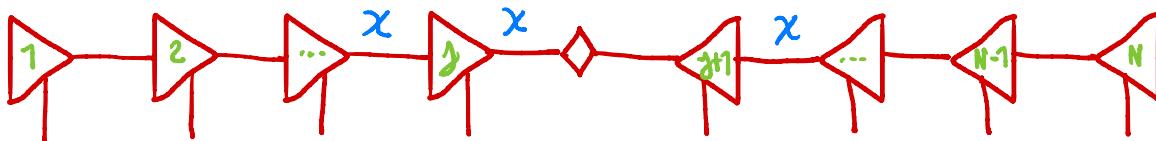
For tri-diagonal T_N , this corresponds to the Lanczos method

Brief Review of Mixed Canonical Form of MPS

From previous lectures and Homework 1, mixed canonical form of tensor

$$\begin{aligned} C_{n_1 n_2 \dots n_N} &= A^{n_1} A^{n_2} \dots A^{n_j} S B^{n_{j+1}} \dots B^{n_{N-1}} B^{n_N} \\ &= \sum_{\alpha_j=1}^x (A^{n_1} A^{n_2} \dots A^{n_j})_{\alpha_j} S_{\alpha_j \alpha_j} (B^{n_{j+1}} \dots B^{n_{N-1}} B^{n_N})_{\alpha_j} \end{aligned}$$

Diagrammatic representation that explicitly shows left (A) and right (B) normalization



Tensor gives amplitudes in state of many-particle quantum system

$$|\Psi\rangle = \sum_{n_1 n_2 \dots n_N=1}^d C_{n_1 n_2 \dots n_N} |n_1 n_2 \dots n_N\rangle$$

Recall Schmidt decomposition of general quantum state. Bipartition at site j

$$|\Psi\rangle = \sum_{k=1}^{\chi} \lambda_k |\psi_{[1,j]}^{L,k}\rangle \otimes |\psi_{[j+1,N]}^{R,k}\rangle$$

The Schmidt vectors are defined by

$$|\psi_{[1,j]}^{L,k}\rangle = \sum_{\alpha_1, \dots, \alpha_j=1}^d (A^{\alpha_1} A^{\alpha_2} \dots A^{\alpha_j})_k |\alpha_1 \alpha_2 \dots \alpha_j\rangle$$

$$|\psi_{[j+1,N]}^{R,k}\rangle = \sum_{\alpha_{j+1}, \dots, \alpha_N=1}^d (B^{\alpha_{j+1}} \dots B^{\alpha_{N-1}} B^{\alpha_N})_k |\alpha_{j+1} \dots \alpha_{N-1} \alpha_N\rangle$$

These vectors constitute an orthonormal basis for the left and right subsystems

Time Dependent Variational Principle (TDVP)

General formalism of quantum mechanics
to solve Schrödinger equation

$$i \frac{\partial}{\partial t} |\Psi(t)\rangle = H |\Psi(t)\rangle$$

Suppose we have intuition of solution, and propose an ansatz which depends on (unknown) variational parameters

$$\{a_j\} = \vec{a}$$

The parametrized equation is $i \frac{\partial}{\partial t} |\Psi(\vec{a}(t))\rangle = H |\Psi(\vec{a}(t))\rangle \quad (*)$

The problem has been shifted to finding the variational parameters. We want an equation for them. From the left hand side (lhs) of the previous equation:

$$\frac{\partial}{\partial t} |\Psi(\vec{a}(t))\rangle = \sum_j \frac{\partial |\Psi(a(t))\rangle}{\partial a_j} \quad \frac{\partial a_j}{\partial t} = \sum_j \dot{a}_j \frac{\partial |\Psi(a(t))\rangle}{\partial a_j} \quad (+)$$

States $\frac{\partial |\Psi(a(t))\rangle}{\partial a_j}$ → **Tangent vectors** (similar to velocities in Euclidean space)

Tangent vectors span a **tangent space**

Lhs of (*) is a tangent vector, but right hand side (rhs) $H|\Psi(\vec{a}(t))\rangle$ may not be

Dirac-Frenkel variational principle: force evolution to remain in tangent space.

General state in tangent space: $|\Phi(\vec{g}; \vec{a})\rangle = \sum_j g_j \frac{\partial |\Psi(a(t))\rangle}{\partial a_j} \quad \vec{g} = \{g_j\}$

$$\rightarrow \frac{\partial}{\partial t} |\Psi(\vec{a}(t))\rangle = |\dot{\Phi}(\vec{a}, \vec{a})\rangle \quad \text{with coefficients } \dot{g}_j = \dot{a}_j$$

The best approximation to the rhs of (*) is

McLachlan's distance

$$\dot{\vec{a}} = \arg \min_{\vec{g}} \| H|\Psi(a(t))\rangle - |\Phi(\vec{g}; \vec{a})\rangle \|$$

Solution of this problem is equivalent to projecting Schrödinger equation to the tangent space

$$iP \frac{\partial}{\partial t} |\Psi(\vec{a}(t))\rangle = P H |\Psi(\vec{a}(t))\rangle$$

$P \rightarrow$ Projector operator
onto tangent space

Lhs remains invariant. Equation becomes $i \frac{\partial}{\partial t} |\Psi(\vec{\alpha}(t))\rangle = P H |\Psi(\vec{\alpha}(t))\rangle$ (X)

Process to solve variational problem

1. Replace (+) into (X)
2. Define and insert properly-defined projector
3. Get equation for variational parameters $\dot{\alpha}_j$
4. Solve the equation, and obtain solution at desired time

For MPS, we will follow a similar development, with

Ansatz \rightarrow MPS

Variational parameters $\rightarrow A_{\alpha \beta}^{\gamma \kappa} [\kappa]$

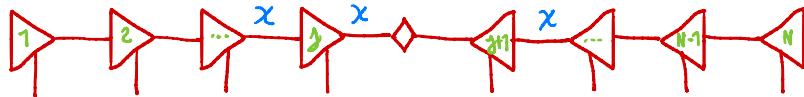
$$j = (\kappa, \gamma, \alpha, \beta)$$

Collective index

Schmidt decomposition

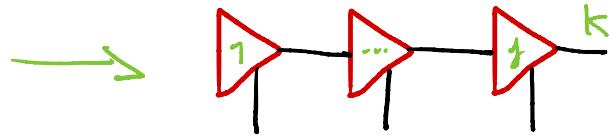
$$|\Psi\rangle = \sum_{k=1}^{\chi} \lambda_k |\varphi_{[1,j]}^{L,k}\rangle \otimes |\varphi_{[j+1,N]}^{R,k}\rangle$$

Orthogonality center is site j



Diagrammatic representation of projectors. For the left projector

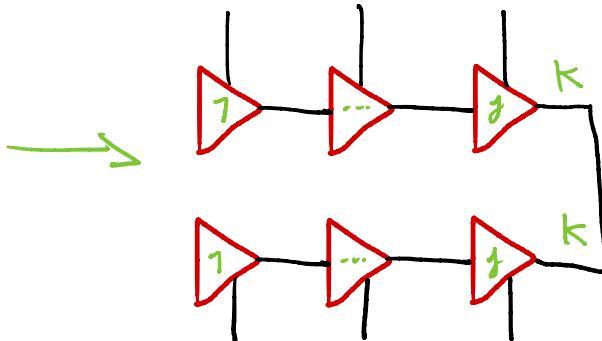
$$|\varphi_{[1,j]}^{L,k}\rangle$$



$$\langle \varphi_{[1,j]}^{L,k} |$$



$$P_j^L = \sum_{k=1}^{\chi} |\varphi_{[1,j]}^{L,k}\rangle \langle \varphi_{[1,j]}^{L,k}|$$



Similar construction for the right projector

We define the following projector onto the tangent space

$$P_{T|\Psi(A)} = \sum_{j=1}^N P_j^L \otimes I_j \otimes P_{j+1}^R - \sum_{j=1}^{N-1} P_j^L \otimes P_{j+1}^R$$

Removes all states that coincide with $|\Psi(A)\rangle$

Filters for all MPS which differ at most on one site from $|\Psi(A)\rangle$

$$P_j^L = \sum_{k=1}^{x_j} |\varphi_{[1,j]}^{L,k}\rangle \langle \varphi_{[1,j]}^{L,k}|$$

with projectors defined from Schmidt vectors

$$P_{j+1}^R = \sum_{k=1}^{x_{j+1}} |\varphi_{[j+1,N]}^{R,k}\rangle \langle \varphi_{[j+1,N]}^{R,k}|$$

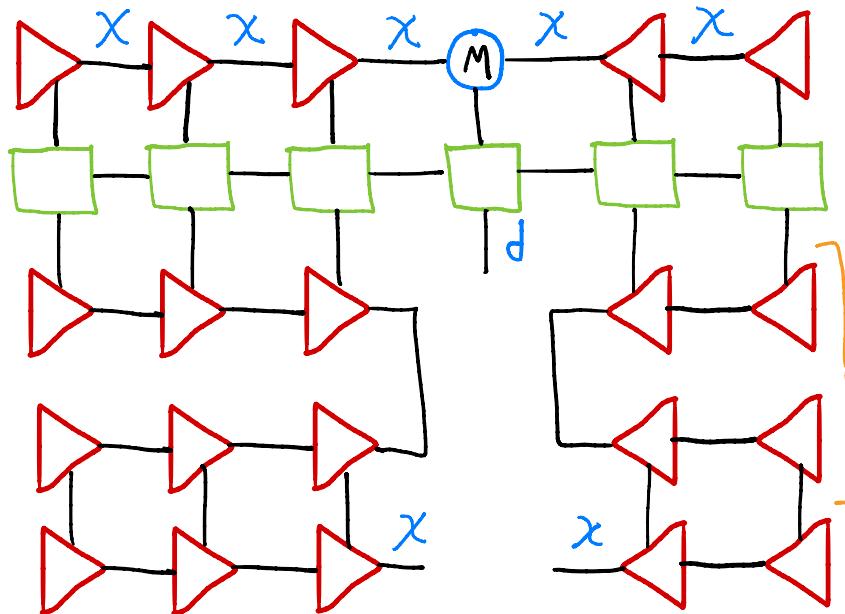
Approximate solution by solving each term of each projector individually and sequentially:

$$\frac{\partial}{\partial t} |\Psi(t)\rangle = -i P_{j-1}^L \otimes I_j \otimes P_{j+1}^R H |\Psi(t)\rangle \rightarrow \text{Forward evolution}$$

$$\frac{\partial}{\partial t} |\Psi(t)\rangle = i P_j^L \otimes P_{j+1}^R H |\Psi(t)\rangle \rightarrow \text{Backward evolution}$$

Diagrammatic representation of example

$$P_3^L \otimes I_4 \otimes P_5^R H |\Psi(t)\rangle$$



$$|\Psi\rangle$$

$$H$$

$$P_3^L \otimes I_4 \otimes P_5^R$$

Multiply by

$$\left\langle \varphi_{[1,3]}^{L,k} \right| \otimes \left\langle \varphi_{[5,N]}^{R,k} \right|$$

to work with effective single site.

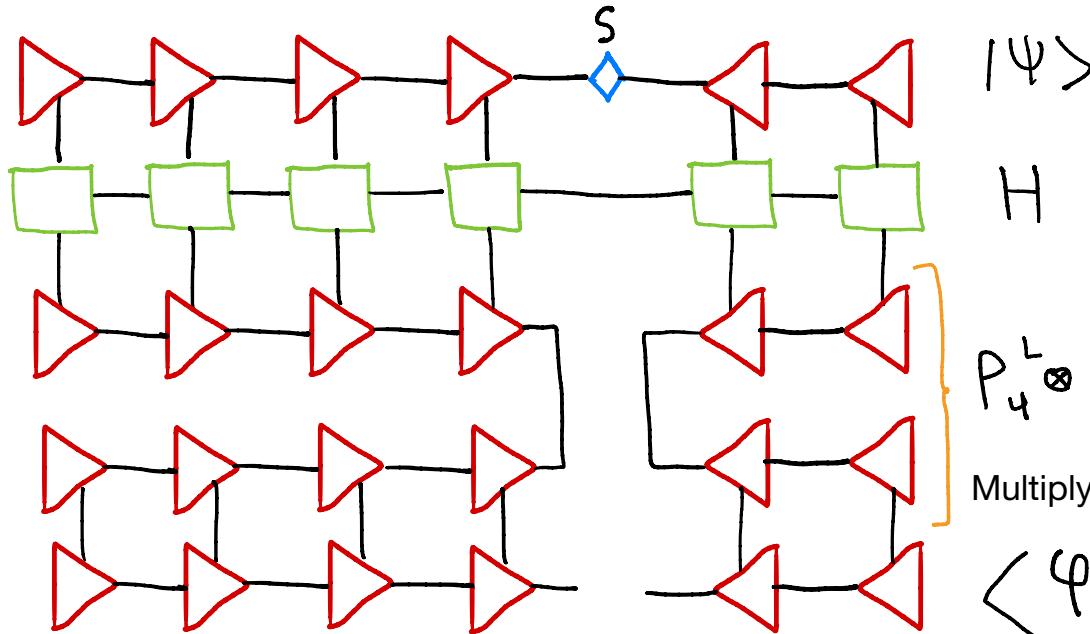
Resulting equation

$$\frac{\partial}{\partial t} M_j = -i H_j^{\text{eff}} M_j$$

Solve with standard
(e.g., Krylov) method

$$P_4^L \otimes P_5^R H |\Psi(t)\rangle$$

$S \rightarrow$ Matrix of singular values when MPS in mixed canonical form



to work with effective single site.

Resulting equation

$$\frac{\partial}{\partial t} S_j = + i N^{\text{eff}} S_j$$

Solve with standard
(e.g., Krylov) method

Important Points About TDVP Algorithm

1. The method directly deals with long-range interactions
2. The previous approach naturally uses Trotter approximation, by evolving each term of the tangent space projector for a small time step Δt . TEBD, in contrast, approximates directly the propagator.
3. TDVP becomes almost identical to one-site DMRG. It just differs in replacing the eigensolver by a routine to calculate time evolution, and in adding the extra step on the singular values.
4. Single-site method does not allow the increase of the bond dimension χ as dynamics is restricted to the tangent space. To allow for the growth of entanglement, manifested in increasing χ , the two-site method is used. Here, the projector is extended to

$$P_{T|\Psi(A)\rangle} = \sum_{j=1}^{N-1} P_j^L \otimes I_j \otimes I_{j+1} \otimes P_{j+2}^R - \sum_{j=2}^{N-1} P_{j-1}^L \otimes I_j \otimes I_{j+1} \otimes P_j^R$$

5. To prevent uncontrolled growth of bond dimension in the two-site method, and keep MPS structure, an SVD and truncation need to be performed after each local time evolution.

6. Similarly to TEBD, error due to time stepping can be decreased by introducing right-to-left sweep after left-to-right sweep, each of time step $\Delta t/2$. The error of each step becomes of $\mathcal{O}(\Delta t^3)$

$M_0 B_0 B_0 B_0 B_0 B_0$

Initial right orthogonalized state

$$\xrightarrow{\text{Forw}} M_1 B_0 B_0 B_0 B_0 B_0 \xrightarrow{\text{svd}} A_1 S_0 B_0 B_0 B_0 B_0$$

Left to right sweep

$$\xrightarrow{\text{back}} A_1 \underline{S_1 B_0} B_0 B_0 B_0 \xrightarrow{\text{absorb}} A_1 M_0 B_0 B_0 B_0$$

$$\xrightarrow{\text{Forw}} A_1 M_1 B_0 B_0 B_0 B_0 \xrightarrow{\text{svd}} A_1 A_1 S_0 B_0 B_0 B_0$$

$$\xrightarrow{\text{back}} A_1 A_1 \underline{S_1 B_0} B_0 B_0 B_0 \xrightarrow{\text{absorb}} A_1 A_1 M_0 B_0 B_0 B_0$$

:

7. There are several sources of error:

a. Projection error, decreased by χ .

c. Truncation error in two-site method, decreased by χ .

b. Trotter error, decreased by Δt .

d. Solution of local equations, decreased by taking more Krylov vectors.