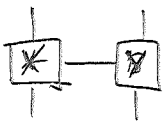
Wrap-up last lecture:

Simulation of time evolution w/ MPS

- Approximate state at every time $|\psi(t)\rangle$ by MPS:

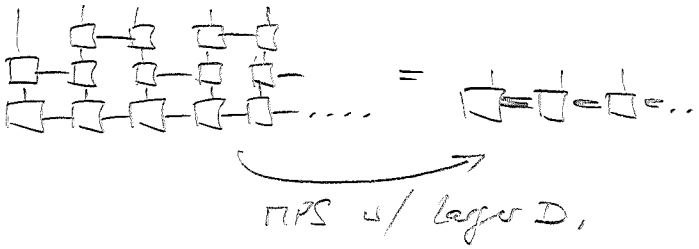
Trotter decomposition:

$$e^{-iHdt} \simeq \prod_i \underbrace{e^{-ih_{i,i+1}dt}}_{=}$$



(SVD)

$$|\psi(t+dt)\rangle = e^{-iHdt}\underbrace{|\psi(t)\rangle}_{\text{MPS}} =$$



⇒ truncate bond dim to D_{max}.

(≡ maximize overlap w/ MPS w/ D_{max} similar to DMRG!

⇒ sweep; quadratic problem!)

Caveats when simulating true evolution:

* We approximate $|\psi(t)\rangle$ by MPS → only works well as long the real $|\psi(t)\rangle$ has low entanglement ($\equiv$ area law)

* When do we expect small / large entanglement?

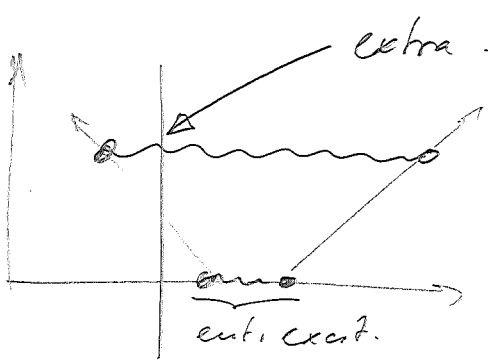
Intuition: $|\psi(0)\rangle$ can be decomposed into excited states of H.

Excited states of $H \overset{(?)}{\simeq}$ Quasi-particle excitations with no / weak interactions.

Quasi-particles * can be entangled
* move according to dispersions.

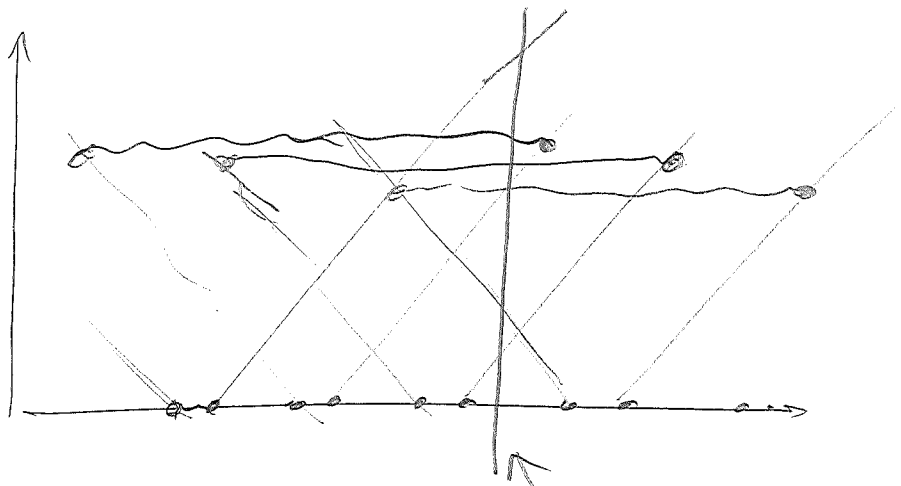
* $|\psi(0)\rangle$ has few excitations (e.g. $|\psi(0)\rangle = O_{local}|\psi_{GS}\rangle$, $|\psi_{GS}\rangle$: GS of H)

⇒ low entanglement at all times.



* $|\psi(0)\rangle$ has constant density of excit. (e.g.: $|\psi(0)\rangle$ is G.S. of $H' \neq H$ — e.g. Ising w/ different field —

⇒ constant density of excitations which can be entangled & move in opposite direction!



excitations per cut =

= entanglement grows linear in time!

$\Rightarrow$ $Ent(|\psi(t)\rangle) \propto t$

$\Rightarrow$ $D_{max} \propto \exp(t)$

$\Rightarrow$ we can only simulate time evolution up to $t \propto \log D_{max}$

Note: We can check how well the simulation works by un-evolving the state again:

$$|\psi(0)\rangle \xrightarrow{e^{-iHt}} |\psi(t)\rangle \xrightarrow{e^{iHt}} |\psi(0)\rangle$$

and verify if we return to the state $|\psi(0)\rangle$

Note 2: There are some neat tricks to extend t_{max}.

More on that (maybe) later!

Imaginary time evolution

This algorithm also work for imaginary time evolution

$$|\psi(\tau)\rangle = e^{-\tau H}\,|\psi(0)\rangle.$$

If $|\psi(0)\rangle$ has overlap w/ G.S., $|\psi(\tau)\rangle \longrightarrow |\psi_{GS}\rangle$!

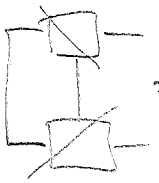
$\Rightarrow$ Alternative method to find ground states!

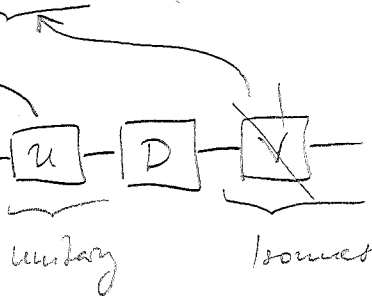
- Advantage: Robust against errors / initial conditions.
- Can also be used to create initial condition for DMRG.

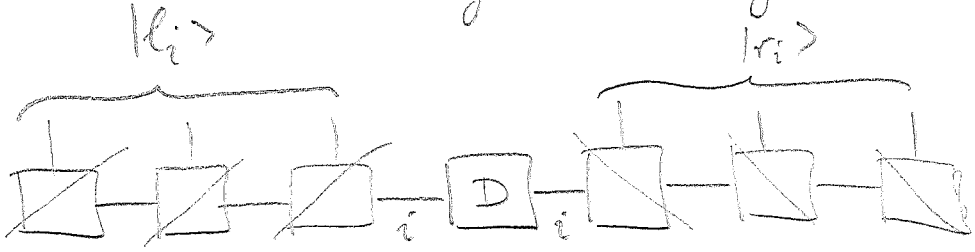
MPS & Schmidt decomposition.

By imposing the isometric gauge from both sides, we can achieve the form

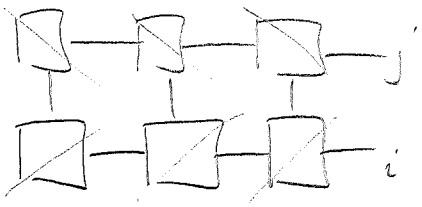
$|\psi\rangle =$ 

w/  = $\mathbb{1}$, etc.



$|\psi\rangle =$ 

we have

$\langle l_j' | l_i \rangle =$  $= \delta_{ij}$

and similarly $\langle r_j' | r_i \rangle = \delta_{ij}$

$\Rightarrow \quad |\psi\rangle = \sum D_{ii} |l_i\rangle |r_i\rangle$ = Schmidt decomposition!

(In part.: D_{ii}^2 are the eigenvalues of the red. density operator.)

$\Rightarrow$ This can be used for a

simple method to reduce the bond dimension:

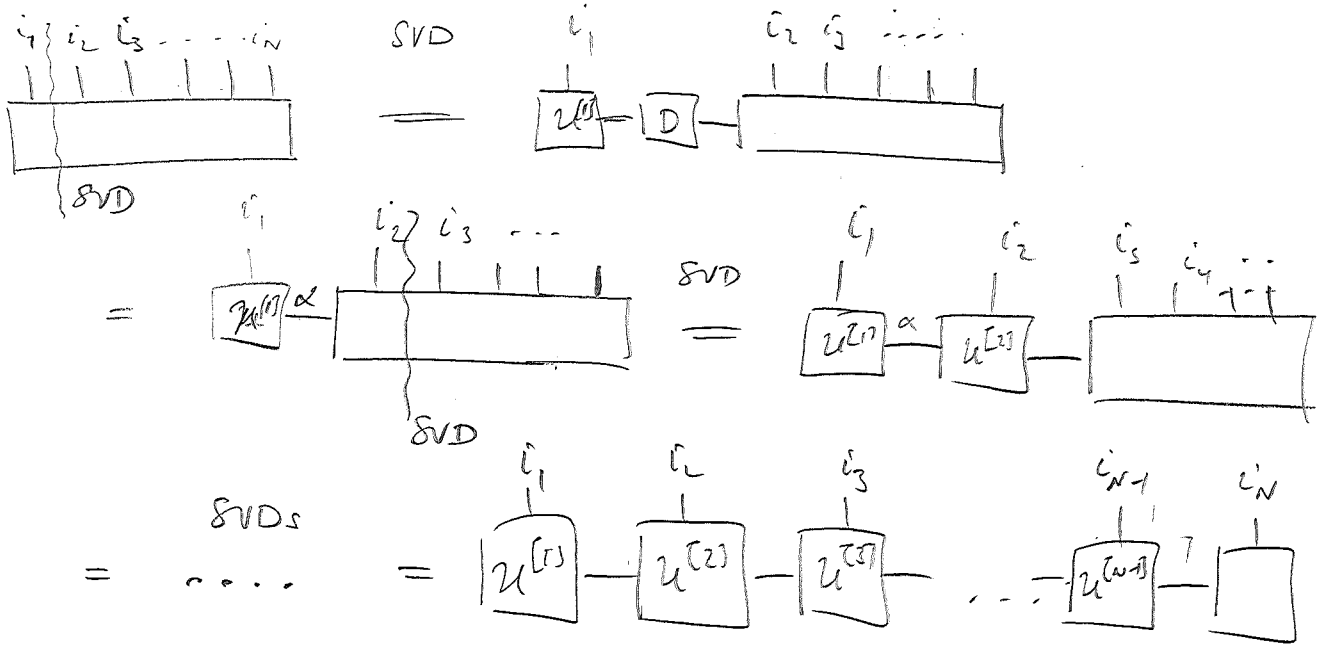
Go from left to right and at each site, only keep the D_{max} largest singular values in D_{ii}!

(Faster than previous method, but possibly worse approximation!)

Representation of arbitrary states by MPS:

Consider arbitrary state $|\psi\rangle = \sum c_{i_1 \dots i_N} |i_1, \dots, i_N\rangle$.

Can we write it as MPS?



$\Rightarrow$ Every state can be written as MPS.

Dimensions of the $A^{[i]}$ from counting dims in SVD:

$$A^{[1]}_{i_1} = 1 \times d$$

$$A^{[2]}_{i_2} = d \times d^2$$

$$\vdots$$

$$A^{[N/2]}_{N/2} = d^{N/2-1} \times d^{N/2}$$

$$A^{[N/2+1]}_{N/2+1} = d^{N/2} \times d^{N/2-1}$$

$$\vdots$$

$$A_{i_N} = d \times 1$$

$\Rightarrow D \sim d^{N/2} \Rightarrow$ exponential in N!

(of course necessary from parameter counting!)

Approximability by MPS & entanglement scaling

We can now truncate D to some D_{max}, using e.g. the aforementioned simple method. What is the error we make?

Consider a fixed cut after site s:

$$|\psi\rangle = \sum_{k=1}^{D} \lambda_k^s \underbrace{|l_k^s\rangle}_{1,\dots,s} \underbrace{|r_k^s\rangle}_{s+1,\dots,N}$$

If we cut at $k = D_{max}$, we obtain a state

$$|\psi'\rangle = \sum_{k=1}^{D_{max}} \lambda_k^s |l_k^s\rangle |r_k^s\rangle .$$

The error (in overlap) is then

$$\underbrace{1 - \langle\psi|\psi'\rangle}_{} = 1 - \sum_{k=1}^{D_{max}} \left(\lambda_k^s\right)^2 = \sum_{k=D_{max}+1}^{D} \left(\lambda_k^s\right)^2 =: \epsilon_s$$

$\Rightarrow$ The error per cut equals the tail of the Schmidt spectrum!

This error also holds for

$$\big||\psi\rangle - |\psi'\rangle\big|^2 = \langle\psi|\psi\rangle + \langle\psi'|\psi'\rangle - 2\,|\langle\psi|\psi'\rangle|$$

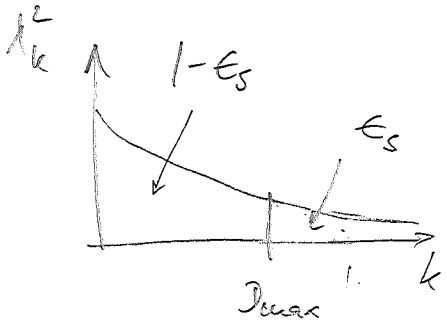
$$= 1 + (1-\epsilon_s) - 2(1-\epsilon_s) = \epsilon_s !$$

Approximate argument: The errors are roughly independent, so the total error in approx. our state $|\psi\rangle$ w/ an MPS w/ bond dim. D_{max}, $|\psi_{D_{max}}\rangle$, is

$$\left| |\psi\rangle - |\psi_{D_{max}}\rangle \right|^2 \approx \sum_{s=1}^{N-1} \epsilon_s$$

(approximate: rigorous bound has a factor 2, cf. exercise sheet)

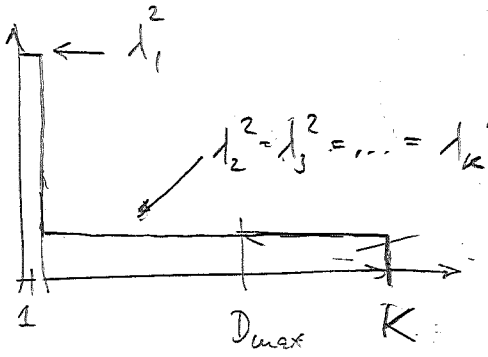
Can we relate ϵ_s — the weight of the tail of the Schmidt coefficients — with the entanglement entropy (cf. area law scaling?)



We want upper bounds on ϵ_s for a given Rényi entropy (i.e., largest possible error in approx. for fixed S)
$\leftrightarrow\!\!\rightarrow$ $\hat{=}$ find minimal S_α for fixed ϵ_s.

Minimal entropy $\leftrightarrow\!\!\rightarrow$ distribution as non-flat (i.e. peaked to the left) as possible:-

$$\lambda_1^2 + (K-1)\mu = 1$$
$$(K - D_{max})\,\mu = \epsilon_s$$



minimize $S_\alpha = \frac{\ln \sum (\lambda_k^2)^\alpha}{1-\alpha}$ for $\alpha < 1 \Longleftrightarrow$ minimize $\sum (\lambda_k^2)^\alpha$

$$\sum (\lambda_k^2)^\alpha = (\lambda_1^2)^\alpha + (K-1)\mu^\alpha \geq D_{max}\mu^\alpha + \epsilon_s \mu^{\alpha-1}$$

$$= e^{(1-\alpha)S_\alpha} \qquad \geq \mu \qquad = \frac{\epsilon_s}{\mu} + D_{max}$$

Minimum is:

$$e^{(1-\alpha)S_\alpha} \geq \frac{D_{max}^{1-\alpha}\,\epsilon_s^\alpha}{(1-\alpha)^{1-\alpha}\alpha^\alpha}$$

$$\Longleftrightarrow \quad e^{S_\alpha} \geq \frac{D_{max}\,\epsilon_s^c}{(1-\alpha)\alpha^c} \quad ; \quad c = \frac{\alpha}{1-\alpha} \; (\to \infty \text{ for } \alpha \to 1)$$

$$\Longleftrightarrow \quad D_{max} \leq \underbrace{(1-\alpha)\alpha^c}_{\leq 1} e^{S_\alpha} \cdot \frac{1}{\epsilon_s^c} \leq \frac{e^{S_\alpha}}{\epsilon_s^c}$$

Using $\delta = \| |\psi\rangle - |\psi_{D_{max}}\rangle \| \leq \sum \epsilon_s$

$\Rightarrow$ optimal choice $\epsilon_s = \delta/N$

$$\Rightarrow D_{max} \leq e^{S_\alpha} \left(\frac{N}{\delta}\right)^c$$

$\Rightarrow$ D scales efficiently in N and δ, as long as

S_α N const (or $S_\alpha \sim \log N$)