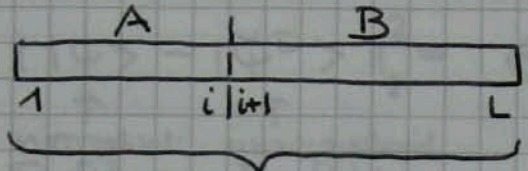
DMRG - A QUANTUM INFORMATION PERSPECTIVE

1. MPS-approximability of quantum statics
2. MPS-approximability of quantum dynamics

Reconsider Schmidt decomposition: $AB \to A+B$



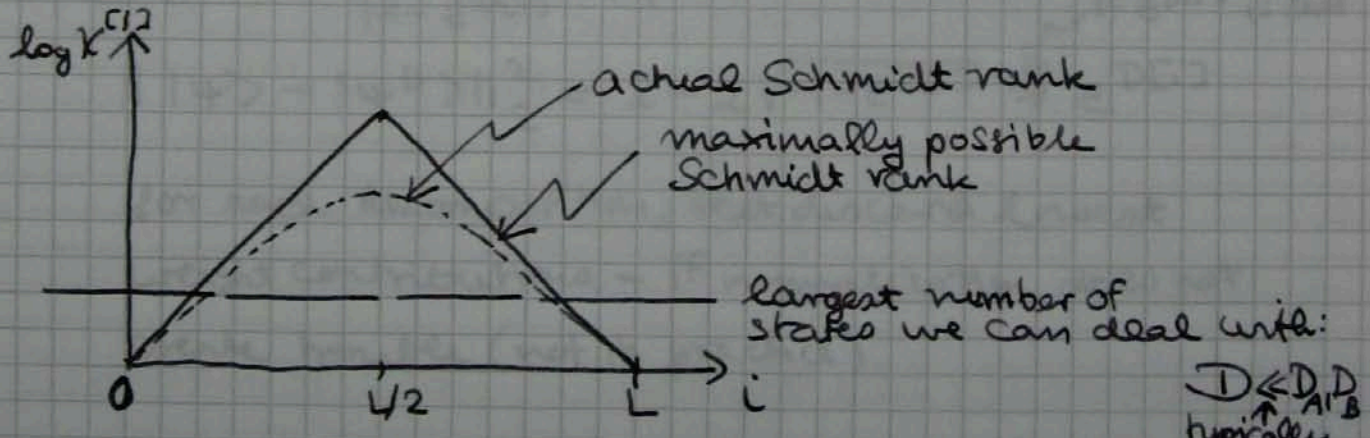
bipartite

$$|\psi\rangle = \sum_{i_A j_B} \psi_{ij} \underbrace{|i_A\rangle}_{\text{ONB's in } A,B} \underbrace{|j_B\rangle}_{\text{ONB's in } A,B} \longrightarrow$$

$$|\psi\rangle = \sum_{m^{[i]}=1}^{\min(D_A, D_B)} \underbrace{\sqrt{w_m^{[i]}}}_{\geq 0} \underbrace{|m_A^{[i]}\rangle}_{\text{can be completed to ONB's in } A,B} \underbrace{|m_B^{[i]}\rangle}_{\text{can be completed to ONB's in } A,B}$$

Schmidt rank $\chi^{[i]}$: # of $\sqrt{w_m^{[i]}} > 0$

$$\chi^{[i]} \leq \min(D_A, D_B) = \min(d^i, d^{L-i})$$



best approximation?

assume decreasing order: $w_1^{[i]} \geq w_2^{[i]} \geq \ldots$
in all of following!

Easy calculation shows: best approx. by

$$|\tilde{\psi}^D\rangle = \sum_{m^{[i]}=1}^{D} \underbrace{\sqrt{w_m^{[i]}}}_{\text{keep the largest ~~eigen~~ Schmidt coefficients}} |m_A^{[i]}\rangle |m_B^{[i]}\rangle$$

how good is the approximation?

$$\| |\psi\rangle - |\tilde{\psi}^D\rangle \|_2^2 = \epsilon^{D[i]}$$

↑ normalized: $\sum w_m^{[i]} = 1$; ↑ unnormalized $\sum w_m^{[i]} \leq 1$

with truncation error

$$\epsilon^{D[i]} = 1 - \sum_{m=1}^{D} w_m^{[i]} = \underbrace{\sum_{m=D+1}^{\max(D_A, D_B)} w_m^{[i]}}_{\text{discarded statistical weight}}$$

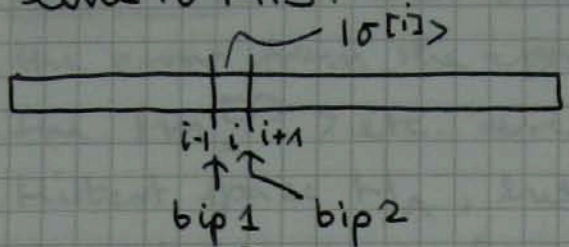
<u>normalized</u> approximation:

$$|\psi^D\rangle = \frac{1}{\sqrt{1-\epsilon^{D[i]}}} |\tilde{\psi}^D\rangle$$

$$\| |\psi\rangle - |\psi^D\rangle \|_2^2 = 2 - 2\sqrt{1-\epsilon^{D[i]}} \overset{\text{if } \epsilon^{D[i]} \text{ is small}}{\approx} \epsilon^{D[i]}$$

for each decomposition, best discard lowest weight contributions – if normalization does not create trouble (not in practice)

link to MPS:



$$|\psi\rangle = \sum^{D} \sqrt{w_m^{[i-1]}}\, |m_A^{[i-1]}\rangle |m_B^{[i-1]}\rangle \quad \text{(bip 1)}$$

$$= \sum^{D} \sqrt{w_m^{[i]}}\, |m_A^{[i]}\rangle |m_B^{[i]}\rangle \quad \text{(bip 2)}$$

$$|m_A^{[i]}\rangle = \sum \underbrace{\langle m_A^{[i-1]} \sigma^{[i]} | m_A^{[i]} \rangle}_{=: (A^{\sigma^{[i]}})_{m_A^{[i-1]}, m_A^{[i]}}} |m_A^{[i-1]}\rangle |\sigma^{[i]}\rangle$$

$\Rightarrow$ defines recursively a MPS

$$|\psi\rangle = \sum_{\{\sigma^{[i]}\}} A^{\sigma^{[1]}} A^{\sigma^{[2]}} \dots A^{\sigma^{[i]}} \underbrace{\psi^{[i]}}_{\substack{\uparrow \\ \text{diagonal} \\ \text{with entries} \\ \sqrt{w_m^{[i]}}}} \tilde{A}^{\sigma^{[i+1]}} \dots \tilde{A}^{\sigma^{[L]}} \times |\sigma^{[1]} \dots \sigma^{[L]}\rangle$$

$A, \tilde{A}$: grow from left, right; different normalization conditions

$$\sum_\sigma A^{[\sigma]\dagger} A^{[\sigma]} = \mathbb{1} \quad \text{vs.}$$

$$\sum_\sigma \tilde{A}^{[\sigma]} \tilde{A}^{[\sigma]\dagger} = \mathbb{1} \quad \text{from ON}$$

position of i can be shifted freely, to obtain

$$|\psi\rangle_{\text{MPS}} = \sum_{\sigma^{[i]}} A^{\sigma^{[1]}} \dots A^{\sigma^{[L]}} |\sigma^{[1]} \dots \sigma^{[L]}\rangle$$

dimension up to $D \times D$

$(1 \times d)(d \times d^2) \dots (d^i \times D)(D \times D) \dots (D \times d^i) \dots (d^2 \times d)(d \times 1)$

for OBC.

important: at each decomposition, we know the error from the approximation – but the $|m_A^{[i]}\rangle$ etc. are not from entire Hilbert space H_A, but themselves from a restricted subset because of construction!

- $|\langle\hat{O}\rangle_{|\psi\rangle} - \langle\hat{O}\rangle_{|\psi^D_{MPS}\rangle}|$ $\qquad \|\hat{O}\|_{op} = \sup_{|\psi\rangle\in H} \frac{\langle\psi|\hat{O}|\psi\rangle}{\langle\psi|\psi\rangle}$

$= |\,\mathrm{tr}(\hat{\psi}\hat{O}) - \mathrm{tr}(\hat{\psi}^D_{MPS}\hat{O})|$ $\qquad (\hat{\psi} = |\psi\rangle\langle\psi|, \dots)$

$= |\sum_i \langle i|\hat{\psi} - \hat{\psi}^D_{MPS}|i\rangle\langle i|\hat{O}|i\rangle|$ $\qquad |i\rangle$: eig. basis of $(\hat{\psi} - \hat{\psi}^D_{MPS})$

$\leq \|\hat{O}\|_{op} \sum_i |\langle i|\hat{\psi} - \hat{\psi}^D_{MPS}|i\rangle|$

$= 2\|\hat{O}\|_{op}\, T(\hat{\psi}, \hat{\psi}^D_{MPS})$ ← trace distance: $T(\hat{\rho},\hat{\sigma}) = \frac{1}{2}\mathrm{tr}|\hat{\rho}-\hat{\sigma}|$, $|\hat{O}| = \sqrt{\hat{O}^\dagger\hat{O}}$

- $\||\psi\rangle - |\psi^D_{MPS}\rangle\|_2^2 = 2 - 2F(|\psi\rangle, |\psi^D_{MPS}\rangle)$

↳ fidelity $F(\hat{\rho},\hat{\sigma}) = \mathrm{tr}\sqrt{\hat{\rho}^{1/2}\hat{\sigma}\hat{\rho}^{1/2}}$

$= |\langle\psi|\varphi\rangle|$ ↳ for pure states

Theorems:

worst-case approximation (for optimal choice) upper bound

$\||\psi\rangle - |\psi^D_{MPS}\rangle\|_2^2 \leq 2\sum_{i=1}^{L-1} \epsilon^{D[i]}$

best-case approximation (for optimal choice) lower bound

$T(\hat{\psi}, \hat{\psi}^D_{MPS}) \geq \frac{1}{2}\max_i \epsilon^{D[i]}$

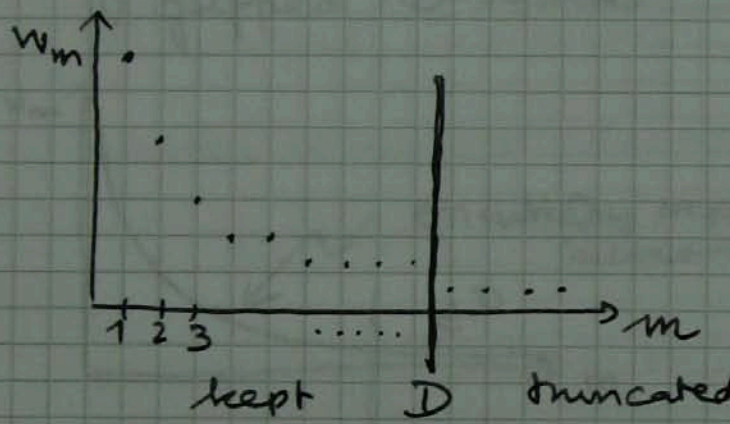
The theorems confirm the intuitive result that approximation quality is linked to the <u>truncation error</u>.

⇓

property of reduced density operator spectra!

$$|\psi\rangle \rightarrow \sum_m \sqrt{w_m}\, |m_A\rangle |m_B\rangle \rightarrow$$

$$\left.\begin{aligned} \hat{\rho}_A &= \sum w_m |m_A\rangle\langle m_A| \\ \hat{\rho}_B &= \sum w_m |m_B\rangle\langle m_B| \end{aligned}\right\} \text{share spectra}$$



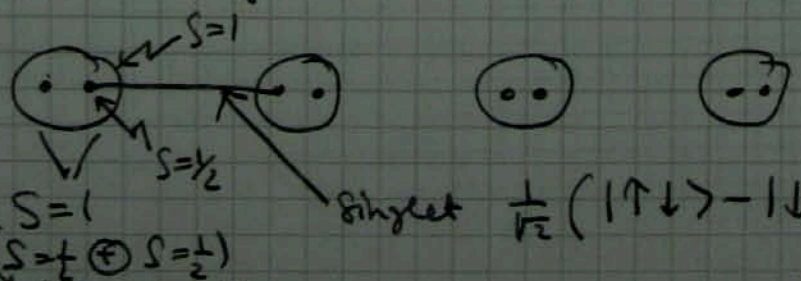
⇒ simulability by MPS will depend on

what do they look like for "real" quantum states (ground states of Hamiltonians that occur in nature)?

i) MPS

example: $H = \sum \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2 \quad (S=1)$

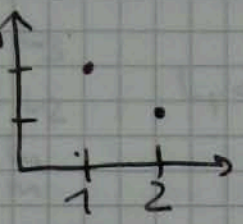
has AKLT-ground state



can be expressed as MPS via:

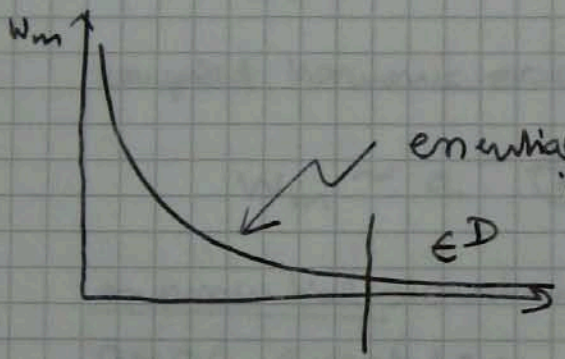
$$A^+ = \begin{bmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix} \qquad A^0 = \begin{bmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \qquad A^- = \begin{bmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{bmatrix}$$

$D = 2$ strictly



but this is rare!

ii) gapped 1D-systems



essentially exponential decay, increasing # of degenerate eigenvalues → not purely exponential!

some exact results: - transverse Ising

- XXZ Heisenberg $S = 1/2$ in AFM gapped regime

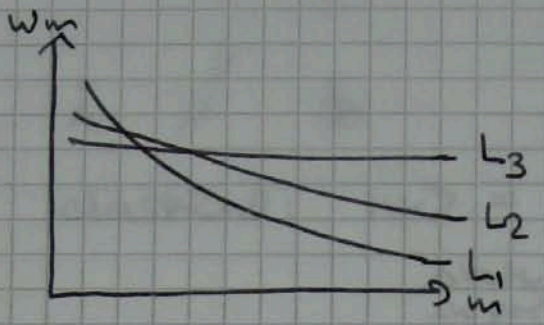
$$\epsilon^D = e^{-3\frac{|\ln z|}{\pi^2}(\ln D)^2}$$

depends on interaction parameter

quite generally:

$$w_m \sim e^{-\text{cst.}(\ln m)^2}$$

iii) critical 1D systems



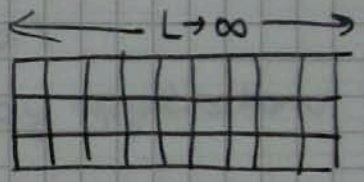
$L_1 < L_2 < L_3$

spectrum becomes flatter with $L \Rightarrow$ discarded weight grows!

iv) gapped 2D systems

coupled harmonic oscillators:

$$w_m \sim e^{-\frac{\text{cst.}}{N}(\ln m)^2}$$



<u>exponential</u> slowdown of eigenvalue decay $\Rightarrow$ DMRG breakdown

can we understand these results generically and perhaps without looking at individual spectra?

Entanglement and area laws

A // B 2 electrons

classical: $|\psi\rangle = |\uparrow_A\rangle \otimes |\uparrow_B\rangle$ or similarly

↑ state factorizes in particular for widely separated particles separability

quantum: $|\psi\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow_A \downarrow_B\rangle + |\downarrow_A \uparrow_B\rangle\right]$

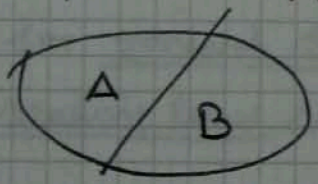
superposition + tensor structure

state does not factorize, <u>entangled</u> (here even <u>maximally</u> entangled)

how do we quantify entanglement?
numerous options, often driven by application

for pure states we focus on
<u>entanglement entropy</u>

$|\psi\rangle = \sum \psi_{ij} |i_A\rangle |j\rangle_B$ ⟹ $\hat{\rho}_A = \mathrm{tr}_B \hat{\rho}$, $\hat{\rho}_B = \mathrm{tr}_A \hat{\rho}$ reduced density operators



$\hat{\rho} = |\psi\rangle\langle\psi| \Rightarrow$

$$(\hat{\rho}_A)_{ii'} = \sum_j \psi_{ij} \psi^*_{i'j} |i_A\rangle\langle i'_A|$$

$$= \sum w_m |m_A\rangle\langle m_A|$$

↑ Schmidt decomp. gives eigenrepresentation!

$$S(|\psi\rangle)_{A|B} := S_{VN}(\hat{\rho}_A) = S_{VN}(\hat{\rho}_B)$$

↑ ent. entropy — ↑ for pure states only! — ↑ von Neumann entropy — ↑ same spectrum!

where $S_{VN}(\hat{\rho}) = -\mathrm{tr}\,\hat{\rho}\log_2\hat{\rho}$

$= -\sum_m w_m \log_2 w_m$.

proxy quantity for (decisive) spectra!

How does $S_{VN}(\hat{\rho}_A)$ depend on system size?

thermal entropy is extensive

$|\psi\rangle = \sum_m^{d^V} \sqrt{w_m}\, |m_A\rangle|m_B\rangle$ — generic quantum state in Schmidt form.

↑ can be imagined like random numbers

$S_{VN}(\hat{\rho}_A) = -\sum_m^{d^V} w_m \log_2 w_m = O(V)$

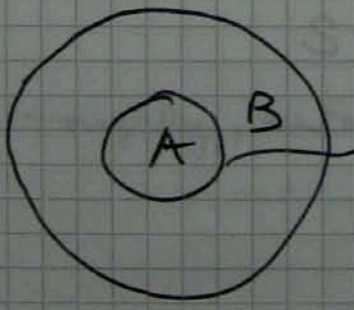
w_m: $O(\frac{1}{d^V})$, $\log_2 w_m$: $O(\frac{1}{d^V})$

extensive for generic states!

BUT

for ground states (low energy states) [of short ranged Hamiltonians] a different scaling law seems to hold (no global proof):

AREA LAW: entanglement entropy scales as the surface of the subsystem, i.e. the boundary

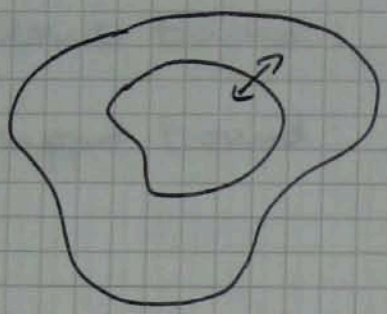


$S_{A|B} \sim L^{d-1}$ area

1d: $S_{A|B} \sim$ cst. (L^0)

2d: $S_{A|B} \sim L$

black hole physics: Bekenstein, Hawking (1974)



short-ranged correlations generate entanglement ⇝

entanglement ∝ surface

(for gapped systems)

<u>corrections</u> for critical systems ($\xi = \infty$)

$$S_{A|B}(L) = \frac{c}{3} \log_2 L + k \qquad (1D)$$

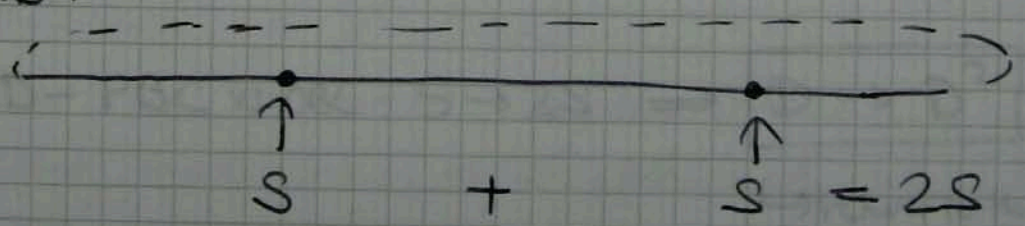
c: central charge of corresponding conformal field theory

(typically small, e.g. 0.5 or 1)

in 2D more complicated:

- log. correction for fermions with 1D Fermi surface
- subleg. correction for fermions with 0D Fermi surface
- no correction for bosons.

special case: periodic boundary conditions in 1D:



roughly, entanglement <u>doubles</u> (exact only in few cases)

von Neumann entropy and spectra:

lower bound: $\{1,0,0,0,\dots\} \to S_{VN}(\hat{\rho}) = 0$

upper bound: $\{\underbrace{\tfrac{1}{D}, \tfrac{1}{D}, \dots}_{D \text{ of them}}\} \to S_{VN}(\hat{\rho}) = \log_2 D$.

completely mixed spectrum

(provable by majorization theorems)

<u>handwaving</u> argument:

for D states, <u>max.</u> entanglement $\log_2 D \Longrightarrow$

for entanglement S, <u>minimally</u> $2^{\propto S}$ states

(but depends on problem!)

$$D \sim 2^S \to D(L) \sim 2^{S(L)}$$

1D-gapped: $D \sim 2^{S(L)} \sim 2^{\text{cst}} \sim$ <u>cst.</u> ✓

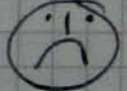
1D-critical $D \sim 2^{S(L)} \sim 2^{\frac{c}{3}\log_2 L} \sim L^{c/3} \sim$

thermodyn. limit not reachable, but good enough for scaling!

This is why DMRG works so well in 1D!

1D-PBC vs. OBC: $S \to 2S \Longrightarrow \boxed{D \to D^2}$

↳ return to that!

2D-gapped: $D \sim 2^{S(L)} \sim 2^L$ 

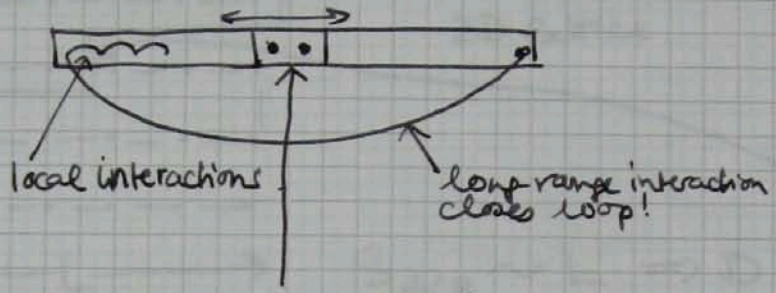
2D-critical, 3D-gapped } even worse 

This is why DMRG fails in 2D and 3D!

What can we do against it?

① periodic boundary conditions

in traditional DMRG:



cut here: D^2 states vs. D ⇒

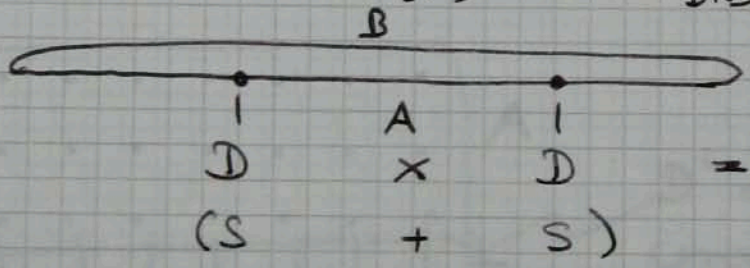
D^6 time vs. D^3 time

(worst case!!!)

or generalize MPS:

$$|\psi\rangle = \sum_{\{\sigma_i\}} \mathrm{tr}\left(A^{\sigma[1]} \cdots A^{\sigma[L]}\right) |\sigma_1 \ldots \sigma_L\rangle$$

$A^{\sigma[1]}$: $D \times D$; $A^{\sigma[L]}$: $D \times D$



$= D^2$ states

<u>natural</u> form for PBC!

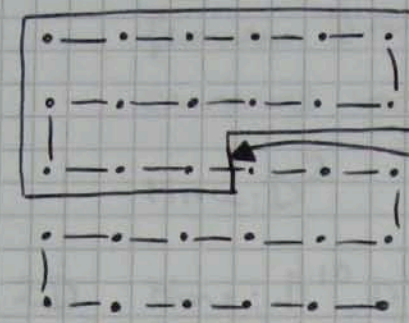
drawback: • D^5 time

• numerically less pleasant

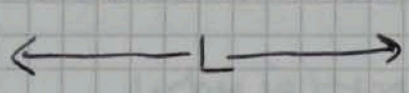
recent improvement to D^3 time with minimal approx. (Pippan et al.)

② higher-dimensional systems

traditional DMRG:

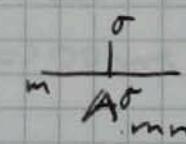


2D lattice



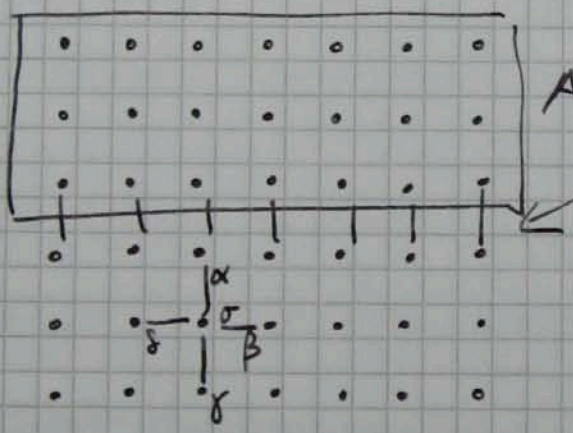
$S_{A/B} \sim L \Rightarrow D \gtrsim 2^L$

same "trick" as for PBC: can we distribute $D \sim 2^L$?

MPS: A matrix: 

indices correspond to neighbours!

generalize to PEPS (Projected Entangled Pair States)



D^L states $\Rightarrow$ $S \propto L$.

correct entanglement scaling!

$A^\sigma_{mn} \rightarrow A^\sigma_{\alpha\beta\gamma\delta}$

$$|\psi\rangle = \sum_\sigma \text{contr}(A^1, A^2, A^3, \ldots A^L)\, |\sigma_1 \ldots \sigma_L\rangle$$

contract over all indices

how to do that efficiently?

CURRENT TOPIC!

Why can we have hope that such algorithms work?

1D: bosons $D \sim 100$, ~~fermi~~ spins $D \sim 200$,
fermions $D \sim 400$ and more (critical systems!)
current record: $D \sim 10000$ (needed for dynamics)

time: D^3

2D time: $D^{10}, D^{12}, \ldots$ (depends on incarnation of algorithm)

why is there hope?

problems become more mean field with increasing dimension: $\boxed{D \to 1}$ $\Rightarrow$ so we expect much smaller D in 2D than in 1D!

2. Simulation of dynamics

How far can we go with time-dependent DMRG?

1. evolving the state: error $O(\Delta t^5) \times \frac{T}{\Delta t} \sim T \cdot \Delta t^4$
   in Trotter,
   even smaller in Krylov.
2. finding the optimal approximation: error $O(\varepsilon^D)$
   ↑ truncation error.

At first sight: <u>very long</u> time dynamics with moderately growing error.

THIS IS - IN GENERAL - NOT THE CASE!

<u>entanglement</u> dynamics

$|\psi(0)\rangle \longrightarrow |\psi(t)\rangle$

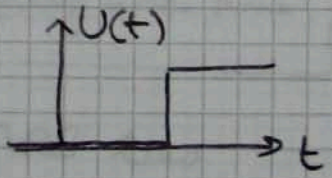
$\rightsquigarrow S(0) \longrightarrow S(t)$

in general, $S(t)$ will be quite different from $S(0)$!

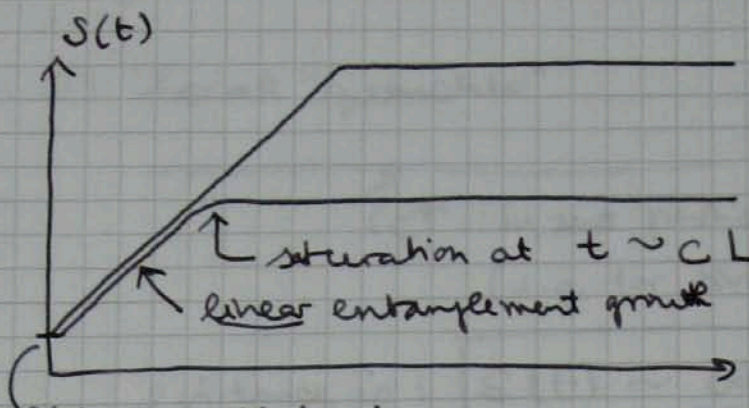
i) <u>global</u> quenches

$$H = -J \sum (b_i^\dagger b_{i+1} + \text{h.c.}) + U(t) \sum_i n_i(n_i - 1)/2$$

Bose-Hubbard model (cold atoms)



- energy changes macroscopically $\propto L$
- $|\psi\rangle$ ground state → highly excited state



L_2

V

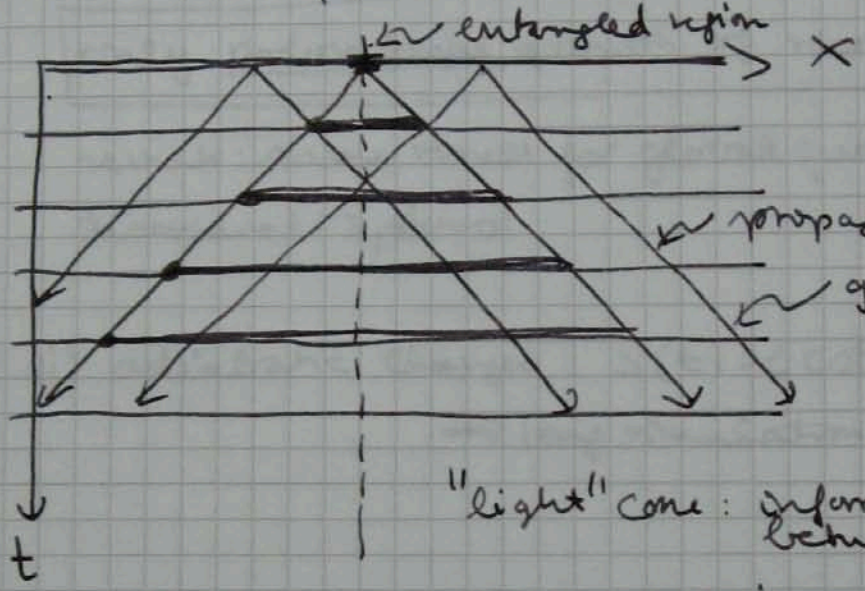
system length L_1

c is typical propagation speed in system

$$S = \text{cst} \cdot t + S_0$$

up to saturation

intuitive picture:



"light" cone: information flow between A and B

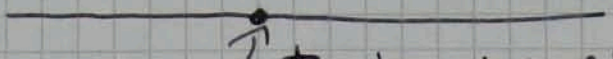
assume certain entanglement "stored" per length unit

$D(t) \sim 2^{S(t)} \Rightarrow D(t) \sim 2^t$

matrix dimension grows exponentially with time!

key limitation of time-dependent DMRG lies in nature of quantum state!

ii) local "quenches"



c_i^+ : insert particle at time t
(e.g. for time-dependent correlators!)

evidence is: $\boxed{S(t) \sim \underline{\text{cst.}} \log t}$ up to saturation.

$\Rightarrow D(t) \sim 2^{S(t)} \rightarrow D(t) \sim t^{\text{cst.}}$

$\boxed{\text{only } \underline{\text{polynomial}} \text{ growth of resources.}}$

remark: same result for global quenches in disordered systems!

iii) adiabatic changes: $S(t) \propto$ cst. (dep on $H(t)$)
$\rightarrow$ long simulation possible