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Tensor Networks → A natural way to represent ~~Both analytic~~ a ~~numerical + Analytic~~ quantum states when there is low entanglement (normally the case): MPS, PEPS, MERA

- 1D Matrix Product States (well understood) time evolution, ground states
- higher dimension
- end of second lecture: slides showing some results for spin liquids

References

U Schollwock arxiv 1008.3477

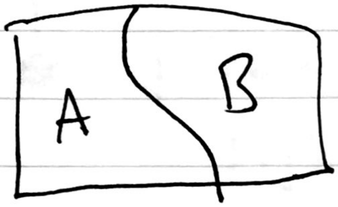
Software: 1) itensor.org

2) julialang.org – very nice new language, esp. for tensor networks

Web site

https://eee.uci.edu/16s/48480

Review: Schmidt Decomp



$$|\psi\rangle = \sum_{a,b} \psi_{ab}\, |a\rangle\, |b\rangle$$

Schmidt Form: $|\psi\rangle = \sum_{\alpha} \lambda_\alpha\, |\alpha\rangle_A\, |\alpha\rangle_B$

- diagonal
- Always possible
- Calculate: ① SVD: $\psi_{ab} = [U D V^T]_{ab}$

$$D = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \end{pmatrix} \qquad U, V \text{ \underline{unitary}} \qquad |\alpha\rangle_A = \sum_a U_{a\alpha} |a\rangle$$

② Reduced density matrix

$$\rho^A_{aa'} = \sum_b \psi_{ab}\, \psi^*_{a'b} = \Big[U D \overbrace{\cancel{V^T V}}^{1} D^T U^T \Big]_{aa'}$$

$$= \left[U D^2 U^T \right]_{aa'}$$

λ_α^2 = eigenvalue of ρ^A and ρ^B

eigenvectors of ρ^A form Columns of U, etc.

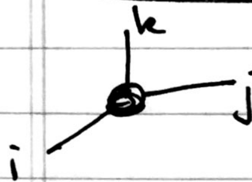
Von Neumann entanglement entropy

$$S = \sum_\alpha -\lambda_\alpha^2 \ln \lambda_\alpha^2 \qquad \lambda_\alpha^2 = \text{prob of } \alpha\text{-pair of states}$$

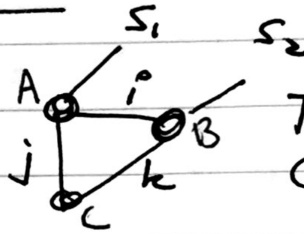
For ground states, $\boxed{S \sim \text{Area Law}}$

Tensor Network Diagrams

$A_{j i s_1}, B_{i s_2 k}$ C_{jk}



Tensor T_{ijk}

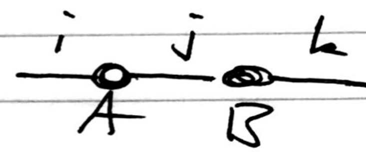


Tensor Contraction

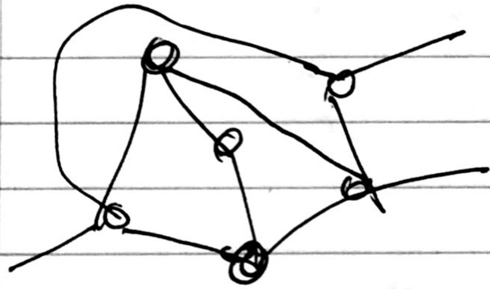
3 tensors. Internal ~~legs~~ indices summed over. External indices define the final tensor result.

~~Matrix~~ Vector 

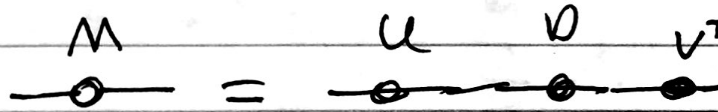
Matrix 

Matrix Product AB 

$$\{AB\}_{ik} = \sum_j A_{ij} B_{jk}$$



Tensor networks can get complicated.

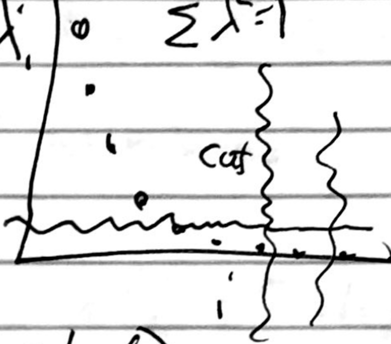
SVD: 

$M = UDV^T$

$\boxed{L|R}$

Truncating Low Probability States

Suppose we have λ_i^2 $\sum \lambda^2 = 1$



$S=1$ chain
$\lambda^2 \sim 10^{-10}$
for 80 λ's.

We want to throw away states with small λ_i^2 (Schmidt states)

~~Error~~ $|\psi\rangle = \sum_{i=1}^{2^{N/2}} \lambda_i \underbrace{|i\rangle_L |i\rangle_R}_{|i\rangle_{LR}} \rightarrow \underbrace{\sum_{i=1}^{m} \lambda_i |i\rangle_L |i\rangle_R}_{\tilde{\psi}}$

Error in $|\psi\rangle$:

$$\left(\langle\psi| - \langle\tilde{\psi}|\right)\left(|\psi\rangle - |\tilde{\psi}\rangle\right)$$

$$\langle\psi|\tilde{\psi}\rangle = \sum_{i=1}^{2^{N/2}} \sum_{i'=1}^{m} \lambda_i \lambda_{i'} \underbrace{{}_{LR}\langle i | i'\rangle_{LR}}_{\delta_{ii'}} = \sum_{i=1}^{m} \lambda_i^2$$

$$= \langle\tilde{\psi}|\tilde{\psi}\rangle$$

$$= \langle\psi|\psi\rangle - \langle\tilde{\psi}|\tilde{\psi}\rangle = 1 - \sum_{i=1}^{m} \lambda_i^2 = \sum_{i=m+1}^{2^{N/2}} \lambda_i^2$$

error in ψ is $\sum_{i=m+1}^{2^{N/2}} \lambda_i^2$ = "truncation error" or "discarded weight"

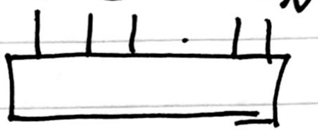
This is ~~sth~~ also the error on the density matrix, roughly.

This is <u>the key TN approximation</u>: a <u>low entanglement approximation</u>

Suppose we had a wavefnct from exact diagonalization of a spin chain

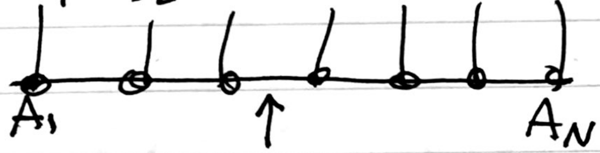
$\psi(s_1, s_2 \ldots s_N)$ 2^N numbers ($N \lesssim \sim 50$)

<u>Diagram</u>



all 2^N degrees of freedom

As an ansatz, lets propose a ~~A~~ Matrix Product State (MPS) is a TN:

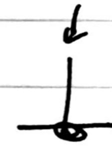


= basic ~~tensor~~ tensor

Algebraically

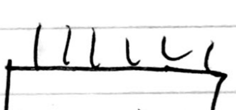
$$\psi(s_1 \ldots s_N) = \underset{\text{row vec}}{\vec{A}^1[s_1]}\, \overleftrightarrow{A}^2[s_2] \cdots \underset{\text{col vec}}{\vec{A}^N[s_N]}$$

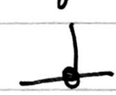
Regard $A^l[s_l]$ as two matrice

$A^l[\uparrow]_{ij}$ =  and $A^l[\downarrow]_{ij}$ 

Given $s_1 \ldots s_N$, pick which matrix to use on each site, take product,

This is a huge compression



$\longrightarrow$  $\times N$

$m^2 \cdot 2 \cdot N$

exp'l improvement [requires low entanglement]

5 Boulder

1

Matrix Product State (MPS)

$$\psi(s_1 \cdots s_N) = \vec{A}_1\{s_1\}\, \overleftrightarrow{A}_2\{s_2\} \cdots \vec{A}_N\{s_N\}$$

Very Simple example: 2 sites, spin singlet

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$$

$$= \sum_{s_1 s_2} \vec{A}_1[s_1] \cdot \vec{A}_2\{s_2\}\ |s_1\rangle |s_2\rangle$$

$$= \underbrace{\left(\sum_{s_1} \vec{A}_1\{s_1\} |s_1\rangle\right)}_{\vec{A}_1} \cdot \underbrace{\left(\sum_{s_2} \vec{A}_2[s_2] |s_2\rangle\right)}_{\vec{A}_2}$$

Let $\vec{A}_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} |\uparrow\rangle \\ -\frac{1}{\sqrt{2}} |\downarrow\rangle \end{pmatrix}$ $\quad \vec{A}_2 = \begin{pmatrix} |\downarrow\rangle \\ |\uparrow\rangle \end{pmatrix}$

By inspection, $|\psi\rangle = \vec{A}_1 \cdot \vec{A}_2$

Three sites: Let $|\psi\rangle = \frac{1}{\sqrt{3}}\left(|\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\rangle\right)$

$\vec{A}_1 = \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix}$ $\quad \vec{A}_3 = \begin{pmatrix} |\uparrow\rangle \\ |\downarrow\rangle \end{pmatrix}$ then $\vec{A}_2 = \frac{1}{\sqrt{3}}\begin{pmatrix} |\downarrow\rangle & |\uparrow\rangle \\ |\uparrow\rangle & 0 \end{pmatrix}$

(use $\vec{A}_1^T$)

More sites: Same structure, much bigger matrices, compressible for low entanglement

6 Dunlkn

In 1D, low entanglement $\Longrightarrow$ MPS

Treat as one big index

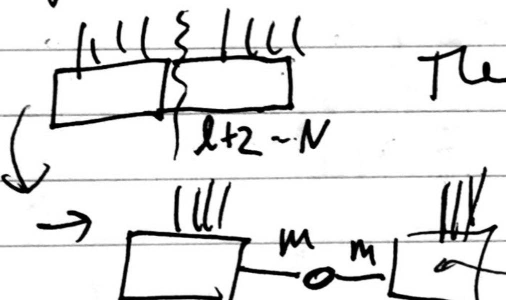
from ED =

Do SVD

Schmidt form

Sites 1 – l can be treated as having only m ~~D~~ states $|\alpha\rangle_L$ $\alpha =$ ~~$1..l$~~

Repeat at one site over



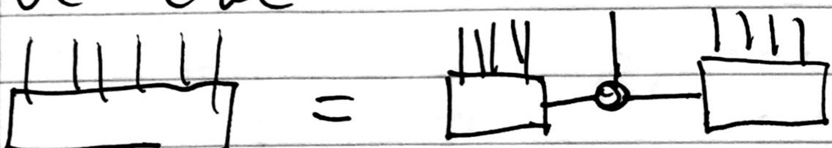
Then site $l+2$ can be treated as having m states

$|\beta\rangle_R$ $\beta = 1 .. m$

Then $$|\Psi\rangle = \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} \sum_{s_{l+1}=\uparrow,\downarrow} \Psi(\alpha, s_{l+1}, \beta) \, |\alpha\rangle_L |s_{l+1}\rangle |\beta\rangle_R$$

$$\Psi(\alpha, s_{l+1}, \beta) \equiv A^{l+1}[s_{l+1}]_{\alpha\beta}$$

We have



To get the full MPS, you just need to repeat on the other sites.

Orthogonality: crucial for effectively using MPS

drop $\dagger$, redefine V

In an SVD, $M = UDV$, U + V ~~are unitary~~ are row/col. unitary

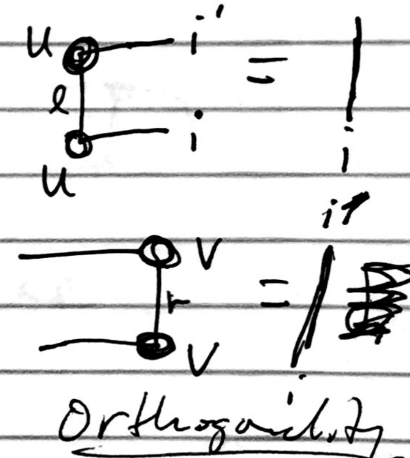
$$U^\dagger U = 1 \qquad V V^\dagger = 1$$

Let U have ~~labels~~ indices $U_{\ell i}$ (left, Schmidt)

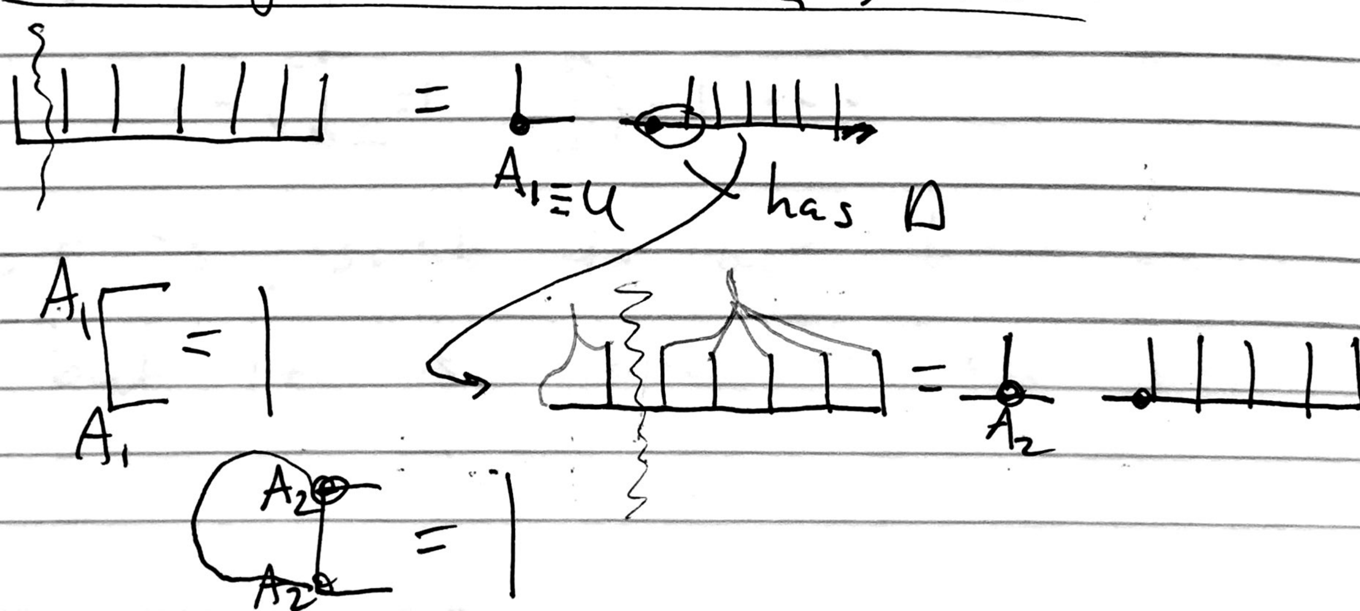
V_{ir} (right)

$\sum_\ell U_{\ell i} U^*_{\ell i'} = \delta_{ii'}$ or

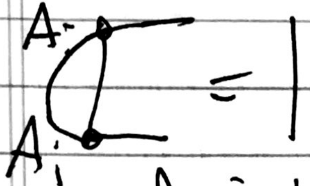
$\sum_r V_{ir} V^*_{i' r} = \delta_{ii'}$ or

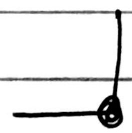


Converting a Wfn to an MPS



Keep going to the end



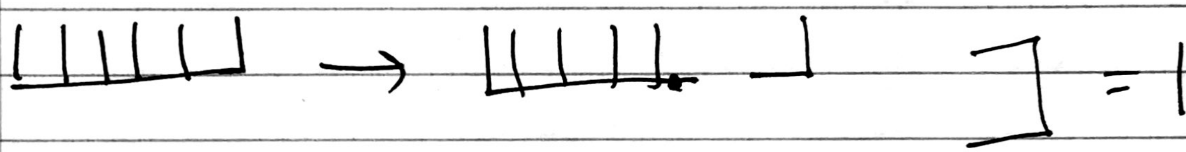


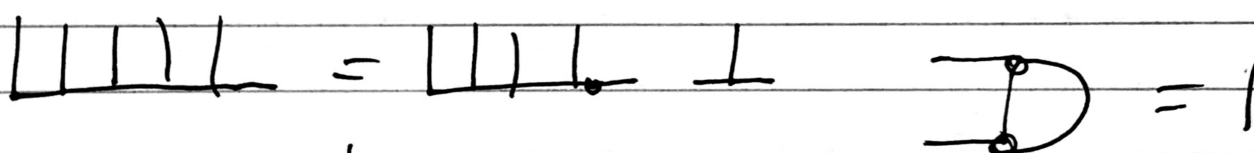
A_N has last D so no orthogonality

for $i = 1, \ldots N-1$

We say site N is the orthogonality center

We could put the OC on site 1

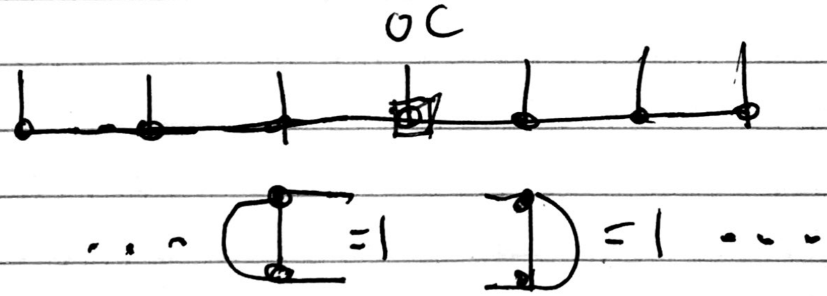




etc.

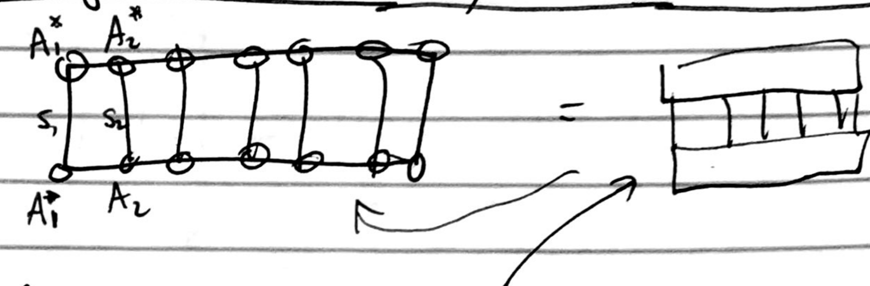
In general, it looks like

OC



It is possible to not have an OC — but it is useful to have one.

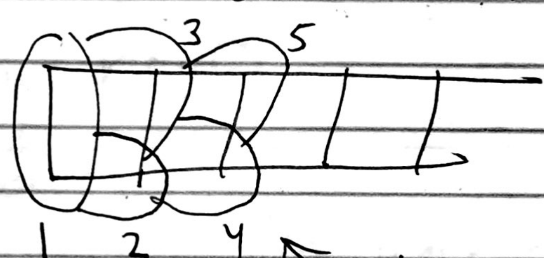
Normalization of an MPS, Measuring Ops

$\langle\psi|\psi\rangle =$ 

$$\sum_{\substack{s_1\dots s_N\\ s_1'\dots s_N'}} \psi^*_{s_1'\dots s_N'}\, \psi_{s_1\dots s_N} \langle s_1'\dots s_N' | s_1 \dots s_N\rangle$$

$$= \delta_{s_1 s_1'} \dots \delta_{s_N s_N'}$$

$= \cancel{\sum_{s_1\dots s_N}}$ To contract: left to right, or right to left. **Not** top, then bottom



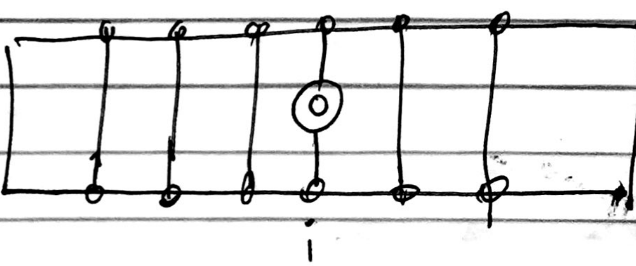
"Bubbling"

Measuring Operators

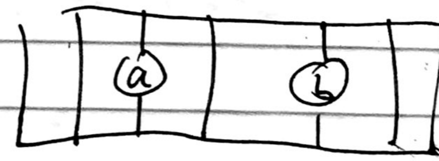
$$\langle s_1'\dots s_N' | O_i | s_1 \dots s_N\rangle$$

$$= \langle s_1' \dots s_N' | s_1 \dots (O_i s_i) \dots s_N\rangle$$

O_i attaches to A_i

$\langle O_i\rangle =$ 

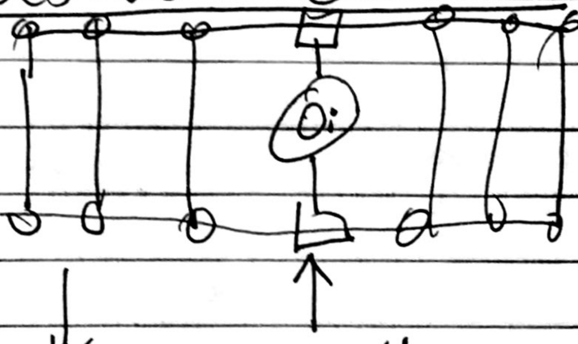
Also



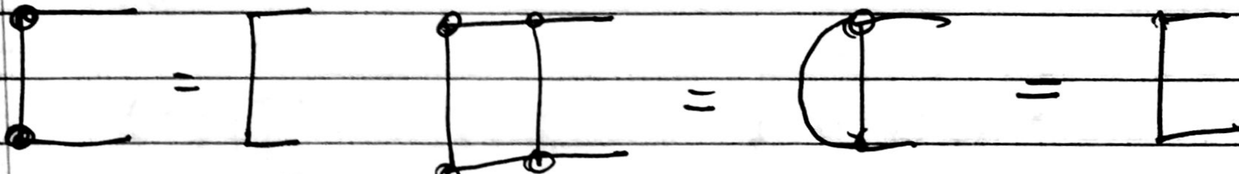
"Bubble" left to right, etc.

Using an OC

$\langle O_i \rangle =$

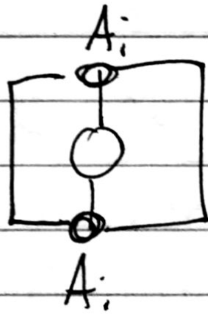


say this is an OC



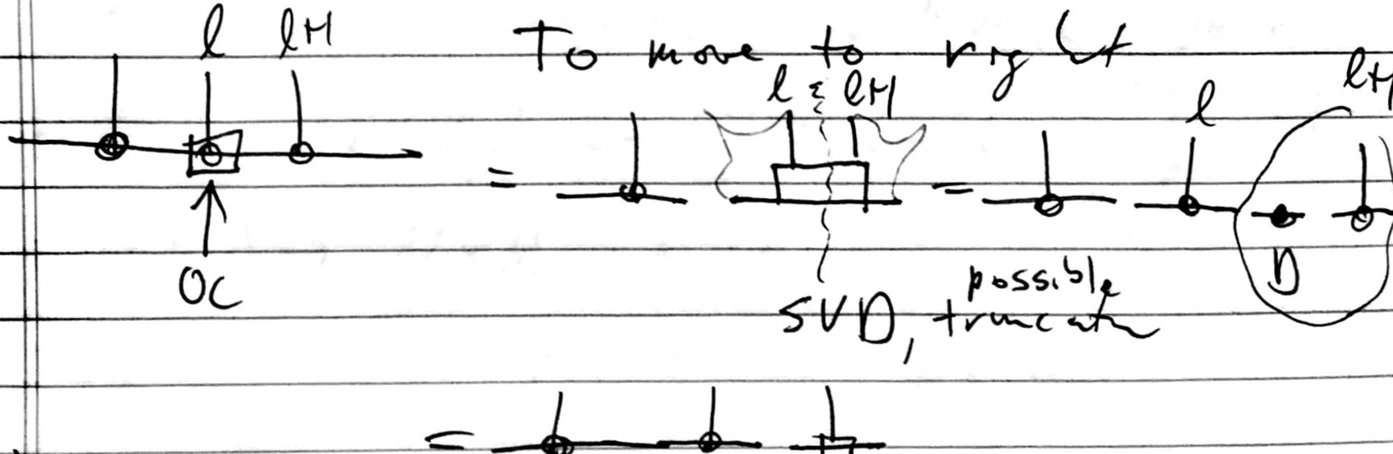
Similarly on right

$\langle O_i \rangle =$



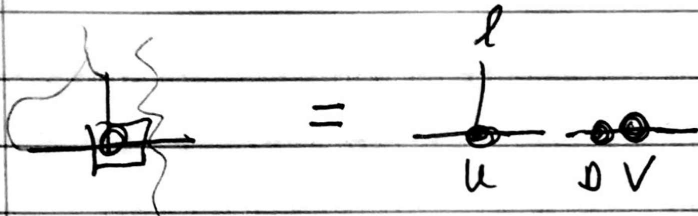
No need to do other contractions

Moving the OC

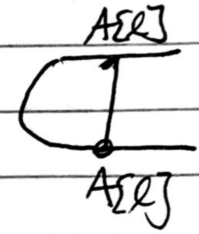


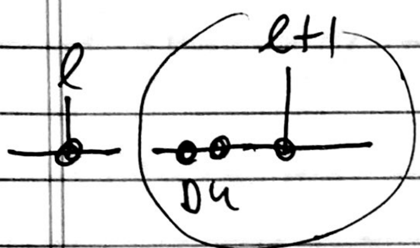
1) Join two adjacent tensors, then split, moving OC.

~~Mov.~~ Using one site

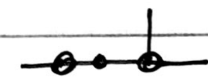


then $A[l] = U$





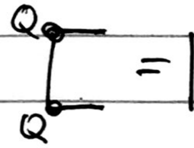
contract

$A[l+1] =$  $D\,U\,\psi[l+1]_{old}$

One site, QR

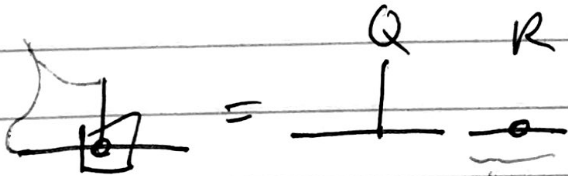
~~$M = QR$, $N \times M$, $N \times M$, $M \times M$, $N \geq M$~~

The QR is a cheaper (than SVD) matrix factorization where Q is [row] orthogonal & R is upper right triangular. The "thin" version ~~D~~ Makes Q column-orthonormal



$$\underset{N \times M}{M} \to \underset{N \times M}{Q}\ \underset{M \times M}{R}$$

$$Q^\dagger Q = 1$$

Then 

plays role of DV (but different)

$A[l] = Q$

$A[l+1] = R\,A[l+1]_{old}$

Getting the ground state Directly in MPS Form

~~TEBD~~ TEBD / tDMRG ~~(Guifre here April 28)~~
time evolving block decimation

Trotter Approximation:

Power method $v' = (1 - \varepsilon H) v$ iterate
$v \to$ grnd state if ε small.

Better $v' = e^{-\beta H} v$ β could be big

$e^{-\beta H}$ is hard for β big, but easy for β small, $\beta \to \tau$ $\tau \ll 1$

$\cancel{e^{-\tau \sum_i \vec{S}_i \cdot \vec{S}}}$ Let $H_i = \vec{S}_i \cdot \vec{S}_{i+1}$, $H = \sum_i H_i$

$$e^{-\tau H} = e^{-\tau \sum_i H_i} \cong \prod_i e^{-\tau H_i}$$

Errors come from $[H_i, H_{i+1}] \neq 0$

$$e^{-\tau(A+B)} = 1 - \tau(A+B) + \tfrac{1}{2}\tau^2 \underbrace{(A+B)^2}_{A^2+B^2+\boxed{AB+BA}} + \cdots$$

$$e^{-\tau A} e^{-\tau B} = \left(1 - \tau A + \tfrac{1}{2}\tau^2 A^2 \cdots\right)\left(1 - \tau B + \tfrac{1}{2}\tau^2 B^2 \cdots\right)$$

$$= 1 - \tau(A+B) + \tfrac{1}{2}\tau^2\left(A^2 + B^2 + \boxed{2AB}\right) \cdots$$

The error is $\propto \tau^2$: $e^{-\tau(A+B)} = e^{-\tau A} e^{-\tau B} + O(\tau^2)$

But to get gnd state, you need to do this $O(\frac{1}{\tau})$ times, so ~~tot~~ total error $\sim \underline{\underline{\tau}}$ [Usually too lousy to use!]

If you do it twice, with a reversal, you get $O(\tau^3)$ per sweep $\rightarrow$ $O(\tau^2)$ total

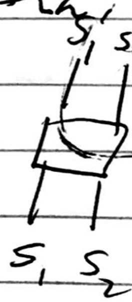
$$e^{-2\tau(A+B+C)} \approx e^{-\tau A} \underbrace{e^{-\tau B}}_{AB} e^{-\tau C} e^{-\tau C} \underbrace{e^{-\tau B} e^{-\tau A}}_{BA}$$

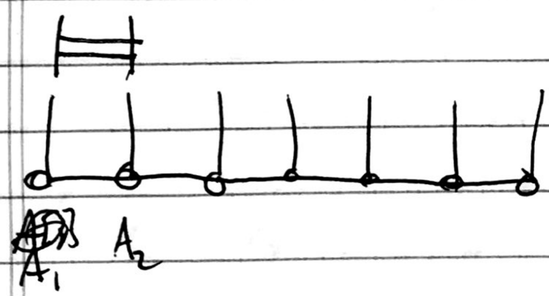
~~has AB+BA~~

has CAB (no CAB)

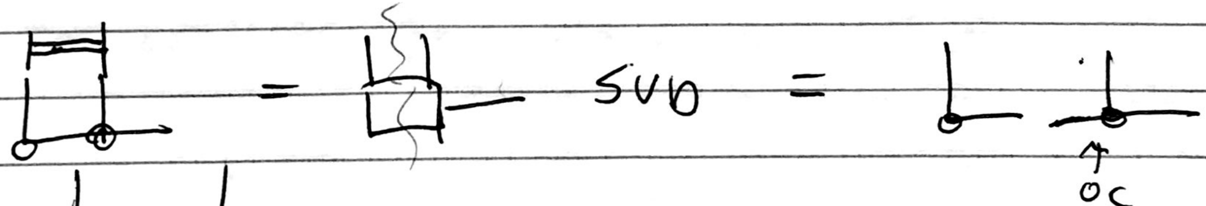
We apply $e^{-\tau H_i}$ one at a time, moving the OC, in a sweeping algorithm.

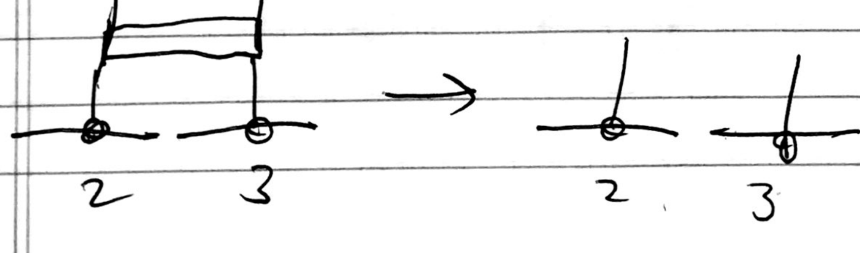
Diagrams $H_{bond} = \vec{S}\cdot\vec{S} =$ 

$e^{-\tau H_{bond}} =$ 

MPS 

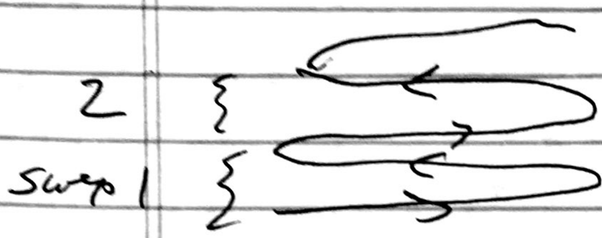
only affects A_1, A_2

step1 

step2 

<u>1 sweep</u> = $i = 1:n$, then $i = n:-1:1$

moving OC in directn of sweeping



Periodically, you need to fix the norm of the state.

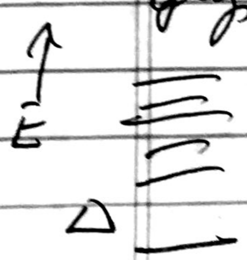
The splitting / moving of the OC needs the two side SVD ; not QR.

QR is only when we don't truncate.

τ controls error in result

But needs to converge in # of sweeps

Need $T = \frac{1}{\beta}$ to be ~~cos~~ less than gap between grnd state & 1st excited state



$T \sim \frac{\Delta}{10}$ $\quad \beta \sim \frac{10}{\Delta}$ $\quad$ # sweeps $\sim \frac{\beta}{\tau} \sim \frac{10}{(\Delta)(\tau)}$