Outline - Two Lectures

Entanglement

Low Entanglement Approximations

Diagrams, Tensor Networks

Matrix Product States

Trotter Time Evolution

Matrix Product Operators

DMRG

References

U. Schollwock, The density matrix renormalization group in the age of Matrix Product States, arxiv 1603.03.039

U. Schollwock, Numerical methods in the study of non-equilibrium strongly interacting quantum many body physics, Les Houches lecture notes

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Entanglement

Product States

The simplest type of states are product state

Examples: $|\uparrow_1 \downarrow_2\rangle = |\uparrow\rangle_1 |\downarrow\rangle_2 = |\uparrow\rangle \otimes |\downarrow\rangle$

or

$$\frac{1}{\sqrt{2}}\left(|\uparrow\rangle_1 - |\downarrow\rangle_1\right)\left(|\uparrow\rangle_2 + |\downarrow\rangle_2\right)\cdot\frac{1}{\sqrt{2}}$$

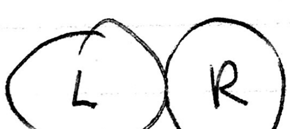
In general, if you can write $|\psi\rangle$ as

$|\psi\rangle = |\phi\rangle_1 |\eta\rangle_2 |\xi\rangle_3 \ldots$ it is a product state
= pure tensor product

Entanglement If $|\psi\rangle$ is not a product state, the system is entangled.

Usually we consider a system divided into two parts, L (left) and R (right)

L + R disjoint spaces



Then $|\psi\rangle \stackrel{?}{=} |\phi_L\rangle |\phi_R\rangle$

Suppose $\hat{O}$ is an op. acting only on L

$$\langle\psi|\hat{O}|\psi\rangle = \langle\phi_R|\langle\phi_L|\,\hat{O}\,|\phi_L\rangle|\phi_R\rangle$$

$$= \langle\phi_R|\phi_R\rangle\langle\phi_L|\hat{O}|\phi_L\rangle = \langle\phi_L|\hat{O}|\phi_L\rangle$$

Conclusion: Product states describe independent systems.

Entangled states – how do you tell if a state is entangled?

<u>Example</u>: 2 spins

Let $|A\rangle = \frac{1}{\sqrt{2}}|\uparrow\uparrow\rangle + \frac{1}{\sqrt{2}}|\downarrow\downarrow\rangle$
and
$|B\rangle = \frac{1}{2}|\uparrow\uparrow\rangle + \frac{1}{2}|\uparrow\downarrow\rangle + \frac{1}{2}|\downarrow\uparrow\rangle + \frac{1}{2}|\downarrow\downarrow$

Which is entangled?

$|B\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)\ \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$

so $|B\rangle$ is a product state, unentangled.

It is easy to see $|A\rangle$ is entangled (exercise).

Show there is no $\alpha, \beta, \gamma, \delta$ so

$|A\rangle = (\alpha|\uparrow\rangle + \beta|\downarrow\rangle)(\gamma|\uparrow\rangle + \delta|\downarrow\rangle)$

To know in general if a state is entangled you need to do a singular value decomposition.

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Singular Value Decomposition (SVD)

Let M be any complex $m \times n$ matrix with $n \geq m$. (If $n < m$, SVD on M^T)

Then there exists $U = m \times m$, $D = m \times n$ with D diagonal, $V = m \times n$ with

$$\boxed{M = UDV}$$

with $D_{ii} \geq 0$, U = unitary, V = row-unitary ($VV^\dagger = 1$) (rows of V orthonormal)

This is the SVD. The D_{ii} are the singular values, unique. $D_{ii} = \lambda_i$

Another form: $\tilde{D} = m \times n$, then $\tilde{V}$ is unitary, $n \times n$

$$M = U \tilde{D} \tilde{V}$$

SVD's have many uses. One is matrix compression. Suppose only a few D_{ii} are nonneglible

$$= \quad (\lambda)$$

Drop rest of matrices

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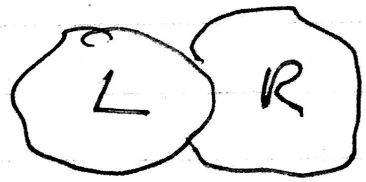
Schmidt Decomposition

Let $|\psi\rangle = \sum_{lr} \psi_{lr} \, |l\rangle |r\rangle$

$|l\rangle$ in L, $|r\rangle$ in R



ψ_{lr} is a wave function, but treat it as a matrix, do SVD

$$\psi_{lr} = [U \tilde{D} \tilde{V}]_{lr}$$

Normalization $\sum_{lr} |\psi_{lr}|^2 = 1 = \mathrm{tr}\{\psi^\dagger \psi\}$

matrix

Let

$$|i\rangle_L \equiv \sum_l U_{li} \, |l\rangle$$

$$|i\rangle_R \equiv \sum_r \tilde{V}_{ir} \, |r\rangle$$

$$|\psi\rangle = \sum_{lr} \sum_i U_{li} \tilde{D}_{ii} \tilde{V}_{ir} \, |l\rangle |r\rangle$$

$$= \sum_i \tilde{D}_{ii} \, |i\rangle_L \, |i\rangle_R = \boxed{\sum_i \lambda_i \, |i\rangle_L |i\rangle_R = |\psi\rangle}$$

this is the Schmidt decomposition

Normalization:

$$1 = \mathrm{tr}\{\psi^\dagger \psi\} = \mathrm{tr}\{\tilde{V}^\dagger \tilde{D}^\dagger \underbrace{U^\dagger U}_{1} \tilde{D} \tilde{V}\}$$

$$= \mathrm{tr}\{\tilde{D}^\dagger \tilde{D}\} \implies \boxed{\sum_i \lambda_i^2 = 1}$$

λ_i^2 is the probability of the Schmidt-state pair $|i\rangle_L |i\rangle_R$

If $|\psi\rangle = |\phi\rangle |\xi\rangle$, it is already in Schmidt decomp form, with $\lambda_1 = 1$, $\lambda_{i>1} = 0$. So this tells us if $|\psi\rangle$ is entangled.

<u>Von Neumann Entanglement Entropy</u>

$$\boxed{S \equiv -\sum_i \lambda_i^2 \ln \lambda_i^2}$$

VN ent. entropy

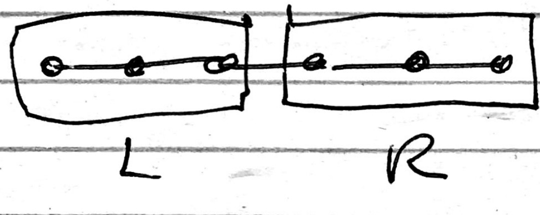
This is the stat mech formula for entropy using λ_i^2 = prob of $|i\rangle$

S measures entanglement. $S=0 \implies$ product state

Entanglement Entropy of Spin Chains

Heisenberg, Open $S=\frac{1}{2}$

Split the system down the middle



1) Find $|GS\rangle$
2) Rewrite in terms of L & R bases
3) SVD

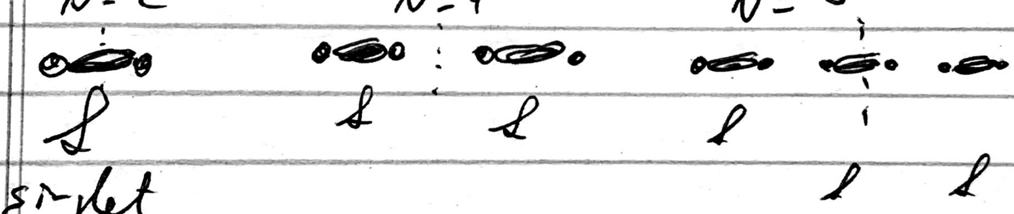
Exercise: Verify this table with Julia

N	S	$S_{max} = \frac{N}{2} \ln 2$
2	0.69	0.69
4	0.32	1.39
6	0.71	2.08
8	0.46	2.77
10	0.74	3.47
12	0.54	4.16
14	0.76	4.85

1) G.S. S is small!

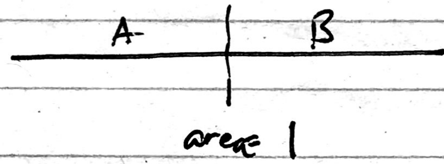
2) Odd-even alternation

RVB picture

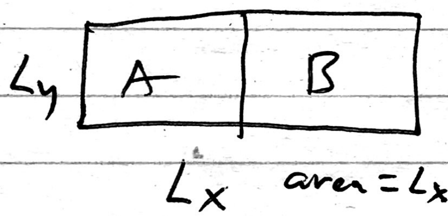


Area Law (Usually True)

The Entropy for a ground state of a system $A+B$, ~~where~~ is proportional to the "area" of the boundary.

1D 

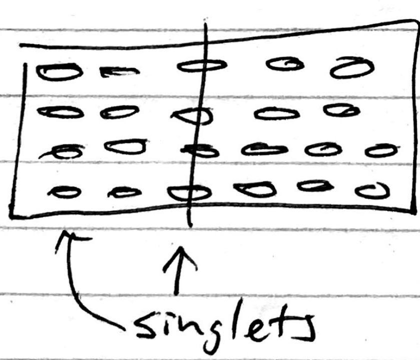
$S \sim$ constant (can be log corrections)

2D 

$S \propto L_y$

3D $S \propto$ Area

Pictorial Justification [lots of more rigorous work — maybe I'll mention some of it later]



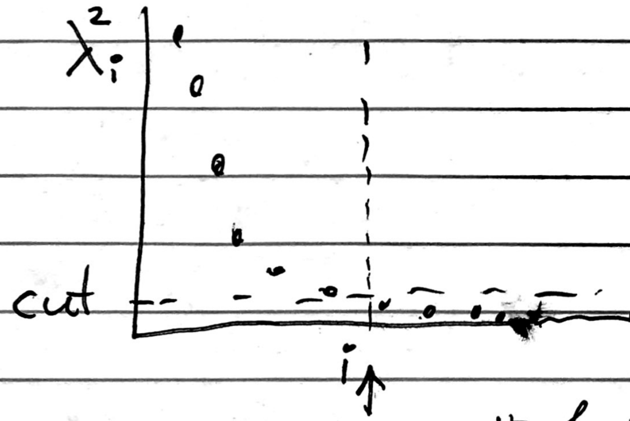
No entanglement unless a singlet bond is cut

The # of cut singlets $\sim$ area

Each contributes $\sim \ln 2$ to S.

Truncating Low Probability Schmidt States

Suppose we have rapidly falling singular values



Then we can throw away the low probability Schmidt states

$$|\psi\rangle = \sum_{i=1}^{2^{N/2}} \lambda_i |i\rangle_L |i\rangle_R \to \sum_{i=1}^{m} \lambda_i |i\rangle_L |i\rangle_R = |\tilde{\psi}\rangle$$

Error in $|\psi\rangle$:

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

$$(\langle\psi| - \langle\tilde{\psi}|)(|\psi\rangle - |\tilde{\psi}\rangle) = \text{error in } \psi$$

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

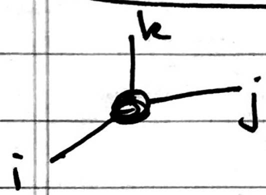
ε = "truncation error" or "discarded weight"

This truncation is the key approximation in Tensor networks & DMRG.

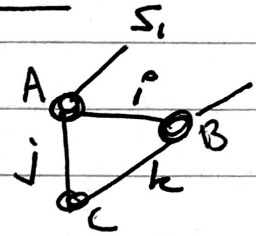
— low entanglement approximation —

Tensor Network Diagrams

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



Tensor
T_{ijk}



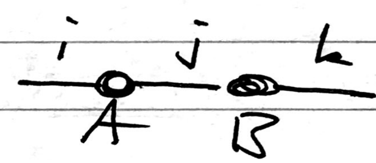
Tensor Contraction

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

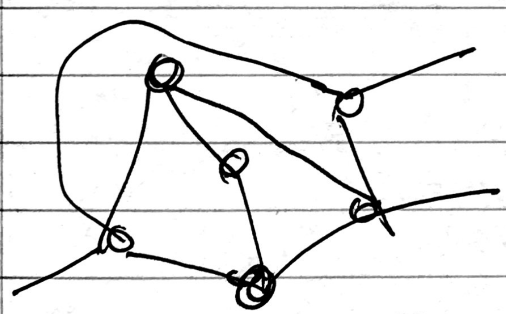
~~Matrix~~ Vector

Matrix

Matrix Product AB

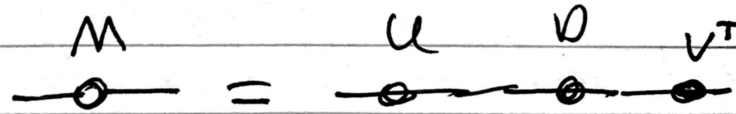


$$\{AB\}_{ik} = \sum_j A_{ij} B_{jk}$$



Tensor networks can get complicated.

SVD:

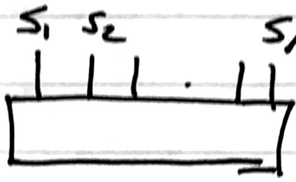


$M = UDV^T$

Suppose we had a wavefunct from exactly diagonalization of a spin chain

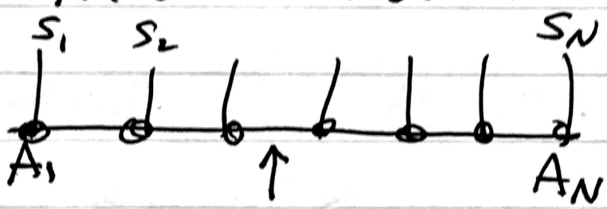
$\psi(s_1, s_2 \ldots s_N)$ $\quad 2^N$ numbers $\quad (N \lesssim \sim 50)$

<u>Diagram</u>



all 2^N degrees of freedom

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

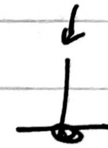


= basic ~~[illegible]~~ tensor

Algebraically

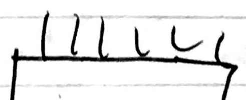
$$\psi(s_1 \ldots s_N) = \overset{\substack{\text{row}\\\text{vec}}}{\vec{A}^1[s_1]}\ \overleftrightarrow{A}^2[s_2] \cdots \overset{\to\ \text{col vec}}{A^N[s_N]}$$

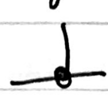
Regard $A^\ell[s_\ell]$ as two matrices

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

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

This is a huge compression



2^N $\longrightarrow$  $\times N$

$m^2 \cdot 2 \cdot N$

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 $\overleftrightarrow{A}_2 = \frac{1}{\sqrt{3}}\begin{pmatrix} |\downarrow\rangle & |\uparrow\rangle \\ |\uparrow\rangle & 0 \end{pmatrix}$

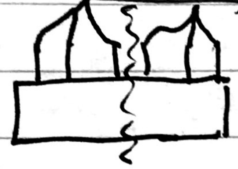
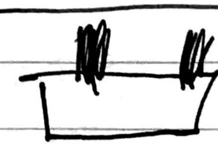
(use $\vec{A}_1^T$)

$$|\Psi\rangle = \vec{A}_1 \cdot \overleftrightarrow{A}_2 \cdot \vec{A}_3$$

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

In 1D, low entanglement $\Rightarrow$ MPS

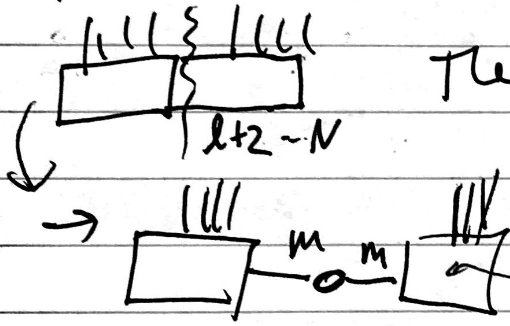
Treat as one big index

 from ED = 

Do SVD  Schmidt form

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

Repeat at one site ~~over~~ to the right



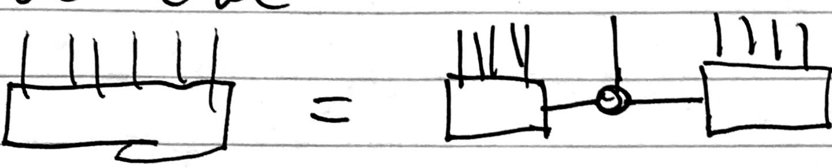
Then site l+2 can be treated as have m states

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

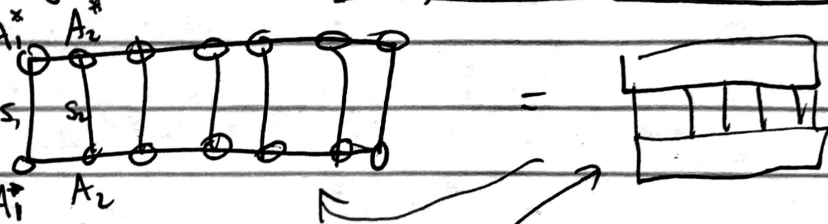
Then $|\psi\rangle = \sum_{\alpha=1}^{m} \sum_{\beta=1}^{m} \sum_{s_{l+1}=\uparrow,\downarrow}$ ~~$\psi A[s_{l+1}]$~~ $\psi(\alpha, s_{l+1}, \beta)$ $|\alpha\rangle_L |s_{l+1}\rangle |\beta\rangle_R$

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

We have

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

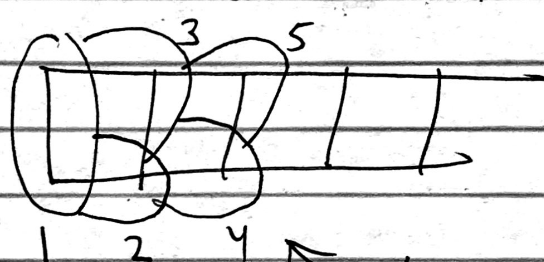
Normalization of an MPS, Measuring Ops

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

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

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

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



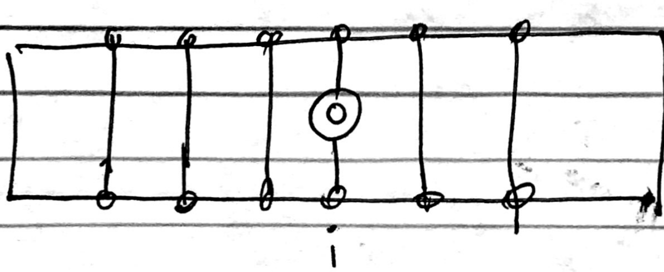
"Bubbling"

Measuring Operators

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

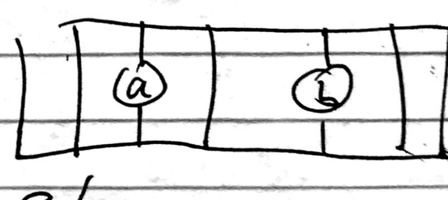
$$= \langle s_1' \ldots s_N' | s_1 \ldots (O_i s_i) \ldots s_N \rangle$$

O_i attaches to A_i

$\langle O_i \rangle =$ 

"Bubble" left to right,

Also



etc.

Orthogonality: crucial for effectively using MPS

drop †, redefine V

In an SVD, $M = UDV$, $U + V$ ~~are unitary~~

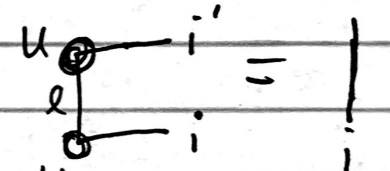
are row/col. unitary

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

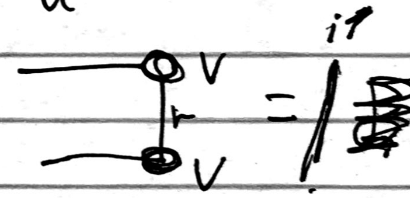
Let U have ~~labels~~ indices $U_{\ell i}$ (left, Schmidt)

V_{ir} (right)

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

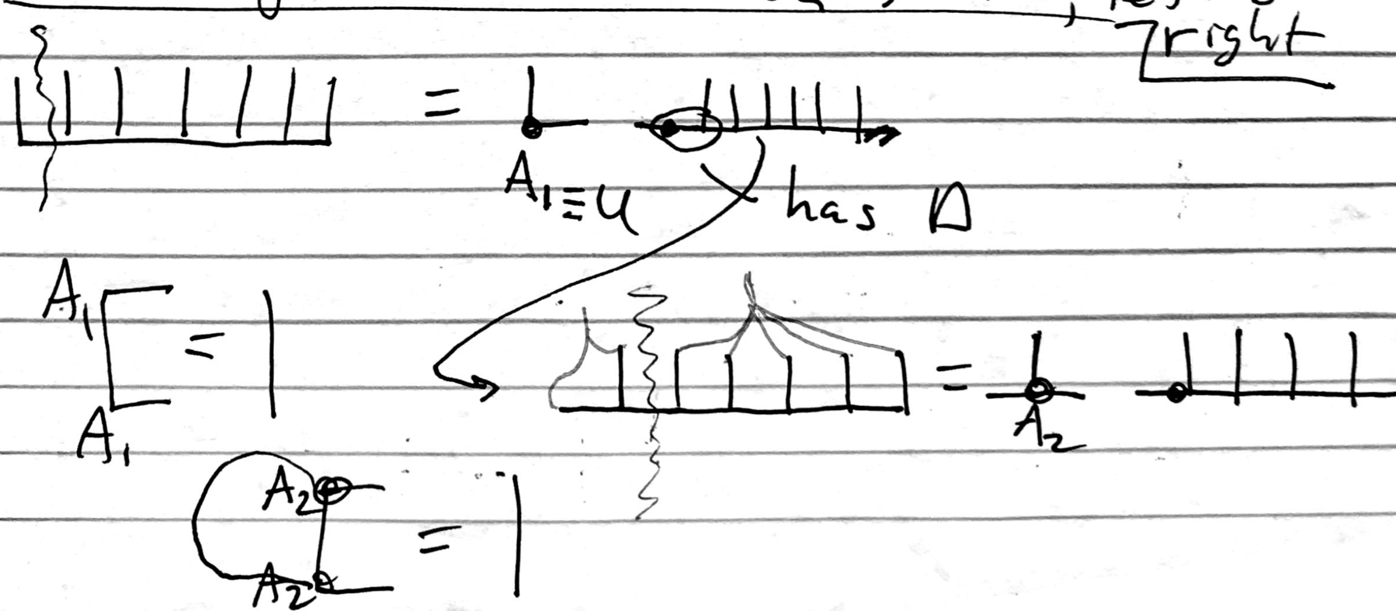


$$\sum_r V_{ir} V^*_{i'r} = \delta_{ii'}$$ or

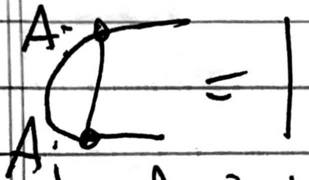


Orthogonality

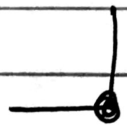
Converting a Wfn to an MPS, left to right



Keep going to the end

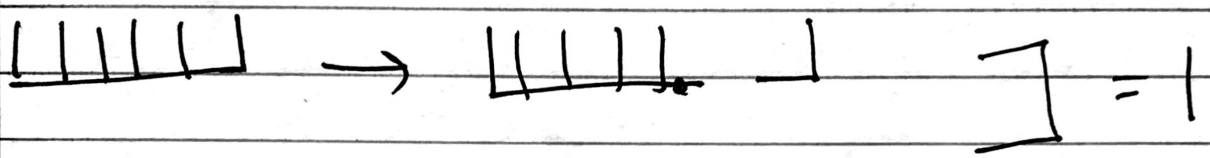


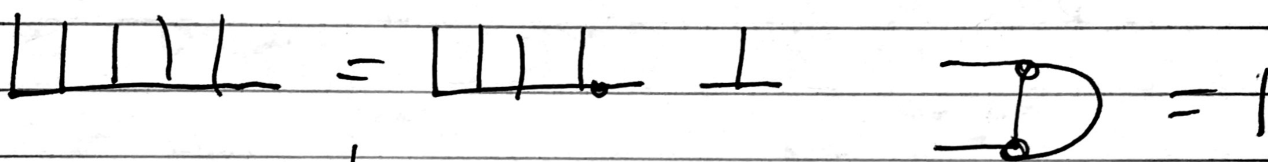
for $i=1,\ldots N-1$

 A_N has last $\square$ so no orthogonality

We say site N is the orthogonality center

We could put ~~it~~ the OC on ~~the~~ site 1

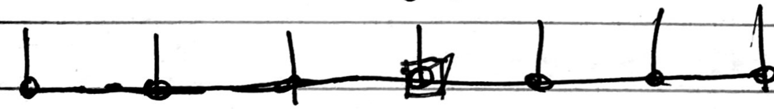


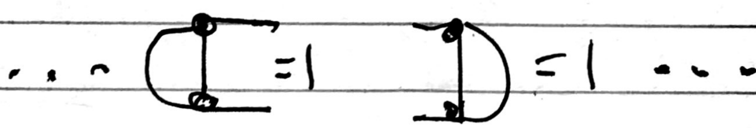


etc.

In general, it looks like

OC

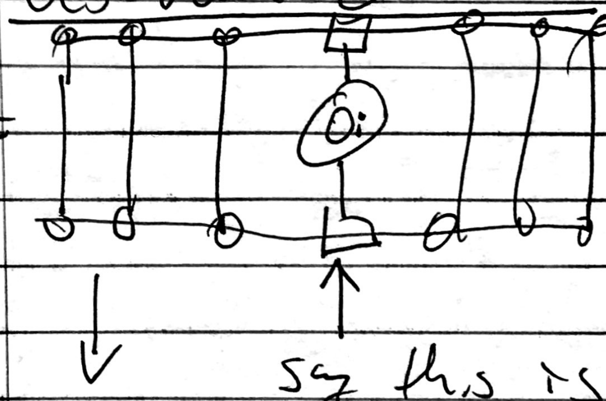


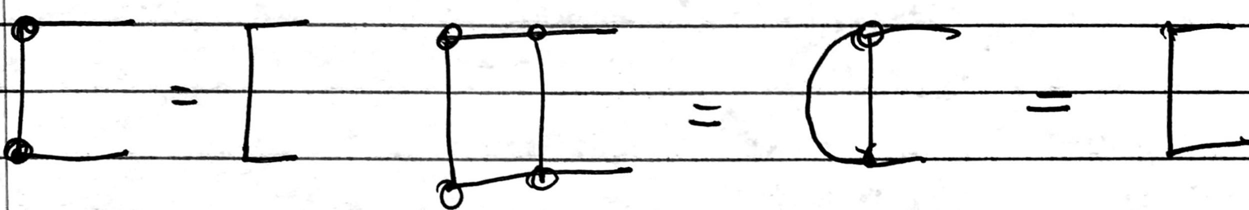


It is possible to not have an OC — but it is useful to have one.

Using an OC

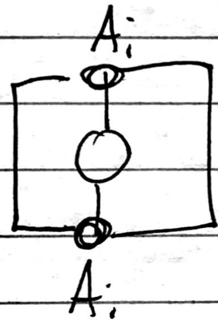
$\langle O_i \rangle =$





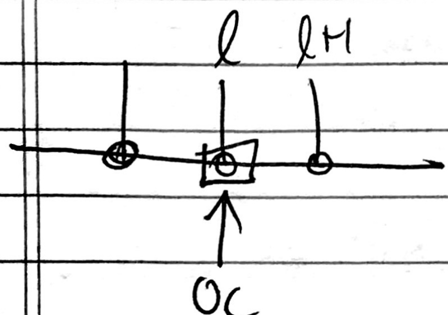
Similarly on right

$\langle O_i \rangle =$

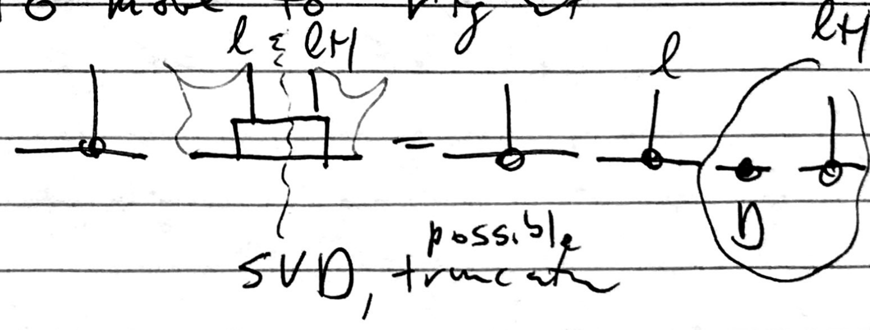


No need to do other contractions

Moving the OC



To move to right



$=$

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

Trotter Time Evolution

time evolving block decimation TEBD, Vidal
& DMRG

Trotter Approx $|\psi\rangle = e^{-\beta H} |\text{almost anything}\rangle$
$\Rightarrow$ ground state as $\beta \to \infty$

How do we apply $e^{-\beta H}$ on an MPS?

$$e^{-\beta H} = \left(e^{-\tau H}\right)^{\frac{\beta}{\tau}} \qquad \tau \text{ small}$$

Let H_i = bond term in H connecting i & $i+1$

Example: $H_i = \vec{S}_i \cdot \vec{S}_{i+1}$. Assume $H = \sum_i H_i$

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

not exact since $[H_i, H_{i+1}] \neq 0$

Errors for one step τ: $\propto \tau^2$

$\#$ steps $\propto \frac{1}{\tau}$ so total $\sim \tau$ not so good

If you reverse, goes to τ^2

$$e^{-2\tau H} = \prod_{i=1}^{N} e^{-\tau H_i} \prod_{i=N}^{1} e^{-\tau H_i} \qquad \text{error} \sim \tau^3$$

$\Rightarrow \tau^2$ OK.

T2

Diagrams $\vec{S}_i \cdot \vec{S}_{i+1}$ =

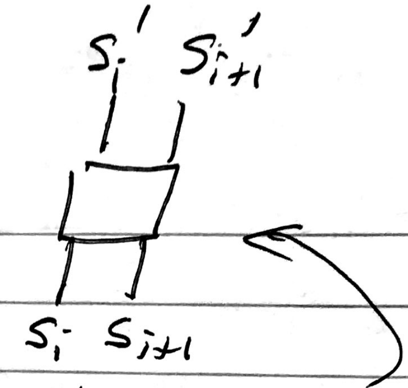
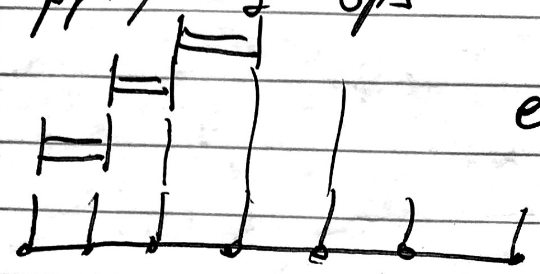
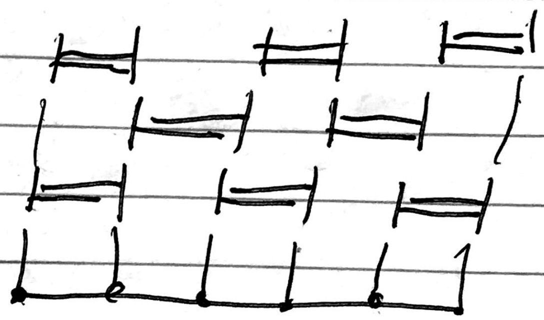


Diagram for $e^{-\tau S \cdot S}$ looks <u>the same</u>

Applying ops



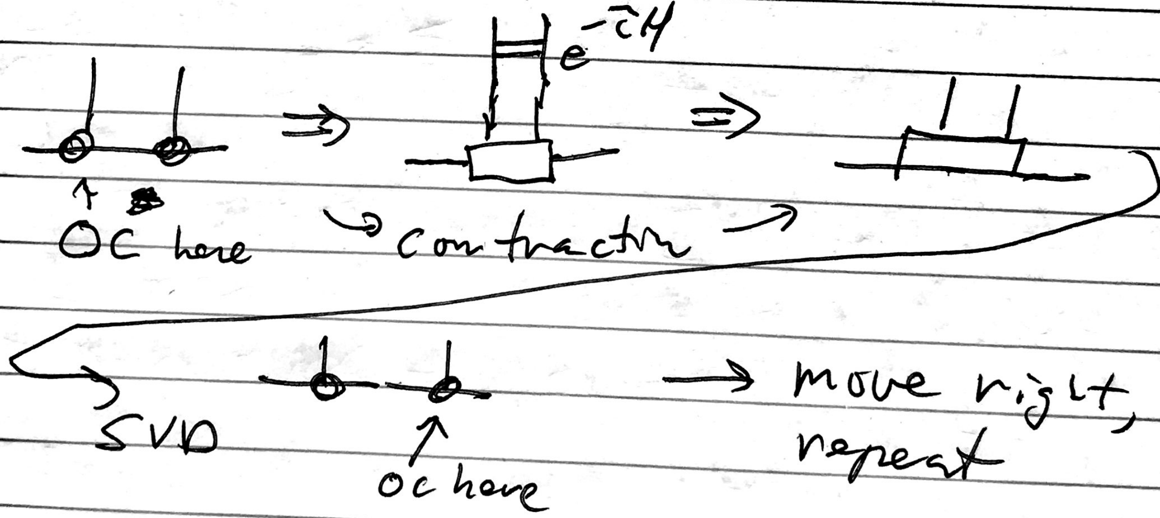
etc, or



forward/back

even/odd

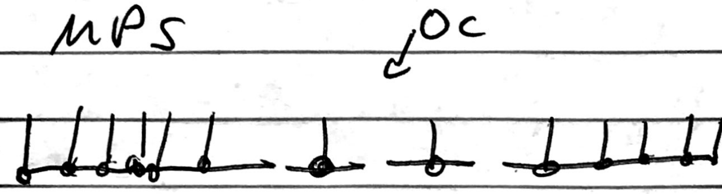
<u>Operators</u>



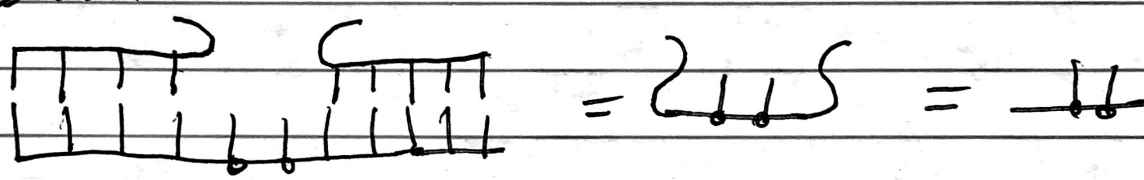
<u>Real time evolution</u>: no difference, apply $e^{-i\tau H}$.

DMRG – finding the ground state

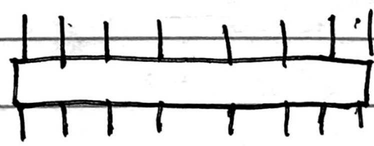
Let's focus on two sites. Given an MPS

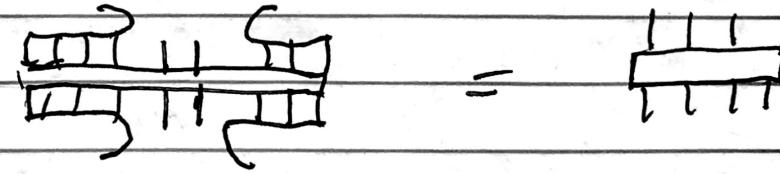


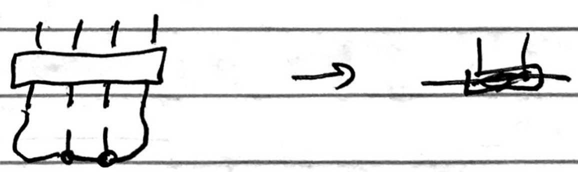
We can regard LIIIL as a change of basis plus a truncation, to a reduced basis. Orthogonal if OC in center at 1 of the 2 sites



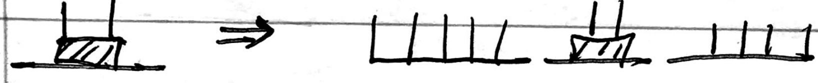
You can use Lanczos to decrease the energy if you know H in the reduced basis

$H =$  Full diagram for any operator

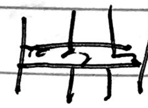
$H^{reduced} =$ 

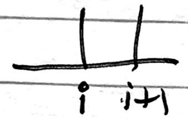
$H^{red} \cdot \psi^{red} =$  ψ'

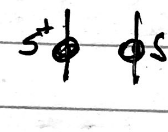
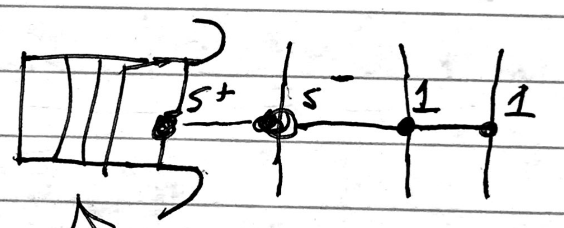
Suppose we reduce the energy in the reduced basis with Lanczos. Then this translates to the same energy in the full basis

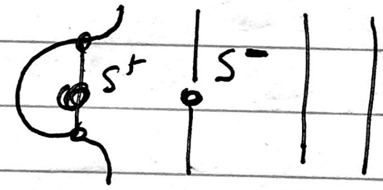


Can go back to full ψ any time.

Constructing  $= H^{\text{reduced}}$ is not hard, since $H = \sum_i \underbrace{H_i}_{\text{only 2 or a few sites involved.}}$

Example:  look at $\frac{1}{2} S^+_{i-1} S^-_i = H_{i-1}$

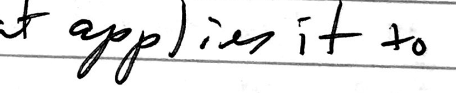
$H^{\text{redu}}_{i-1} \Rightarrow$  $\Rightarrow$ 

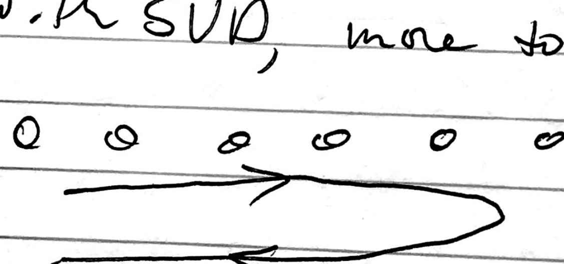
$H^{\text{red}}_{i-1} =$ 

contract with orthogonality

$+\ S^- S^+$ term $+\ S^z S^z$ term

For efficiency, we don't construct H^{red}, we write a function that applies it to ψ

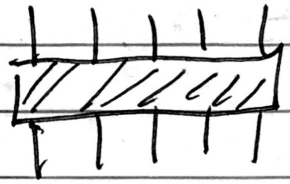
After Lanczos, split up  with SVD, move to next site.



sweep

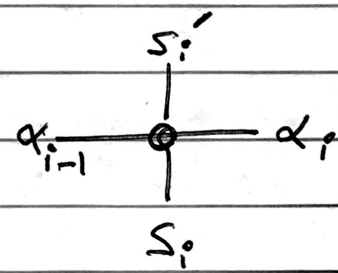
Matrix Product Operators

Full ~~M~~ diagram for H is

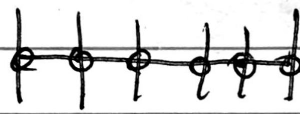


Can we write this as a matrix product?

Basis tensor



Yes

MPO = 

Example: 4 site Ising Let $S^z = Z$

$$H = Z_1 Z_2 + Z_2 Z_3 + Z_3 Z_4$$

$$MPO = (0\ Z_1\ 1)\underbrace{\begin{pmatrix} 1 & 0 & 0 \\ Z_2 & 0 & 0 \\ 0 & Z_2 & 1 \end{pmatrix} \underbrace{\begin{pmatrix} 1 & 0 & 0 \\ Z_3 & 0 & 0 \\ 0 & Z_3 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ Z_4 \\ 0 \end{pmatrix}}_{\begin{pmatrix} 1 \\ Z_3 \\ Z_3 Z_4 \end{pmatrix}}}_{\begin{pmatrix} 1 \\ Z_2 \\ Z_2 Z_3 + Z_3 Z_4 \end{pmatrix}}$$

elements of each matrix are site operators

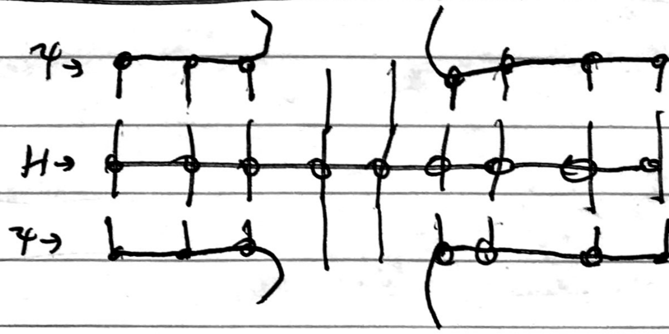
$m = 3$ MPO.

$$= Z_1 Z_2 + Z_2 Z_3 + Z_3 Z_4$$

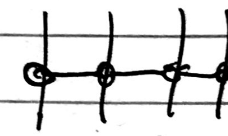
These are easy to construct for short range Hams.

DMRG with MPOs

H^{red} =

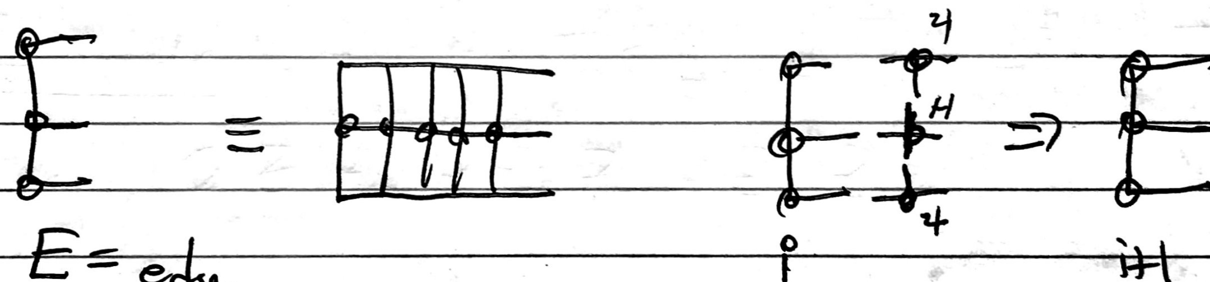


=



short MPO

Both operator DMRG & MPO DMRG allow recursive construction of H^{red}_{i+1} from H^{red}_{i}. For example



E = edge tensor