Entanglement and Tensor Networks in Cond-Mat. (Pohang '17)

*) Goal: basics on quant-many-body entang., TNs, and associated numerical methods and future prospects.

*) Some ref's:

- RO, arXiv: 1306.2164 (Ann. Phys. 349, 117 (2014))
- U. Schöllwock, Ann. Phys. 326, 96 (2011)
- RO, arXiv: 1407.6552 (EPJB 87: 280 (2014))
- (...)

1.- Entanglement.

1.1) Entang. and its quantification.

*) Given $|\psi\rangle_{AB} \in \mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$, $|\psi\rangle_{AB}$ is entangled iff

$$|\psi\rangle_{AB} \neq |\phi\rangle_A \otimes |\phi\rangle_B, \; |\phi\rangle_A \in \mathcal{H}_A, \; |\phi\rangle_B \in \mathcal{H}_B.$$

*) Considerations:

(i) it can also be multipartite, e.g. $|\psi\rangle_{ABC} \neq |\phi\rangle_A \otimes |\phi\rangle_B \otimes |\phi_C\rangle$, etc.

(ii) A full classification of ent. states is only possible in particular cases, e.g.

- 2 qubits $\longrightarrow$ EPR states, $|\psi^-\rangle = \frac{1}{\sqrt{2}}(|0\rangle|1\rangle - |1\rangle|0\rangle)$
- 3 qubits $\longrightarrow$ GHZ, W states $\longrightarrow$ $|GHZ\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$;

$$|W\rangle = \frac{1}{\sqrt{3}}(|001\rangle + |010\rangle + |100\rangle).$$

(iii) Ent. is non-local: it does not change under local unitary op's:

$$E(|\psi\rangle_{AB}) = E(U_A \otimes U_B \, |\psi\rangle_{AB}).$$

Therefore cannot be created locally. Formally: "ent. does not increase under Local Op's & Classical Comm (LOCC)". $\rightarrow$ includes measurements and mixed states.

*) Bipartite pure states & Schmidt decomp

Theorem: $|\psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$, $|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$,

$\exists$ always a decomposition such that $|\psi\rangle_{AB} = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_A |\alpha\rangle_B$,

with ${}_A\langle\alpha|\alpha'\rangle_A = {}_B\langle\alpha|\alpha'\rangle_B = \delta_{\alpha\alpha'}$ ($\perp$ Basis), $\lambda_\alpha > 0$

$$\begin{cases} \lambda_\alpha \equiv \text{Schmidt Coeff.} \\ \chi \equiv \text{Schmidt Rank} \leq \min(d_A, d_B),\ d_{A/B} \equiv \dim(\mathcal{H}_{A/B}). \\ \{|\alpha\rangle_{A/B}\} \equiv \text{Schmidt basis for } A/B. \end{cases}$$

Examples: $|\psi\rangle_{AB} = |0\rangle_A |0\rangle_B \rightarrow \chi = 1,\ \lambda_1 = 1$

$|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}\left(|0\rangle_A|0\rangle_B + |1\rangle_A|1\rangle_B\right) \longrightarrow \chi = 2,\ \lambda_1 = \lambda_2 = \frac{1}{\sqrt{2}}$

Lemma: $\boxed{\chi = 1 \Longleftrightarrow |\psi\rangle_{AB} \text{ is separable.}}$

*) Proof of the S.D:

$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$; $\psi_{ij} \equiv$ Matrix. Let's do an SVD:

Singular Value Decomp (SVD):

$$\underset{\substack{\uparrow \\ d_A \times d_B}}{\psi} = U \Lambda V^\dagger, \text{ with } UU^\dagger = \mathbb{I}_{d_A},\ V^\dagger V = \mathbb{I}_{d_B},\ \Lambda \text{ diag, } \chi\times\chi, > 0.$$

$\Lambda_{\alpha\beta} = \lambda_\alpha \delta_{\alpha\beta}$, $\lambda_\alpha \equiv$ Singular Values > 0

Then: $\psi_{ij} = \sum_{\alpha=1}^{\chi} U_{i\alpha} \lambda_\alpha (V^\dagger)_{\alpha j}$

Then: $|\psi\rangle_{AB} = \sum_{i=1}^{d_A} \sum_{j=1}^{d_B} \sum_{\alpha=1}^{\chi} U_{i\alpha} \lambda_\alpha (V^\dagger)_{\alpha j} |i\rangle_A |j\rangle_B =$

$$= \sum_{\alpha=1}^{\chi} \lambda_\alpha \underbrace{\left(\sum_{i=1}^{d_A} U_{i\alpha} |i\rangle_A\right)}_{|\alpha\rangle_A} \underbrace{\left(\sum_{j=1}^{d_B} (V^\dagger)_{\alpha j} |j\rangle_B\right)}_{|\alpha\rangle_B} = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_A |\alpha\rangle_B \checkmark$$

*) Comment : χ is a discontinuous measure of entang.

*) Von Neumann (Entang.-) Entropy :

Given $|\psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$, with rdms ρ_A and ρ_B,

$\rho_A = \mathrm{tr}_B(|\psi_{AB}\rangle\langle\psi_{AB}|)$; $\rho_B = \mathrm{tr}_A(|\psi_{AB}\rangle\langle\psi_{AB}|)$

The von Neumann entropy is $\boxed{S(\rho_A) = -\mathrm{tr}(\rho_A \log \rho_A) = S(\rho_B)}$

- In terms of eigenvalues ν_α of ρ_A: $\boxed{S(\rho_A) = -\sum_{\alpha=1}^{\chi} \nu_\alpha \log \nu_\alpha .}$

- Moreover, $\rho_A = \sum_{\alpha=1}^{\chi} \underbrace{|\lambda_\alpha|^2}_{\nu_\alpha} |\alpha\rangle\langle\alpha|_A$; $\rho_B = \sum_{\alpha=1}^{\chi} \underbrace{|\lambda_\alpha|^2}_{\nu_\alpha} |\alpha\rangle\langle\alpha|_B$, thus

$\boxed{\mathrm{rank}(\rho_A) = \mathrm{rank}(\rho_B), \text{ and same spectrum} \Rightarrow S(\rho_A) = S(\rho_B).}$ (as expected

- $\boxed{S(\rho_A) \le \log \chi}$ Saturated by a flat distribution of coefficients.

$$|\psi_{AB}^{max}\rangle = \frac{1}{\chi} \sum_{\alpha=1}^{\chi} |\alpha\rangle_A |\alpha\rangle_B .$$ Maximally Entang. State.

- $S(\rho_A)$ is a measure of ent. between A & B. It's the only one that

$\left\{ \begin{array}{l} \text{(i) does not increase under LOCC} \\ \text{(ii) is continuous} \\ \text{(iii) Subadditivity: } S(\rho_{AB}) \le S(\rho_A) + S(\rho_B) \end{array} \right.$

1.2) Entanglement in quantum many-body.

(a) 1d Systems.

--- o o o o o o o --- spinchain, fermionic chain, etc

→

⊛ <u>Setting</u> : <u>entropy of a block for the ground state</u> :

$$\cdots \circ \quad \circ \quad \underbrace{(\circ \quad \circ \quad \circ \quad \circ \quad \circ \quad \circ \quad \circ)}_{L} \quad \circ \quad \circ \quad \circ \cdots \qquad |\psi_0\rangle$$

$$\downarrow$$

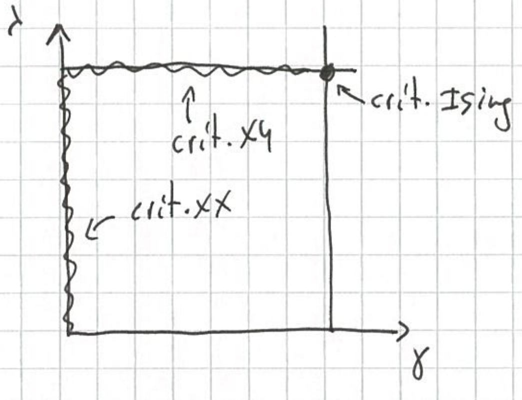
$$\rho_L = \mathrm{tr}_{N-L}(|\psi_0\rangle\langle\psi_0|)$$

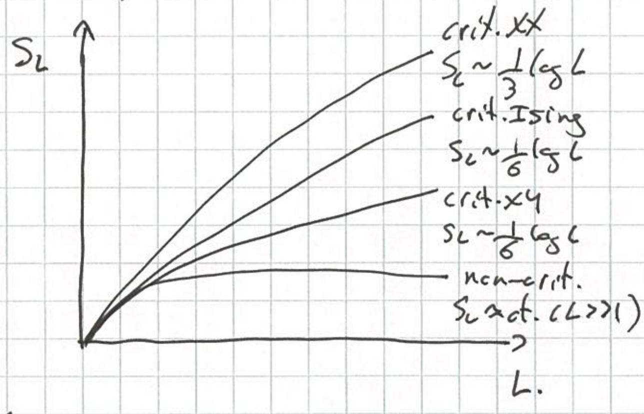
$$\downarrow$$

$$S_L \equiv -\mathrm{tr}(\rho_L \log \rho_L).$$

•) <u>Example: XY Model.</u>

$$H = -\sum_{i=1}^{\infty} \left(\frac{1+\gamma}{2}\right)\sigma_i^x\sigma_{i+1}^x + \left(\frac{1-\gamma}{2}\right)\sigma_i^y\sigma_{i+1}^y + \lambda\sigma_i^z$$





•) <u>General Result: Conformal Field Theory</u>

$$\text{For } L \gg 1, \begin{cases} S_L \approx \frac{c}{3}\log L + a + O(1/L) & \text{at quant. crit. points} \\ S_L \approx \frac{c}{3}\log \xi + a + O(1/L) & \text{close to criticality (but gapped).} \end{cases}$$

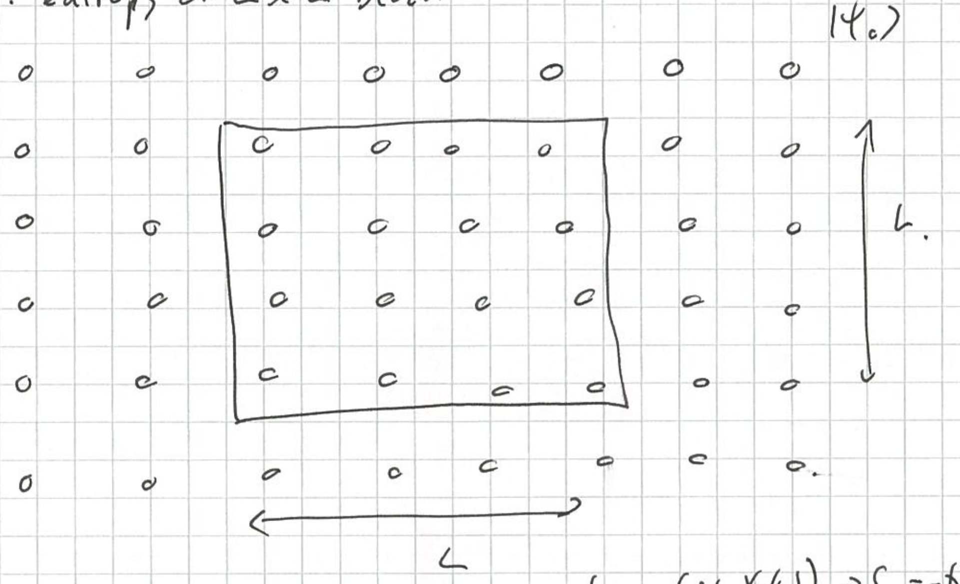
c = central charge of the (1+1)d-CFT.

$$\begin{cases} c = 1/2 \longrightarrow S_L \sim \frac{1}{6}\log L \longrightarrow \text{Ising \& XY QPT} \Longleftrightarrow \text{Free Fermion QFT} \\ c = 1 \longrightarrow S_L \sim \frac{1}{3}\log L \longrightarrow \text{XX} \Longleftrightarrow \text{Free Boson QFT.} \end{cases}$$

→

(b) 2d Systems:

+) Setting: entropy of $L \times L$ block.



$\hookrightarrow \rho_L = \mathrm{tr}_{N-L}(|\Psi_0\rangle\langle\Psi_0|) \rightarrow S_L = -\mathrm{tr}(\rho_L \log \rho_L)$

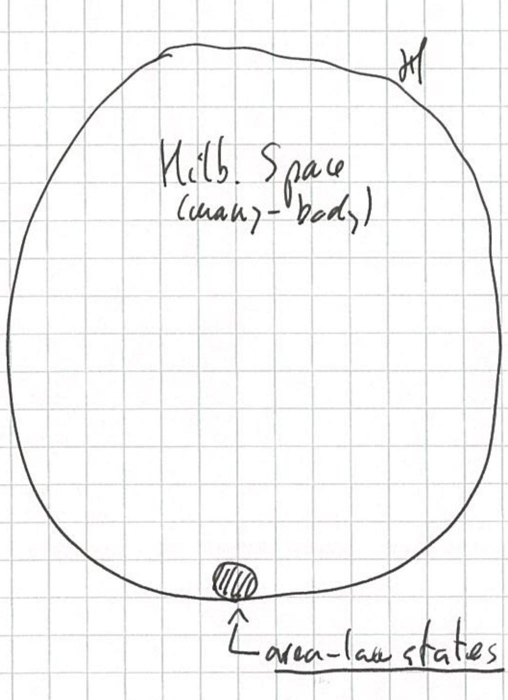
+) Generic Result: For H with local interactions, one typically has

$$\boxed{S_L \approx a \cdot L - S_\gamma + O(1/L)}$$

both at and away from criticality.

- It's a 2d - Area Law.
- $S_\gamma \equiv$ Topological entropy.

1.3) Physical Picture



- Relevant corner at low energies is exp. small!
- "Exploration time" is also exp. large (via local H's).
- Putting numbers: $T \sim 10^N \sim 10^{10^{23}}$ sec.
  $T_{univ} \sim 10^{17}$ sec. (wiki) ?
- Target relevant corner directly $\rightarrow$ TNs,

$\uparrow$ area-law states $\rightarrow$ relevant corner at low energies

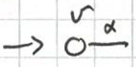
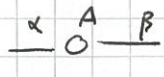
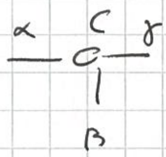
2.- Tensor Networks (TN)

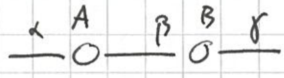
2.1) TN theory

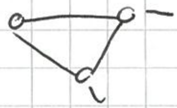
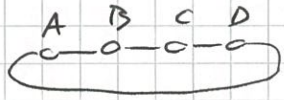
*) <u>Tensor</u> = multidimensional array of $\mathbb{C}$ numbers, e.g.,

v_α ≡ vector, $A_{\alpha\beta}$ ≡ matrix, $C_{\alpha\beta\gamma}$ ≡ 3-index tensor.

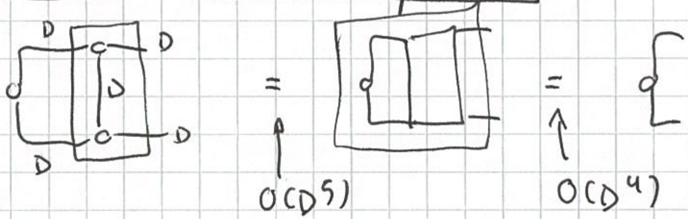
*) <u>Diagrammatic notation</u>:

$v_\alpha \to$  ; $A_{\alpha\beta} \to$  ; $C_{\alpha\beta\gamma} \to$ 

 $\equiv \sum_\beta A_{\alpha\beta} B_{\beta\gamma}$ (index contraction).

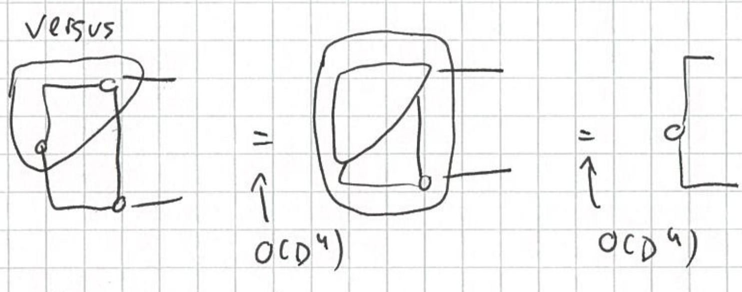
Similarly:  , etc. <u>Example</u>:  $= tr(ABCD)$.

*) <u>Contraction order is important</u>:



$\Rightarrow O(D^5)$ op's.

versus

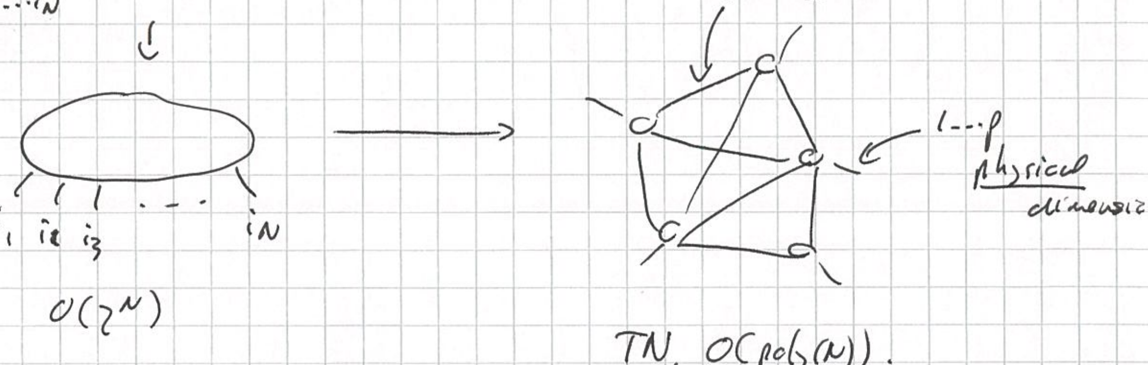


$\Rightarrow O(D^4)$ op's. (!!)

Optimal contraction order → always pairwise contractions.

*) Idea of TNs: <u>break the wavefunction in fundamental pieces</u>.

$|\psi\rangle = \sum_{i_1 \cdots i_N} C_{i_1 \cdots i_N} |i_1\rangle \cdots |i_N\rangle$



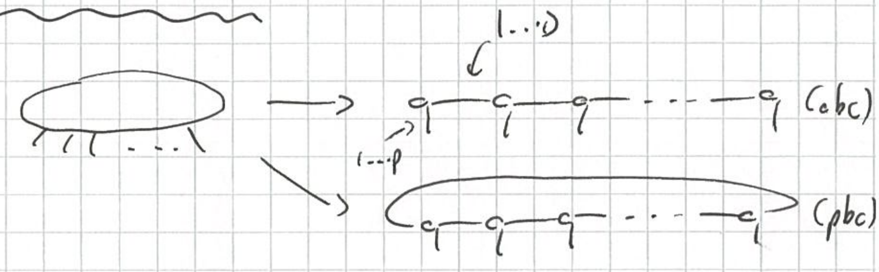
$O(2^N)$

TN, $O(poly(N))$.

- Depending on the situation, the inherent TN structure of $|\psi\rangle$ will be one or the other.
- TNs account for the <u>entanglement amount & structure</u> in $|\psi\rangle$.

2.2) Matrix Product States (MPS).

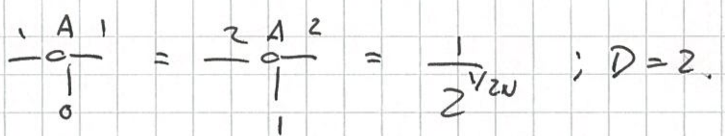
*) MPS are 1d TNs:



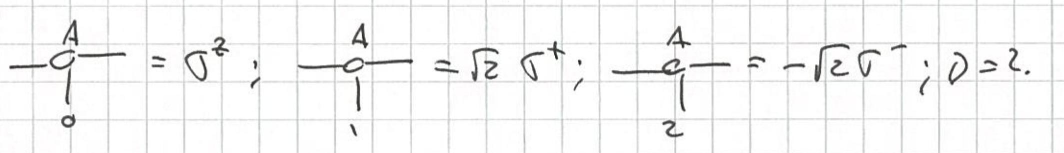
with equations, e.g. for pbc: $C_{i_1\ldots i_N} = \mathrm{tr}\left(A^{[1]i_1}\cdots A^{[N]i_N}\right)$.

*) <u>Examples</u>:

(i) <u>GHZ</u>. $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\ldots0\rangle + |1\ldots1\rangle\right)$;



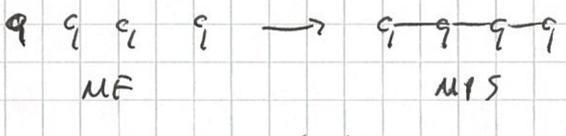
(ii) <u>AKLT</u>: unique g.s. of $H = \sum_i \vec{S}_i\cdot\vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i\cdot\vec{S}_{i+1}\right)^2$, spin-1



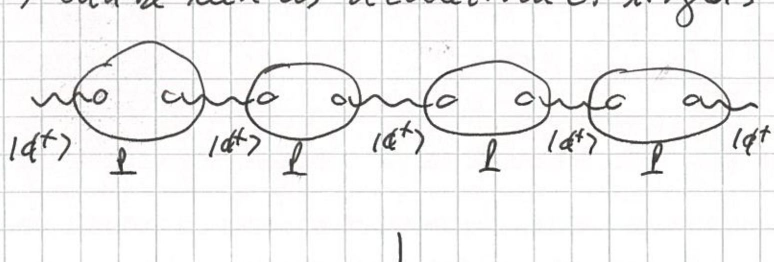
*) <u>Motivations for MPS</u>:

0) ~~#~~ parameters $O(pD^2N)$.

1) Generalizes Mean-field, taking entang. into account:

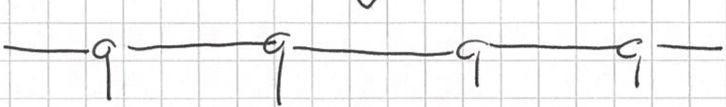


2) Can be seen as a collection of singlets with projectors:



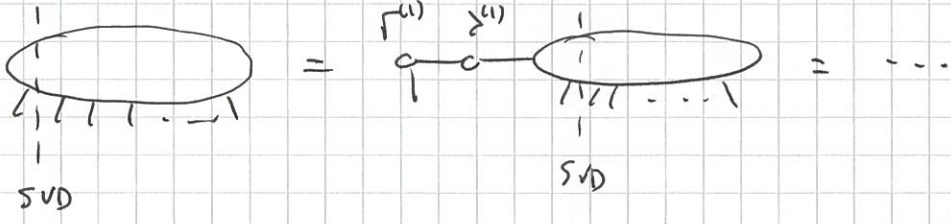
$|\phi^+\rangle \equiv \frac{1}{\sqrt{D}}\sum_{\alpha=1}^{D} |\alpha\rangle|\alpha\rangle$

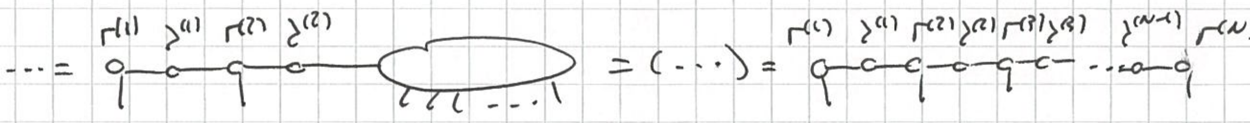
$(P)^i_{\alpha\beta}\ |i\rangle\langle\alpha|\langle\beta| \equiv P$.



→

3) For obc → MPS come from a sequence of SD's:



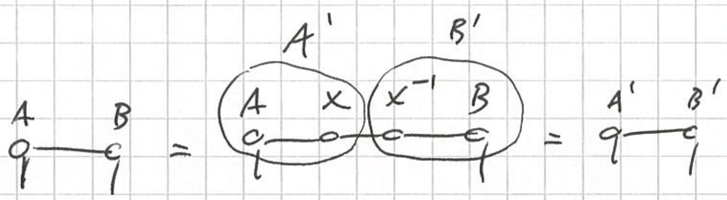


- If ∀ Schmidt Rank is upper-bounded by a constant D, then this is also an MPS. They call this the <u>MPS canonical form</u>.

- This looks very arbitrary. <u>But</u> for 1d systems in a gapped phase, this is exactly the case!.

*) <u>Properties of MPS</u>:

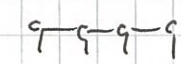
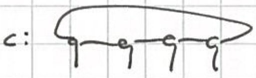
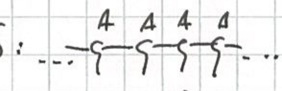
1) <u>Gauge-invariance</u> :



Same state, different tensors.

2) $\boxed{S_L(MPS) \leq 2\log D}$ 1d- Area Law.

(I'll show the proof tomorrow for 2d).

3) obc:  phc:  ; iMPS: 

(unit cell).

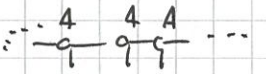
4) <u>~~Gapped~~ Ground States of gapped TI local Hamiltonians can be approximated with exp. accuracy by MPS with finite D</u>.

5) $\boxed{\xi \text{ is finite for all MPS}}$ ⇝ Again, 1d gapped phases.

→

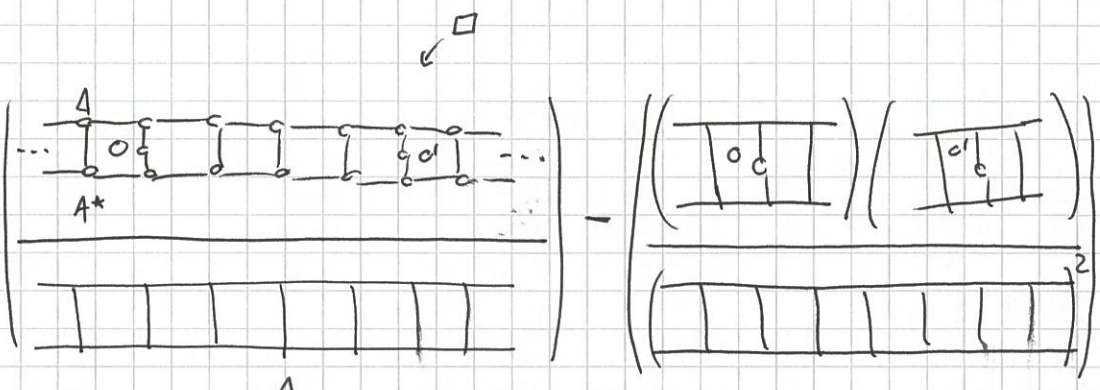
Proof:

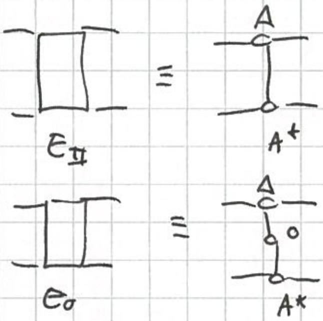
$C(r) = \langle O_i \, O'_{i+r} \rangle - \langle O_i \rangle \langle O'_{i+r} \rangle$?

MPS: 

: MPS, 1-site unit cell (assume).

Then:

$C(r) =$ 

Define: 

MPS Transfer Matrix.

Then $\langle \psi | \psi \rangle = \lim_{N \to \infty} \mathrm{tr}\left((E_{II})^N \right)$.

Spectral dec: $E_{II} = \sum_{\mu=1}^{D^2} \lambda_\mu \, |r_\mu)(l_\mu|$; $\lambda_1 > \lambda_2 \geq \dots$

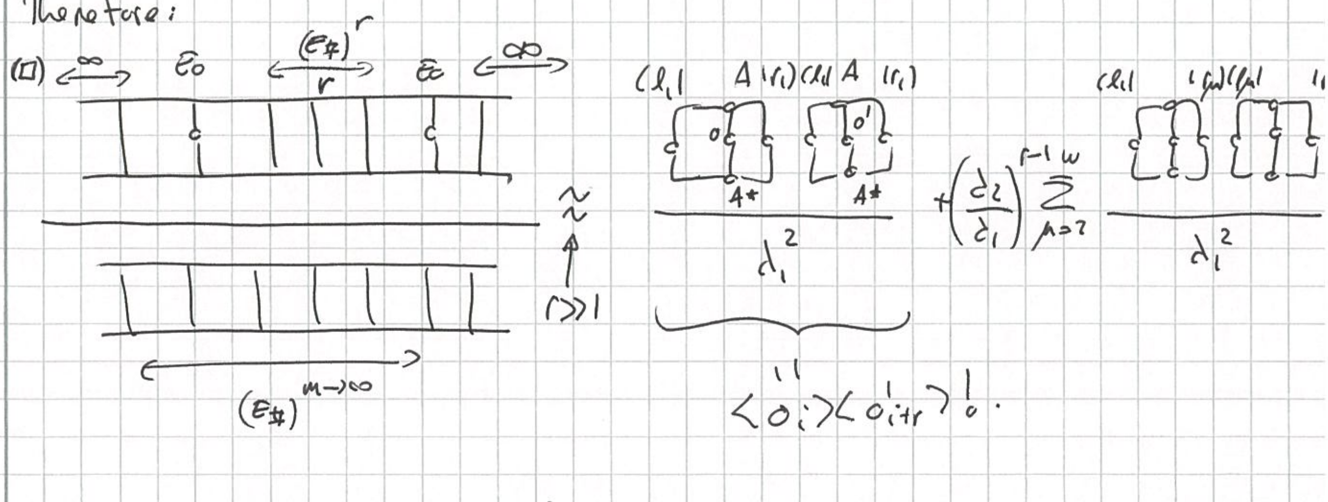
$(l_\mu | r_\nu) = \delta_{\mu\nu}$ (left/right eigenvectors).

Then: $(E_{II})^m = (\lambda_1)^m \sum_{\mu=1}^{D^2} \left(\frac{\lambda_\mu}{\lambda_1} \right)^m |r_\mu)(l_\mu|$ (assume λ_1 non-deg.)

For $m \gg 1 \Rightarrow (E_{II})^m \approx (\lambda_1)^m \left(|r_1)(l_1| + \left(\frac{\lambda_2}{\lambda_1} \right)^m \sum_{\mu=2}^{w} |r_\mu)(l_\mu| \right)$.

deg. of λ_2

Therefore:



$= \langle O_i \rangle \langle O'_{i+r} \rangle$!

—D.

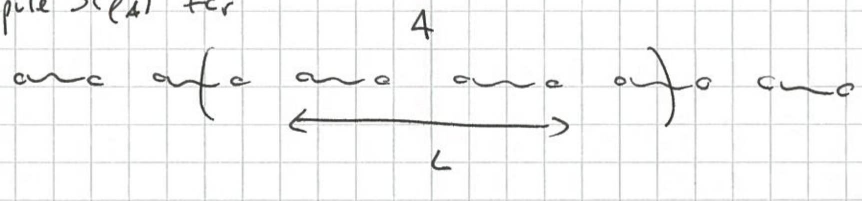
Therefore:

$$C(r) \approx \left(\frac{\lambda_2}{\lambda_1}\right)^{r-1} \sum_{\mu>2}^{w} \Big(\qquad \Big) = f(r)\cdot a\cdot e^{-r/\xi}$$

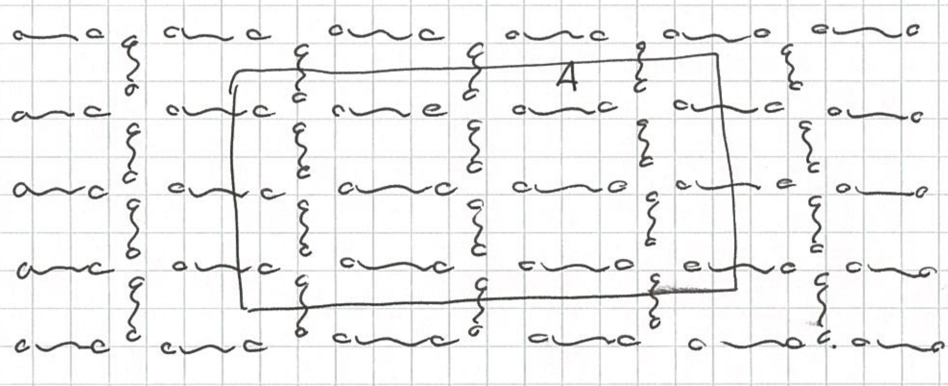
with $a = O(w)$, and $\boxed{\xi \equiv \dfrac{-1}{\log\left|\lambda_2/\lambda_1\right|}}$ MPS Corr. Length.

Exercises:

1) Compute $S(\rho_A)$ for



and



2) Compute the 3-point Corr. Funct. of an MPS:

$$C(r,s) \equiv \langle O_i\, O'_{i+r}\, O''_{i+r+s}\rangle - \langle O_i\rangle\langle O'_{i+r}\rangle\langle O''_{i+r+s}\rangle .$$

for $r \gg 1$, $s \gg 1$.

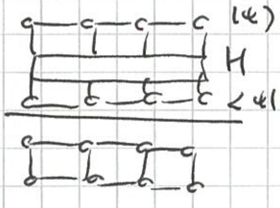
3.- MPS algorithms.

3.1) Density Matrix Ren-Group (DMRG).

*) DMRG → ground states. Originally developed by White 'al, using an RG picture. Later it was realized that it's a variational algorithm over MPS.

1) Task: for a finite MPS of N-sites, with bond dim. D, find the one that minimizes

$$E(|\psi\rangle) = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} =$$



for a given Hamiltonian H (ideally 1d, but could also be something else).

*) Comments:

(i) $|\psi\rangle \in$ MPS variational wavefunc; var. param ≡ tensor coeff.

(ii) $O(ND^2p)$ var. parameters.

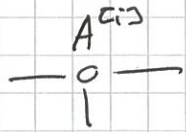
(iii) D ⇒ controls entang. & var. param.

(iv) Strategy of DMRG: sweep-optimization.

*) Algorithm:

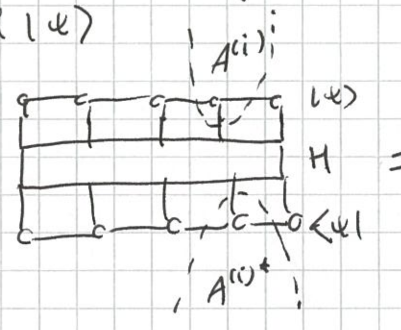
1) Fix ∀ tensor except at site "i". We will optimize this tensor:

$A^{[i]} \rightarrow$



2) Write $\langle\psi|H|\psi\rangle$

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

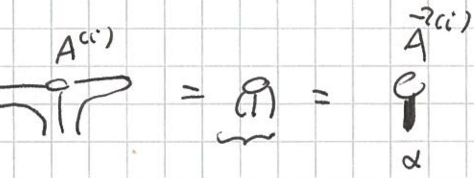


(obc, simpler).

Key!

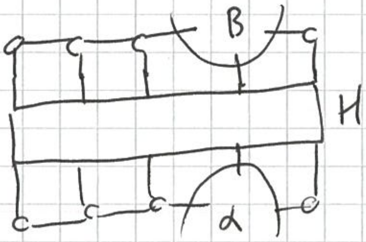
$$= \underline{\vec{A}^{(i)\dagger} \cdot H_{eff} \cdot \vec{A}^{(i)}}$$

where $\vec{A}^{(i)}$ is the vector



(fuse legs).

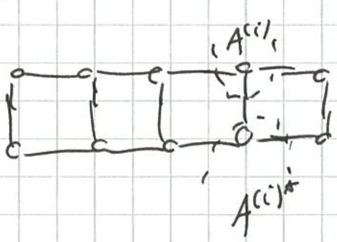
and H_{eff} is the TN for $\langle\psi|H|\psi\rangle$ after removing $A^{(i)}$ and $A^{(i)\dagger}$, written as a matrix:



$$\equiv \left(H_{eff}\right)_{\alpha\beta}$$

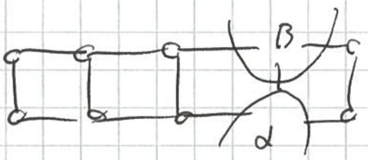
3) Similarly, write $\langle\psi|\psi\rangle$:

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



$$= \vec{A}^{(i)\dagger} \cdot N \cdot \vec{A}^{(i)}$$

where N is a <u>normalization matrix</u> given by



$$= (N)_{\alpha\beta}$$

4) We are then minimizing $E(|\psi\rangle) = \dfrac{\vec{A}^{(i)\dagger} \cdot H_{eff} \cdot \vec{A}^{(i)}}{\underbrace{\vec{A}^{(i)\dagger} \cdot N \cdot \vec{A}^{(i)}}_{\text{norm. constraint}}}$

This is equivalent to minimize the functional

$$F(|\psi\rangle) = \langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle = \vec{A}^{(i)\dagger} H_{eff} \vec{A}^{(i)} - \lambda \vec{A}^{(i)\dagger} N \vec{A}^{(i)}$$

λ: Lagrange mult. (constraint)

This is a <u>quadratic problem</u>. Minimizing:

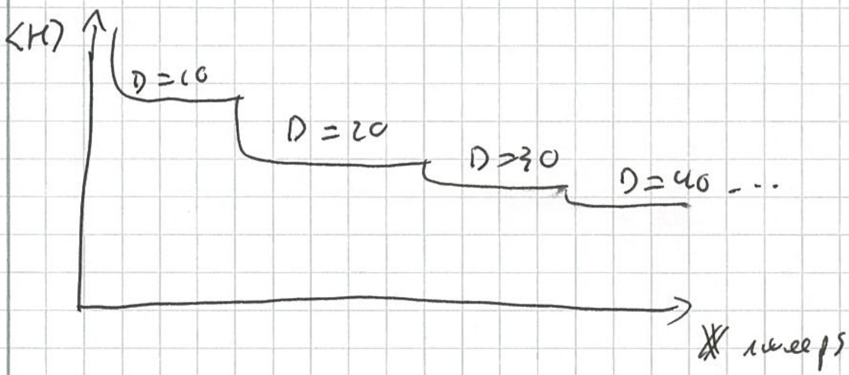
$$\frac{\partial F}{\partial \vec{A}^{(i)\dagger}} = 0 \Rightarrow H_{eff} \cdot \vec{A}^{(i)} - \lambda N \vec{A}^{(i)} = 0$$

$$\Rightarrow \boxed{H_{eff} \cdot \vec{A}^{(i)} = \lambda N \vec{A}^{(i)}}$$ <u>Generalized</u> <u>Eig. Problem</u>.

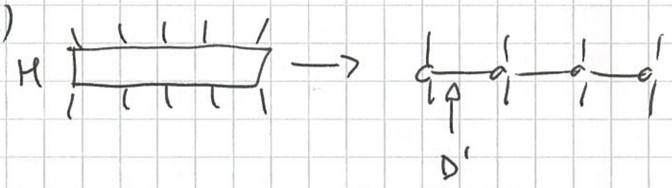
5) Solve the gen. eig. problem → find optimal $A^{(i)}$

6) Replace the new tensor, move to site "i+1", and repeat.

7) Iterate sweeping back and forward until convergence.

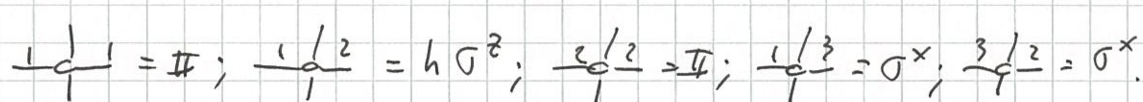


*) Remarks:

1) 

Matrix Product Operator (MPO).

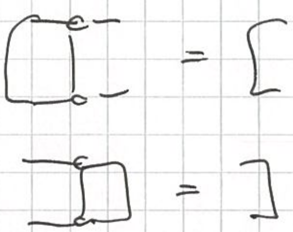
Example: $H = \sum_i \sigma_i^x \sigma_{i+1}^x + h \sum_i \sigma_i^z$



2) Comp. cost

$$\begin{cases} O(ND^3) & \text{obc} \\ O(ND^5) & \text{pbc} \end{cases} \qquad O(D^3) \text{ for infinite-DMRG.}$$

3) Stability: sometimes N is ill-conditioned. The solution is to work in a "canonical gauge" → $N = \mathbb{I}$ (obc). Gauge such that



∀ sites < "i"

∀ sites > "i".

Mixed Canonical Form.

(always possible).

3.2) Time-Evolving Block Decimation (TEBD)

*) Time-evol. of an MPS (Vidal' 2004) in canonical form

*) Task: given an initial MPS $|\psi(0)\rangle$, and a Hamiltonian

$$H = \sum_i h^{(i,i+1)}$$

Compute $|\psi(T)\rangle = e^{-iHT} |\psi(0)\rangle$.

*) Algorithm:

1) Write $H = \sum_i h^{(i,i+1)} = H_{odd} + H_{even}$

with $H_{odd} = \sum_{i \in odd} h^{(i,i+1)}$, $H_{even} = \sum_{i \in even} h^{(i,i+1)}$.

(sums of mutually-commuting terms).

2) Trotterize the time-evol. operator:

$$e^{-iHT} \underset{\delta t \ll 1}{=} \left(e^{-iH\delta t}\right)^{T/\delta t} \approx \left(e^{-iH_{odd}\delta t} e^{-iH_{even}\delta t}\right)^{T/\delta t} + O(\delta t^2) =$$

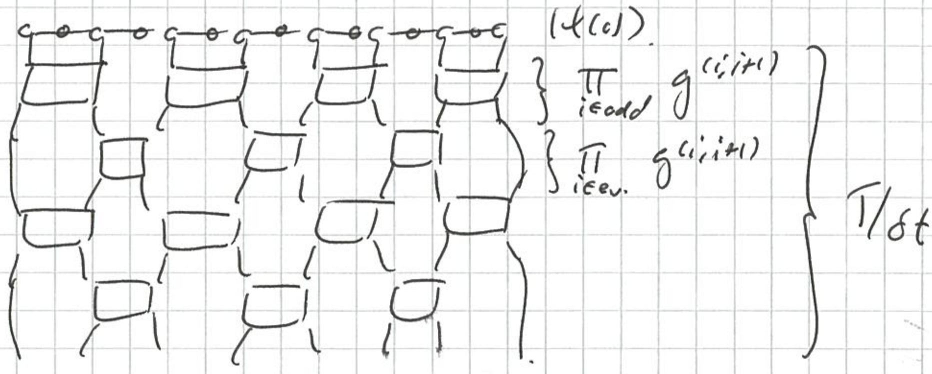
$$= \left[\left(\prod_{i \in odd} g^{(i,i+1)}\right)\left(\prod_{i \in even} g^{(i,i+1)}\right)\right]^{m = T/\delta t} + O(\delta t^2)$$

with $g^{(i,i+1)} \equiv e^{-ih^{(i,i+1)}\delta t}$ 2-body gate.

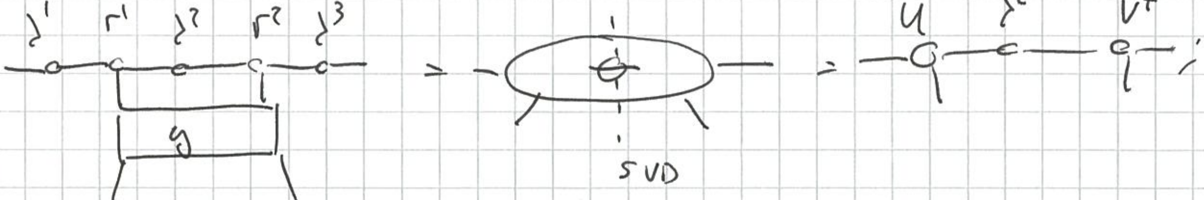
$\rightarrow$

3) Apply row-by-row to the MPS:

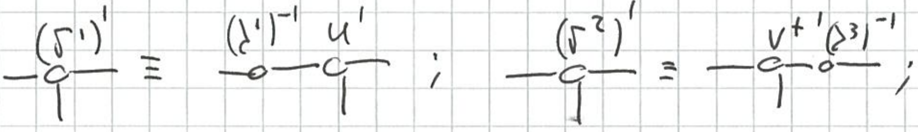
$|\psi(T)\rangle =$



4) For every 2-body gate, update as follows:



Truncate $\tilde{\lambda}^2$ in the D largest ones $\longrightarrow \lambda^{(2)'}$. (similarly U', $(V^\dagger)'$).



5) Apply for all required sites at each step until reaching time T.

*) <u>Remark</u>: it can also be used to approximate g.s. via imaginary-time evolution:

$$|\psi_0\rangle = \lim_{T\to\infty} \frac{e^{-HT}\,|\psi(0)\rangle}{\|\qquad\|^{1/2}}.$$