Quantum information: from qbits to space-time.

(Southampton, 23 - 25 May, 2016). My email: roman.orus@uni-mainz.de.

⊛ **Goal**: intro to q-info, entang. in many-body, TNs, and how all this relates to AdS/CFT and Gravitation.

⊛ Some references:

J. Eisert, arXiv: 1308.3318
N. Schuch, arXiv: 1306.5551
RO, arXiv: 1306.2164, arXiv: 1407.6592
Cirac & Verstraete, J. Phys. A 42, 504004 (2009).
Verstraete, Cirac, Murg, Adv. Phys. 57, 143 (2008)
U. Schollwöck, Annals of Physics 326, 96 (2011).

} Basic ones, ∃ more (I'll give more tomorrow).

+ „classics" such as Nielsen & Chuang on Q. Comp., etc.

⊛ We'll start from the very basic, and start building structure until ending up in quite complex things.

① Basics on Q.M. (refreshment).

⊛ All the information about a physical system is encoded in its wave function or quantum state: $|\psi\rangle \in \mathcal{H}$.

- For 2-level systems (e.g. spin-1/2):

$$|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle \,;\ \{|\uparrow\rangle, |\downarrow\rangle\} \text{ basis of } \mathcal{H} = \mathbb{C}^2,\ \alpha, \beta \in \mathbb{C}.$$

This defines a qubit, or quantum bit. Usually, $|\uparrow\rangle = |0\rangle$, $|\downarrow\rangle = |1\rangle$, and then $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$. (it's a superposition of 0's & 1's).

⊛ Usual stuff of Q.M.: measurements are projections on the state, evolutions are unitary, probabilities, etc.

→

⊛ *Composite Systems* : are obtained by *tensor product* of $\mathcal{H}$'s.

$|\psi_1\rangle \in \mathcal{H}_1$, $|\psi_2\rangle \in \mathcal{H}_2$; Composite system $|\psi_3\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 = \mathcal{H}_3$.

In terms of basis: (qbits)

$$\left.\begin{array}{l} \{|0\rangle_1, |1\rangle_1\} \in \mathcal{H}_1 \\ \{|0\rangle_2, |1\rangle_2\} \in \mathcal{H}_2 \end{array}\right\} \{|0\rangle_1 \otimes |0\rangle_2, |0\rangle_1 \otimes |1\rangle_2, |1\rangle_1 \otimes |0\rangle_2, |1\rangle_1 \otimes |1\rangle_2\} \in \mathcal{H}_3.$$

$\dim(\mathcal{H}_3) = \dim(\mathcal{H}_1) \cdot \dim(\mathcal{H}_2)$. → *product* of dimensions.

- Some possible states in $\mathcal{H}_3$ are:

$$\left\{\begin{array}{l} |\psi\rangle = |0\rangle_1 \otimes |0\rangle_2 \\ |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_1 \otimes |0\rangle_2 + |0\rangle_1 \otimes |1\rangle_2\right) \equiv |0\rangle_1 \otimes \overset{\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle).\ \swarrow}{|+\rangle_2}. \\ |\psi\rangle = \frac{1}{2}\left(|0\rangle_1 \otimes |0\rangle_2 - |0\rangle_1 \otimes |1\rangle_2 - |1\rangle_1 \otimes |0\rangle_2 + |1\rangle_1 \otimes |1\rangle_2\right). \\ |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_1 \otimes |0\rangle_2 + |1\rangle_1 \otimes |1\rangle_2\right). \\ \qquad \text{etc.} \end{array}\right.$$

⊛ Whenever $|\psi\rangle = |\phi\rangle_1 \otimes |\phi\rangle_2$, we say it's separable. Otherwise, we say it's *entangled*.

- Examples:

$$\left\{\begin{array}{l} \rightarrow |\psi\rangle = |0\rangle|0\rangle \quad \text{sep.} \\ \rightarrow |\psi\rangle = \frac{1}{2}\left(|0\rangle|0\rangle + |0\rangle|1\rangle + |1\rangle|0\rangle + |1\rangle|1\rangle\right) = |+\rangle|+\rangle \quad \text{sep.} \\ \rightarrow |\psi\rangle = \frac{1}{2}\left(|0\rangle|0\rangle - |0\rangle|1\rangle - |1\rangle|0\rangle + |1\rangle|1\rangle\right) = |-\rangle|-\rangle \quad \text{sep.} \\ \rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|0\rangle + |1\rangle|1\rangle\right) \quad \text{ent. (EPR Pair, Bell State)} \\ \rightarrow |\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle|1\rangle - |1\rangle|0\rangle\right) \quad \text{ent. (" \quad " , Singlet)} \end{array}\right.$$

- Entanglement is *non-local* and has no classical analoge.

- Entanglement *is a resource*

Ⓐ **Variational Principle**: given H (Hamiltonian) and E_0 its lowest energy eigenvalue, then

$$\langle\psi|H|\psi\rangle \geq E_0 \quad \forall|\psi\rangle.$$

Proof: $\langle\psi|H|\psi\rangle = \sum_i E_i \langle\psi|i\rangle\langle i|\psi\rangle = \sum_i E_i \underbrace{|\langle\psi|i\rangle|^2}_{\geq 0} \geq \dots$

$$\dots \underset{\substack{\uparrow \\ E_i \geq E_0 \ \forall i}}{\geq} \sum_i E_0 |\langle\psi|i\rangle|^2 = E_0 \sum_i |\langle\psi|i\rangle|^2 = E_0 \checkmark.$$

Ⓐ **Reduced density Matrix**: given a quantum state $|\psi\rangle$ for many parties (e.g. $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$), the rdm ρ of a subsystem is obtained by doing the partial trace on $|\psi\rangle\langle\psi|$ of the other subsystems (environment).

$$\rho_A = \mathrm{tr}_{(All-A)}(|\psi\rangle\langle\psi|) \equiv \sum_i \langle i|\psi\rangle\langle\psi|i\rangle$$, where $\{|i\rangle\}$ is a orthonormal basis for the $\mathcal{H}$ of "all - A".

- Example: $|\psi\rangle = \alpha|0\rangle|1\rangle + \beta|1\rangle|0\rangle$.

$$\rho_1 = \mathrm{tr}_2(|\psi\rangle\langle\psi|) = {}_2\langle 0|\psi\rangle\langle\psi|0\rangle_2 + {}_2\langle 1|\psi\rangle\langle\psi|1\rangle_2 =$$

$$= {}_2\langle 0|\left(|\alpha|^2 |01\rangle\langle 01| + |\beta|^2 |10\rangle\langle 10| + \alpha^*\beta |10\rangle\langle 01| + \beta^*\alpha |01\rangle\langle 10| \right)|0\rangle_2 +$$

$$+ {}_2\langle 1|\left(\quad " \quad\quad " \quad\quad " \quad \right)|1\rangle_2 =$$

$$= |\beta|^2 |1\rangle_1\langle 1| + |\alpha|^2 |0\rangle_1\langle 0| = \begin{array}{cc} \begin{pmatrix} |\alpha|^2 & 0 \\ 0 & |\beta|^2 \end{pmatrix} & \begin{array}{c} |0\rangle \\ |1\rangle \end{array} \\ \begin{array}{cc} |0\rangle & |1\rangle \end{array} & \end{array}.$$

- Properties:
  - (i) $\rho = \rho^\dagger$, $\mathrm{tr}(\rho) = 1$.
  - (ii) $\mathrm{eig}(\rho) \geq 0$
  - (iii) $\langle O\rangle_\rho \equiv \mathrm{tr}(O\cdot\rho)$ Expec. Values.
  - (iv) ρ contains all the info. available if I only look at the subsystem.

(2.-) Entanglement

Let's remind the definition:

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

$$|\psi\rangle \neq |\phi\rangle_A \otimes |\phi\rangle_B , \quad |\phi\rangle_A \in \mathcal{H}_A, \ |\phi\rangle_B \in \mathcal{H}_B .$$

⊛ Considerations:

(i) it can also be multipartite, e.g.: $|\psi\rangle \neq |\phi\rangle_A \otimes |\phi\rangle_B \otimes |\phi\rangle_C$, etc

(ii) a full classific. of ent. states is only possible in particular cases (e.g. 2, 3 qbits) → EPR (2 qubits), GHZ+W (3 qubits).

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

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

Therefore, it cannot be created locally. Formally one says that "entanglement does not grow under Local Op's & Classical Comm. (LOCC)" (includes measurements).

⊛ Bipartite pure states & Schmidt decomposition.

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

Theorem: ∃ always a decomp. such that

$$|\psi\rangle_{AB} = \sum_{\alpha=1}^{\chi} \lambda_\alpha \, |\alpha\rangle_A \, |\alpha\rangle_B$$

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

$\lambda_\alpha \equiv$ Schmidt coeff. $\chi \equiv$ Schmidt Rank. $= \min(d_A, d_B)$
($d_A = \dim(\mathcal{H}_A)$, $d_B = \dim(\mathcal{H}_B)$).

$\{|\alpha\rangle_A\}$, $\{|\alpha\rangle_B\}$ → Schmidt basis

→

Before proving it, <u>example</u>:

$$|\psi\rangle_{AB} = |0\rangle_A\,|0\rangle_B\,,\quad \chi=1,\ \lambda_1=1.$$

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

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

⊛ <u>Lemma</u>: $\boxed{\chi = 1 \iff |\psi\rangle_{AB} \text{ is separable}}$ (great!).

⊛ <u>Proof</u> of the Schmidt Dec:

$|\psi\rangle_{AB} = \sum_{ij} \psi_{ij}\,|i\rangle_A|j\rangle_B$; ψ_{ij} = Matrix. Let's do a <u>Singular Value Decomp.</u>:

$$\psi = U\,\Lambda\,V^\dagger,\ \text{with } U^\dagger U = \mathbb{I}_{d_A},\ V^\dagger V = \mathbb{I}_{d_B},\ \Lambda \text{ diag. } \chi\times\chi,$$

with real positive entries (<u>Singular values</u>)

$d_A \times d_B$ matrix

$\chi = \min(d_A, d_B)$.

Then: $$\psi_{ij} = \sum_{\substack{\alpha=1\\ \beta=1}}^{d_A,\,d_B} U_{i\alpha}\,\Lambda_{\alpha\beta}\,(V^\dagger)_{\beta j} = \sum_{\alpha=1}^{\overbrace{\min(d_A,d_B)}^{\chi}} U_{i\alpha}\,\lambda_\alpha\,(V^\dagger)_{\alpha j}$$

$\Lambda_{\alpha\beta} = \lambda_\alpha\,\delta_{\alpha\beta}$

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

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

⊛ <u>Comment</u>: χ is, in fact, a <u>measure of entang.</u>

→.

⊛ Von Neumann Entropy :

Given $|\psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B$, with rdm ρ_A & ρ_B, the von Neumann Entropy is

$$\boxed{S(\rho_A) = -\text{tr}(\rho_A \log \rho_A) = S(\rho_B).}$$ (also "entang. entropy")

In terms of the eigenvalues $\nu_{A\alpha}$ of ρ_A:

$$\boxed{S(\rho_A) = -\sum_{\alpha=1}^{\nu_A} \nu_\alpha \log \nu_\alpha .}$$

- Moreover, if $|\psi\rangle_{AB} = \sum_{\alpha=1}^{\chi} \lambda_\alpha |\alpha\rangle_A |\alpha\rangle_B$ (S.D) then.

$$\rho_A = \sum_{\alpha=1}^{\chi} \underbrace{|\lambda_\alpha|^2}_{\nu_\alpha} |\alpha\rangle\langle\alpha|_A \; ; \; \rho_B = \sum_{\alpha=1}^{\chi} \underbrace{|\lambda_\alpha|^2}_{\nu_\alpha} |\alpha\rangle\langle\alpha|_B$$ (direct!).

$$\boxed{\text{rank}(\rho_A) = \text{rank}(\rho_B), \text{ and they share the eigenvalues} \Rightarrow S(\rho_A) = S(\rho_B).}$$

- Moreover, $\boxed{S(\rho_A) \le \log \chi.}$ (easy to prove). This is saturated by a flat spectrum of Schmidt coefficients: $\boxed{|\psi^{max}\rangle_{AB} = \frac{1}{\chi}\sum_{\alpha=1}^{\chi} |\alpha\rangle_A |\alpha\rangle_B}$

↳ This is a Maximally Ent. State, like EPR for χ-level subsystems.

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

$$\begin{cases} \text{(a) invariant under LOCC} \\ \text{(b) continuous} \\ \text{(c) additive} : S(|\psi_{AB}\rangle \otimes |\phi_{A'B'}\rangle) = S(\psi_{AB}) + S(\phi_{A'B'}). \end{cases}$$

↳ Droppin (c) ∃ more: concurrence, Rényi entropies, etc.

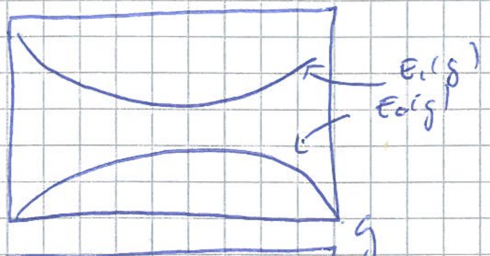
③.- Entang. in Quantum Many-Body Systems.

What happens when I have many particles at $T=0$?

⊛ Quantum phase transitions (descriptive):

$H = H(g)$. Let's plot the first 2 energy levels $E_1(g)$ & $E_0(g)$.

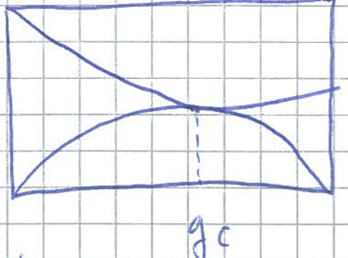
(a)



$\Delta(g) \equiv E_1(g) - E_0(g)$ (Gap) > 0 always.

Gapped phase, $\xi(g)$ finite $\forall g$.

(b)

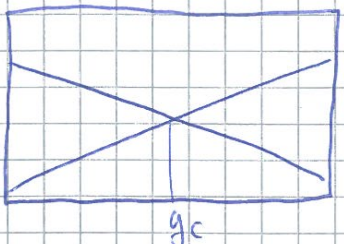


$\Delta(g=g_c)=0$, $\left.\frac{d^r E_0(g)}{dg}\right|_{g_c}$ continuous $(r<m)$.

$\left.\frac{d^m E_0(g)}{dg^m}\right|_{g_c}$ discontinuous.

Continuous QPT, $\xi(g_c) \to \infty$.

(c)



$\Delta(g=g_c)=0$, $\frac{d E_0(g)}{dg}$ discontinuous.

1st order QT, $\xi(g_c) = $ Finite.

⊛ In (b), $\exists$ a QPT $\Rightarrow$ it's at $T=0$, and caused only by quantum fluctuations.

At $g = g_c \Rightarrow \xi \to \infty \Rightarrow$ scale invariance ($\approx$ CFTs).

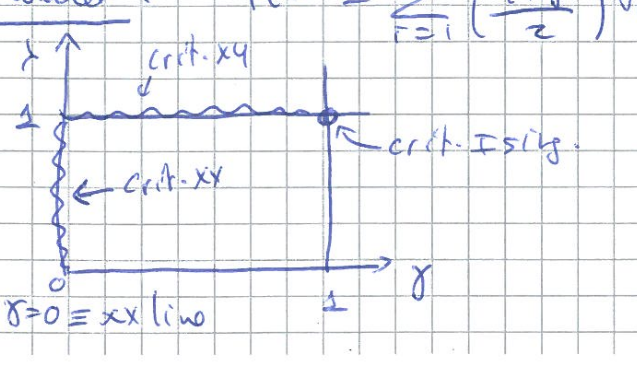
⊛ One can define critical exponents, universality classes, and so on.

⊛ Examples of ent. in many-body:

(a) 1d

- - - o o o o o - - - (spin chain, chain of fermions, etc).

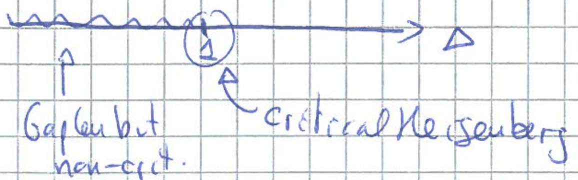
Example: XY-model:
$$H = -\sum_{i=1}^{\infty} \left(\frac{1+\gamma}{2}\right) \sigma_i^x \sigma_{i+1}^x + \left(\frac{1-\gamma}{2}\right) \sigma_i^y \sigma_{i+1}^y + \lambda \sigma_i^z.$$



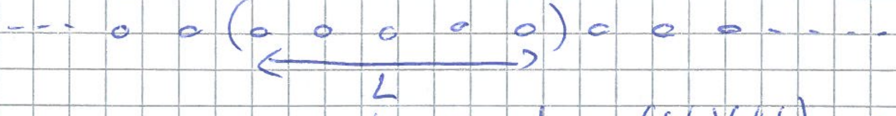
→

Example: Anisotropic Heisenberg model

$$H = \sum_{i=1}^{\infty} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z), \Delta \geq 1.$$



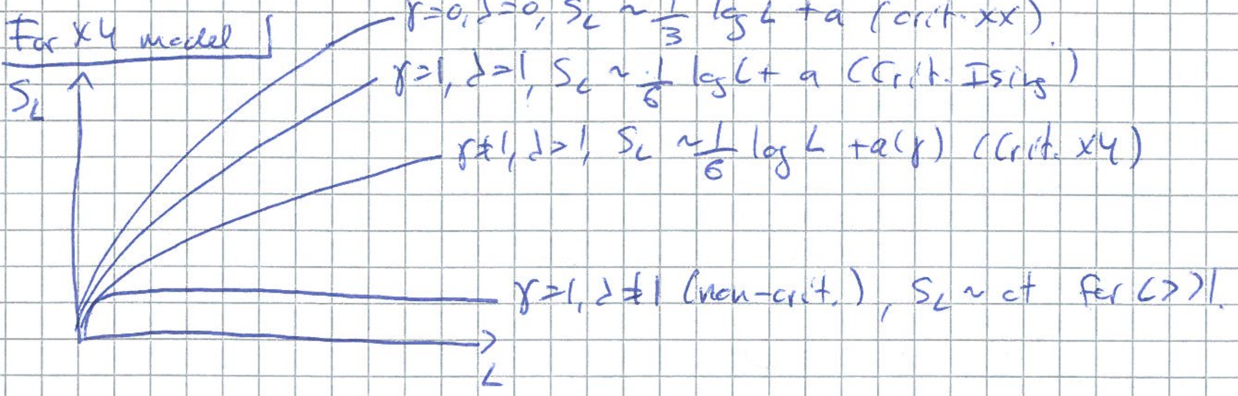
⊕ We will compute the entang. entropy of a block:



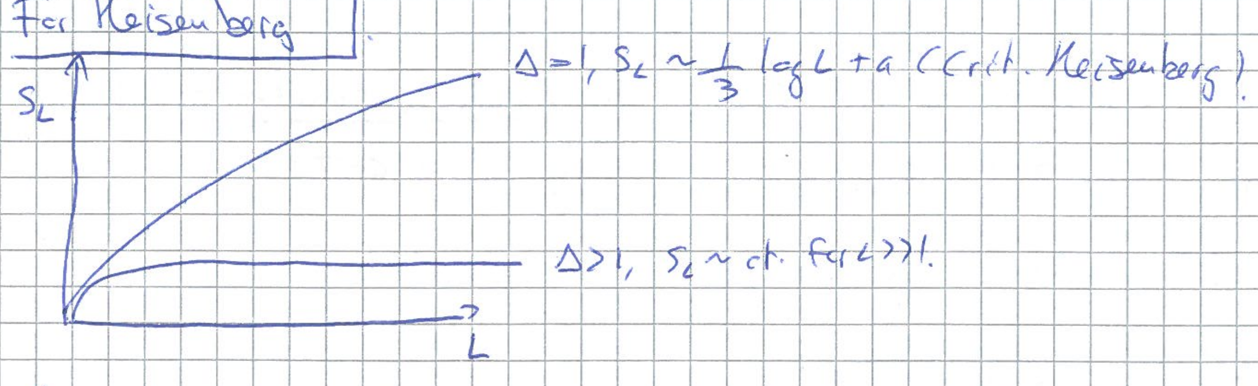
$$L \rightarrow \rho_L = tr_{N-L}(|\psi_0\rangle\langle\psi_0|) \longrightarrow S_L \equiv -tr(\rho_L \lg \rho_L).$$

Scaling? Critical vs non-Critical?

For XY model



For Heisenberg



This rings a bell:

(i) $S_L \sim cte$ for non-critical (ξ finite, $\Delta \neq 0$) $\rightarrow$ 1d area-law.

(ii) $S_L \sim \lg L$ for $\xi \rightarrow \infty$.

(iii) Pre factor of $\lg L \longleftrightarrow$ Universality class.

$\rightarrow$.

⑨

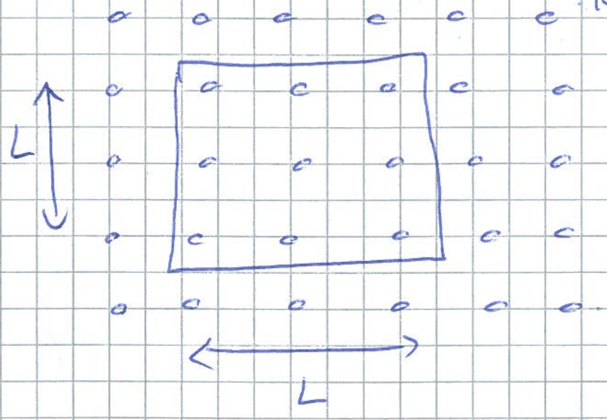
⊛ General result: Conformal Field Theory (Calabrese & Cardy)

For $L \gg 1$, $$\begin{cases} S_L \sim \frac{c}{3} \log L + a & \text{at quant. crit. points.} \\ S_L \sim \frac{c}{3} \log \xi + a & \text{close to criticality.} \end{cases}$$

$c \equiv$ Central charge of the $(1+1)$-dimensional CFT.

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

(b) 2d | In 2d: S_L of an $L \times L$ block. (Hamiltonians with local interactions)



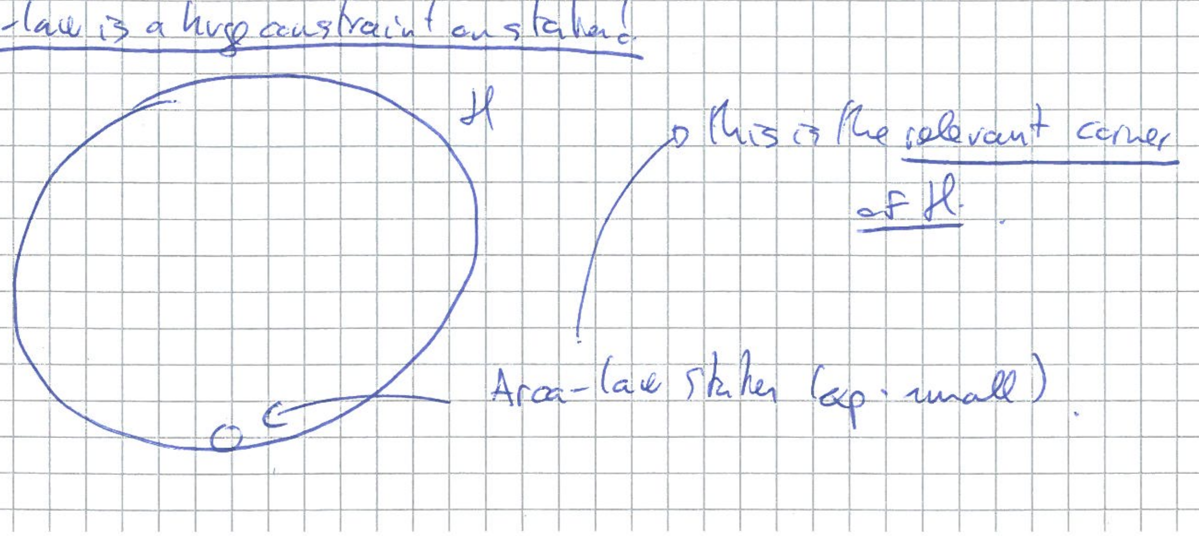
$\longrightarrow \rho_L = \text{tr}_{N-L}(|\psi_0\rangle\langle\psi_0|) \longrightarrow S_L = -\text{tr}(\rho_L \log \rho_L)$.

Generic Result: $\boxed{S_L \sim a \cdot L + O(1/L)}$

↳ at, and away from criticality.
this is a 2d-area-law (like Black-Hole Entropy!).

- For higher dims → similar conclusions.
- there are exceptions, e.g. 2d fermions, bose metals, etc.

⊛ ~~Thus~~ Area-law is a huge constraint on states!



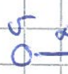
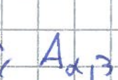
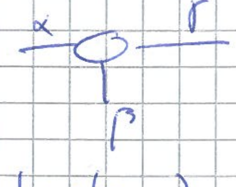
④.- Tensor Networks.

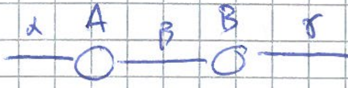
(!) The relevant corner in H satisfying the area-law → tensor network states.

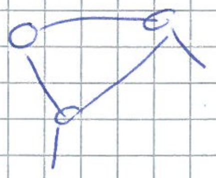
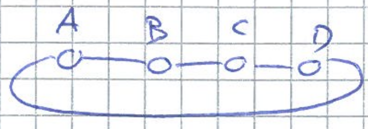
- **Tensor**: multidimensional array of ℂ numbers.

  e.g. v_α (vector), $A_{\alpha\beta}$ (matrix), $C_{\alpha\beta\gamma}$ (3-index tensor).

- **Diagrammatic notation:**

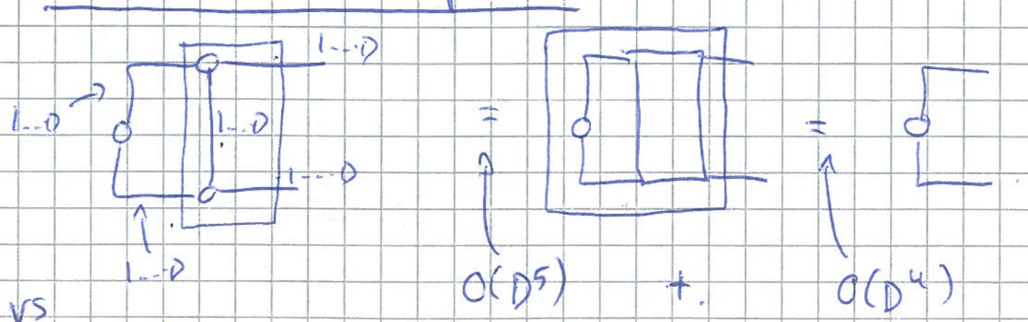
$v_\alpha \rightarrow$  ; $A_{\alpha\beta} \rightarrow$  ; $C_{\alpha\beta\gamma} \rightarrow$  .

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

Similarly,  , etc. Example:  =

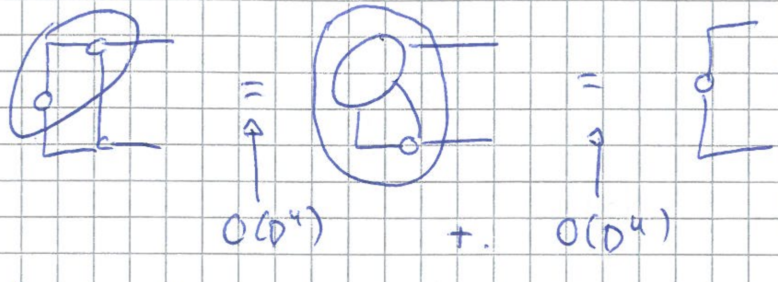
= tr(ABCD).

- **Contraction order is important:**



⇒ $O(D^5)$ operations

vs

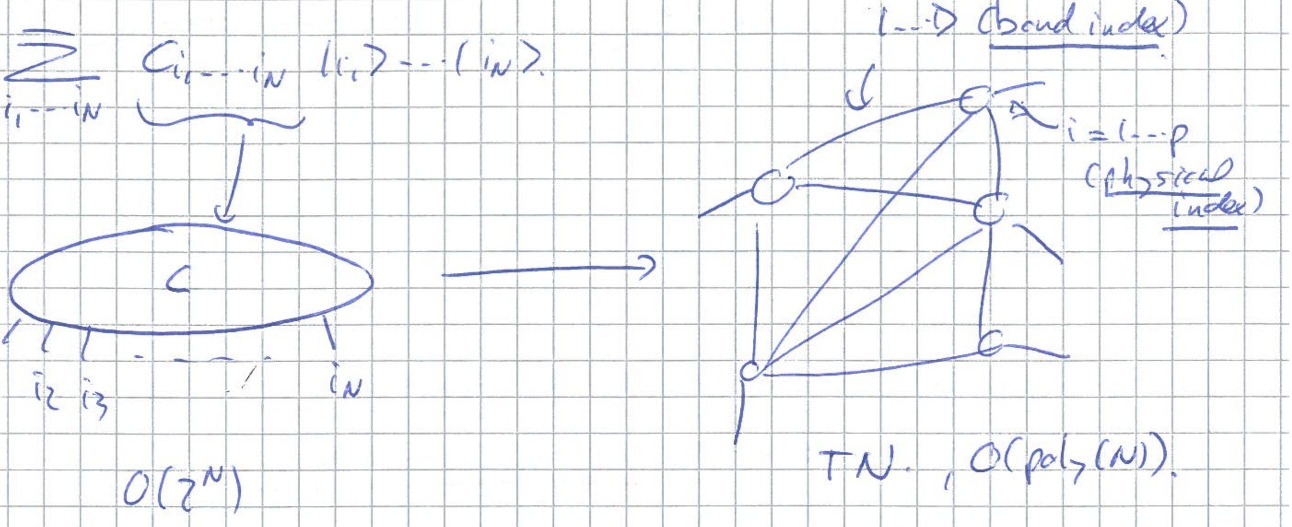


⇒ $O(D^4)$ operations!!!

Optimal contraction order → always pairwise contractions.

⊛ Idea of TNs: <u>break the wave function in fundamental pieces.</u>

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

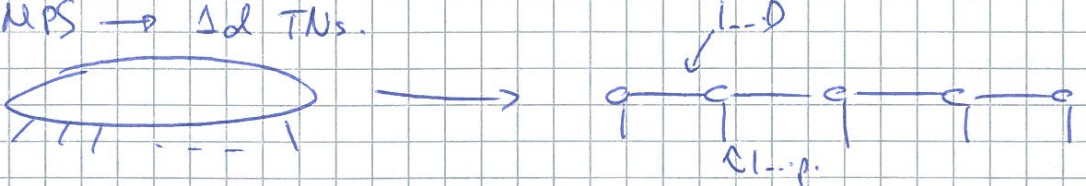


- Depending on the situation, the inherent TN structure of $|\psi\rangle$ will be one or the other.

Moreover, TN accounts for the entanglement amount & structure in $|\psi\rangle$.

⑤.- Matrix Product States (MPS).

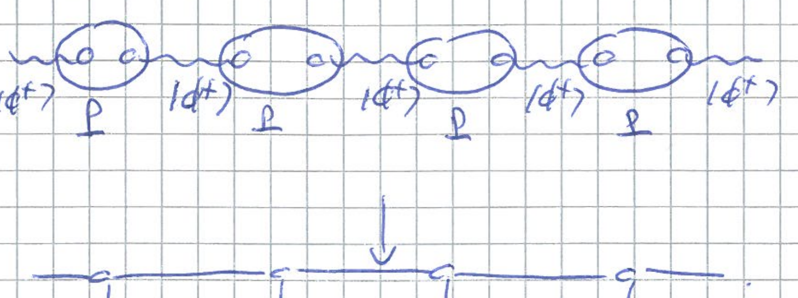
⊛ MPS → 1d TNs.



<u>Motivation (0)</u>: the number of parameters is $O(N)$.

<u>Motivation (1)</u>: ansatz generalizing mean-field,  taking into account correlations.

<u>Motivation (2)</u>: can be seen as a collection of singlets with projectors.

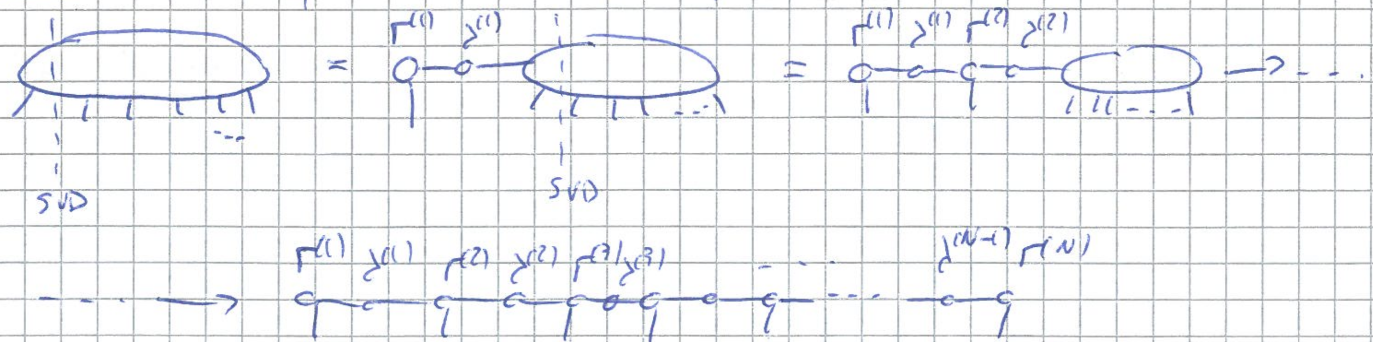


$$|\phi^+\rangle = \frac{1}{\sqrt{D}} \sum_{\alpha=1}^{D} |\alpha\rangle|\alpha\rangle.$$

$$(P)^{i}_{\alpha\beta} = |i\rangle\langle\alpha\beta| = P.$$

→e.

Motivation (3): sequential Schmidt Decompositions.

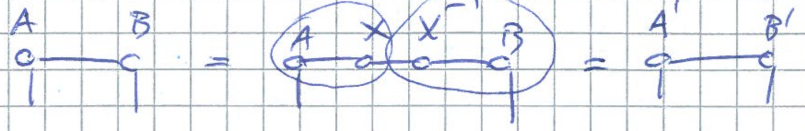


If ∀ Schmidt rank is bounded by a constant D, then this is also an MPS. They call this the MPS Canonical Form.

- For a system with low entanglement: D ~ ct. Otherwise, D grows.

⊛ Properties:

(i) Gauge invariance:



Same state, different tensors.

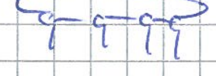
(ii) $\boxed{S_L(|\psi_{mps}\rangle) \leq 2 \log \chi}$ (I'll prove this in 2d tomorrow!).

this is a 1d area-law $\Rightarrow$ $\boxed{\text{MPS are good for gapped 1d Systems.}}$

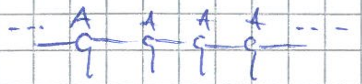
(one can actually put this formally).

(iii) obc

pbc



infinite system:



(or other unit cells).

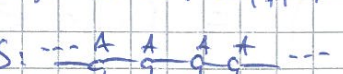
(iv) $\boxed{\xi \text{ is finite for an MPS}}$

→

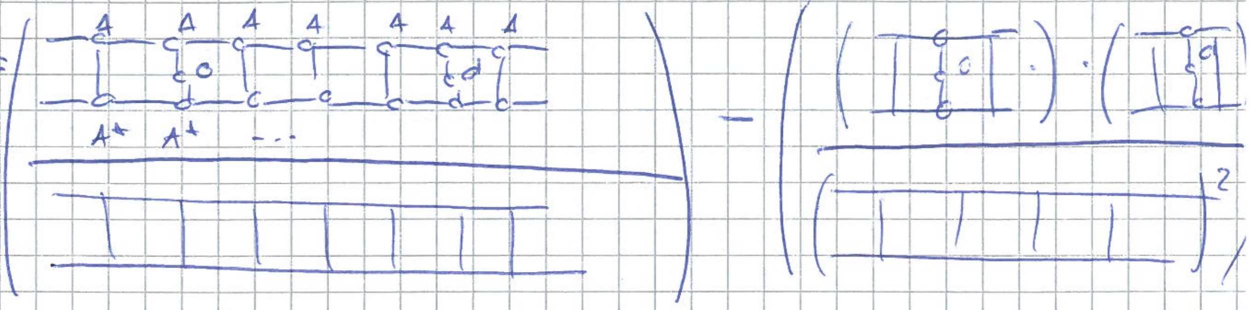
▸ **Proof:**

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

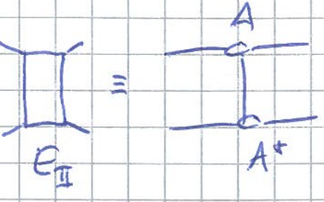
MPS:



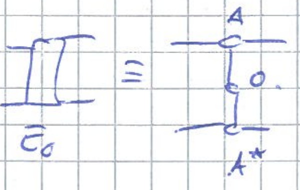
then: $C(r) =$



Define



MPS transfer matrix ;



then: $\langle\psi|\psi\rangle = \lim_{N\to\infty} \mathrm{tr}\left((E_{II})^N \right)$; $E_{II} = \sum_{\mu=1}^{D^2} \lambda_\mu \underbrace{|r_\mu)(l_\mu|}$ $\lambda_1 \geq \lambda_2 \geq \dots$

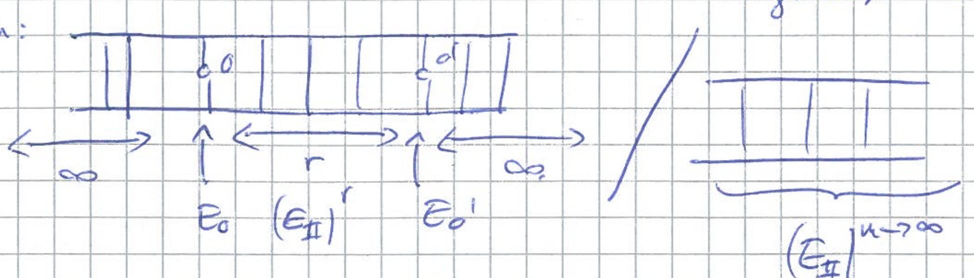
$(l_\mu|r_\nu) = \delta_{\mu\nu}$. (right- and left-eigenvectors.

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

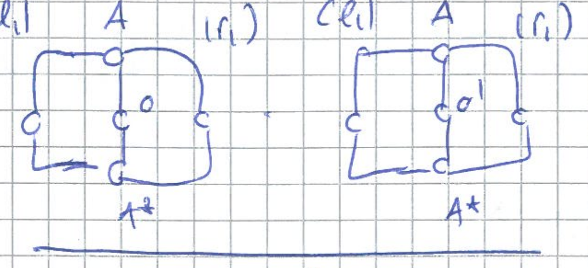
degeneracy of λ_2.

Then:

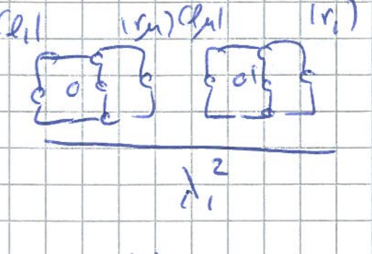


$\approx$ $r \gg 1$

$\approx$



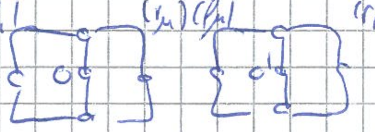
$+ \left(\frac{\lambda_2}{\lambda_1}\right)^{r-1} \sum_{\mu=2}^{w}$



(the rest cancels!).

The First term is nothing but $\langle O_i \rangle \langle O'_{i+r} \rangle$. Therefore:

$$C(r) \approx \left(\frac{d_2}{d_1}\right)^{r-1} \sum_{\mu=2}^{\omega} \frac{\square}{d_1^2} = f(r)\, a \cdot e^{-r/\xi}.$$

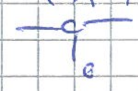


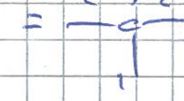
with $a = O(\omega)$, and $\boxed{\xi = \frac{-1}{\log|d_2/d_1|}}$ MPS corr. length

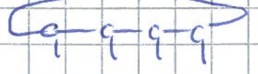
(—)

⊛ Examples:

(i) **GHZ** $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|0\cdots0\rangle + |1\cdots1\rangle\right)$, $\square = \square = \frac{1}{2^{1/2N}}$,

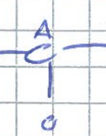


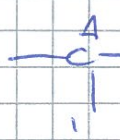


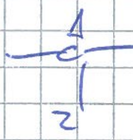

pbc.

(ii) **AKLT**: unique g.s. of $H = \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2$ spin = 1.

$\square = \sigma^z$, $\square = \sqrt{2}\,\sigma^+$, $\square = -\sqrt{2}\,\sigma^-$.







etc. (eg cluster states, Majumdar-Gosh...).

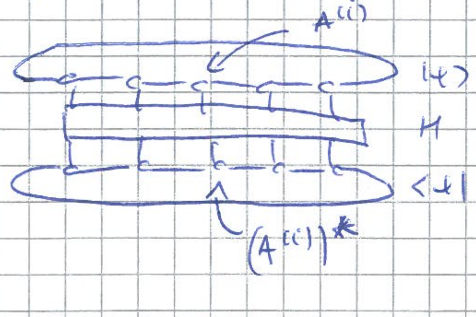
Ⓐ MPS Optimization: DMRG Algorithm:

- **Task**: for a *finite* MPS of N sites with band dimension D, find the one that minimizes $\langle\psi|H|\psi\rangle / \langle\psi|\psi\rangle$. → Algorithm to approx. ground states.

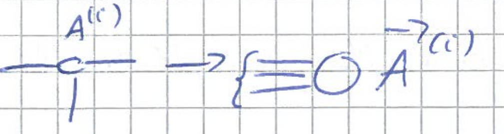
- **Optimal Strategy**: sweep-optimization.

1) Fix ∀ tensor except at site "i". Optimize this tensor: $A^{[i]} \rightarrow$

2) Write $\langle\psi|H|\psi\rangle = \square = \vec{A}^{(i)\dagger} \cdot H_{eff} \cdot \vec{A}^{(i)}$

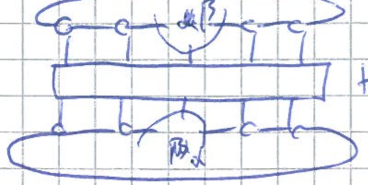


→

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

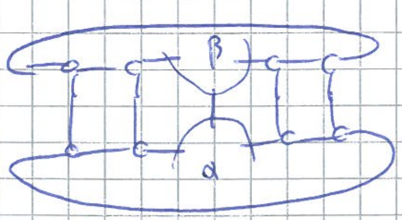
(fuse legs).

- Heff = TN for $\langle\psi|H|\psi\rangle$ after removing $A^{(i)}$ & $(A^{(i)})^*$:



$= (\text{Heff})_{\alpha\beta}$

3) Write $\langle\psi|\psi\rangle = \vec{A}^{(i)\dagger} \cdot N \cdot \vec{A}^{(i)}$, N = Normalization matrix.



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

4) Minimize $F = \langle\psi|H|\psi\rangle - \lambda\langle\psi|\psi\rangle = \vec{A}^{(i)\dagger}\, \text{Heff}\, \vec{A}^{(i)} - \lambda\, \vec{A}^{(i)\dagger} N \vec{A}^{(i)}$

$\uparrow$ Lagrange mult.

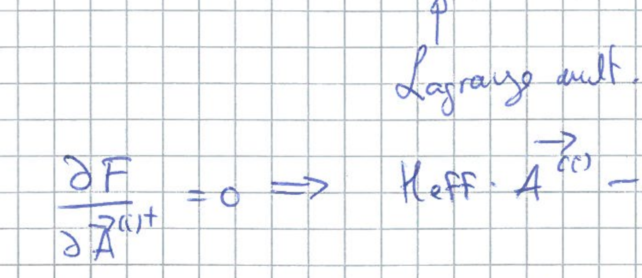
$$\frac{\partial F}{\partial \vec{A}^{(i)\dagger}} = 0 \Longrightarrow \text{Heff} \cdot \vec{A}^{(i)} - \lambda N \vec{A}^{(i)} = 0 \Rightarrow \boxed{\text{Heff}\, \vec{A}^{(i)} = \lambda N \vec{A}^{(i)}}$$

Generalized Eig. Problem.

5) Solve the g.e.p. → <u>find $A^{(i)}$</u>.

6) Replace tensor $A^{(i)}$ at site "i", & move to "i+1" & repeat.

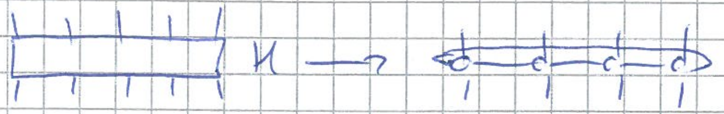
The algorithm follows by sweeping over the whole system. At every iteration step, the $\langle H\rangle$ decreases. Typically one gets plots like this:



This is the DMRG Algorithm (S. White).

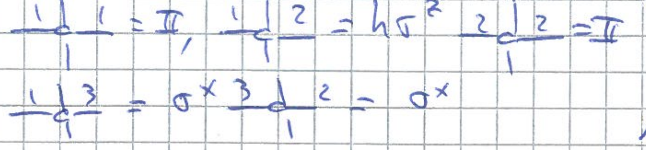
(Can also be generalized to minimize distance, time evol., etc.)

- **Comment**: H can normally be written as a Matrix Product Operator (MPO):



this simplifies a lot!

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



)

- **Comment**: $O(D^3)$ for obc, $O(D^5)$ for pbc.

- There are also many ways to improve the stability (e.g. canonical form).
- one can also do time evolution (TEBD, t-DMRG, etc).