MPS & PEPS — Autrans summer school
David Perez-Garcia (notes © 2016 Toby Cubitt)
Note Title 11/07/2016

Fix $D\times D$ matrices $A_1,\dots,A_d$

$$|MPS_A\rangle \propto \sum_{i_1,\dots,i_N=1}^{d} \mathrm{tr}(A_{i_1}\cdot A_{i_2}\cdots A_{i_N})\,|i_1,\dots,i_N\rangle$$

Expectation value of observable θ_r on site r:

$$\frac{\langle MPS_A|\,\theta_r\otimes \mathbb{1}_{rest}\,|MPS_A\rangle}{\langle MPS_A|MPS_A\rangle}$$

$$\langle MPS_A|\,\theta_r\,|MPS_A\rangle$$

$$= \sum_{\substack{i_1\dots i_N\\ j_1\dots j_N}} \overline{\mathrm{tr}(A_{i_1}\dots A_{i_N})}\,\mathrm{tr}(A_{j_1}\dots A_{j_N})\,\langle i_1\dots i_N|\,\theta_r\,|j_1\dots j_N\rangle$$

$$= \sum_{\alpha,\beta}\cdots\sum_{\substack{i_{r+1}\\ j_{r+1}}} A^\dagger_{i_{r+1}} \sum_{\substack{i_r\\ j_r}} \langle i_r|\theta_r|j_r\rangle A_r^\dagger\Big(\cdots$$

$$\cdots\Big(\sum_{\substack{i_2\\ j_2}} A^\dagger_{i_2}\Big(\sum_{\substack{i_1\\ i_2}} A^\dagger_{i_1}\,|\alpha\rangle\langle\beta|\,A_{i_1}\Big)A_{j_2}\Big)\cdots A_{j_r}\Big)A_{j_{r+1}}\cdots$$

$$= \sum_{\alpha,\beta} \langle\alpha|\,E\circ\cdots\circ E\circ E_r\circ E\cdots E(|\alpha\rangle\langle\beta|)\,|\beta\rangle$$

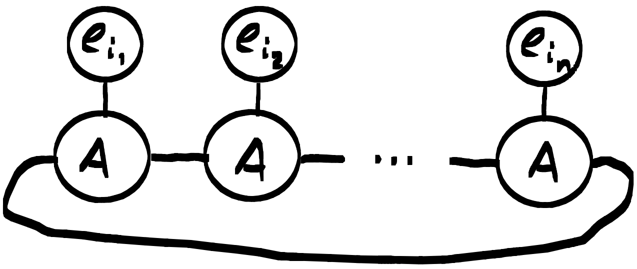
Transfer operator:

$$E(X) = \sum_i A_i^\dagger X A_i$$

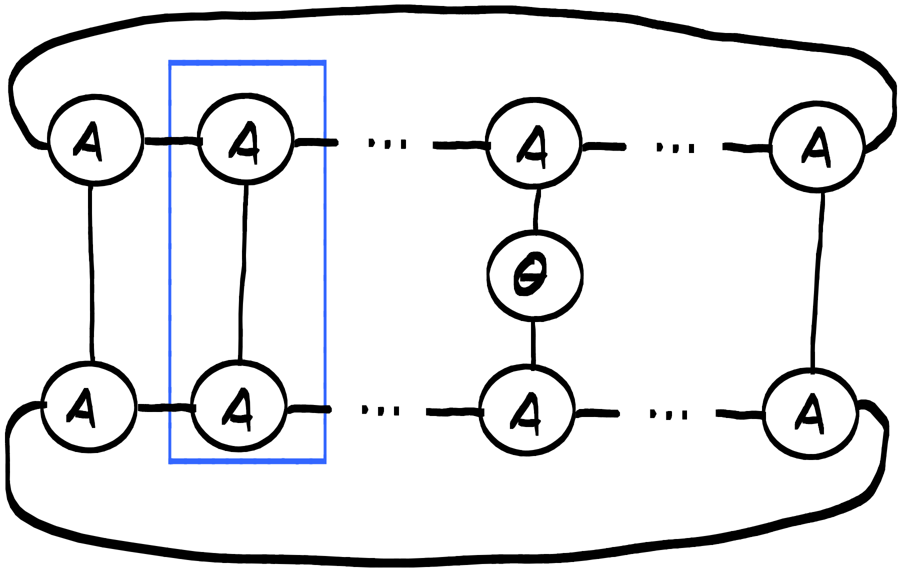
$$E_\theta(X) = \sum_{i,j} \langle i|\theta|j\rangle A_i^\dagger X A_j$$

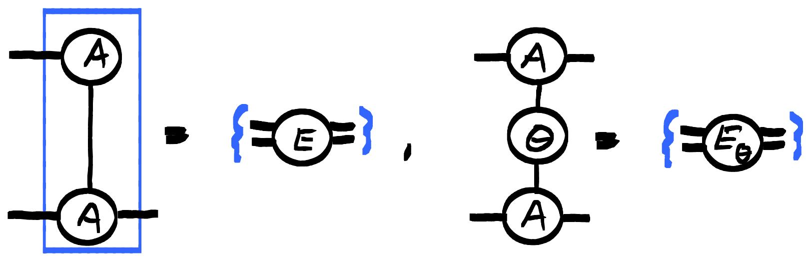
$$= \sum_{\alpha,\beta} \langle\alpha|\,E^{n-r}\circ E_\theta\circ E^{r-1}\,|\beta\rangle.$$

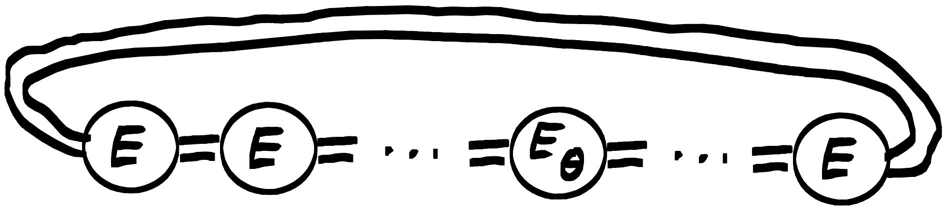
In the usual graphical notation for tensor contractions,

$|MPS_A\rangle =$ 

$\langle MPS_A | \Theta_r | MPS_A \rangle$

$=$ 



$=$ 

E is the matrix of lin. op. $\mathcal{E} : M_D \to M_D$ in canonical basis

CP map

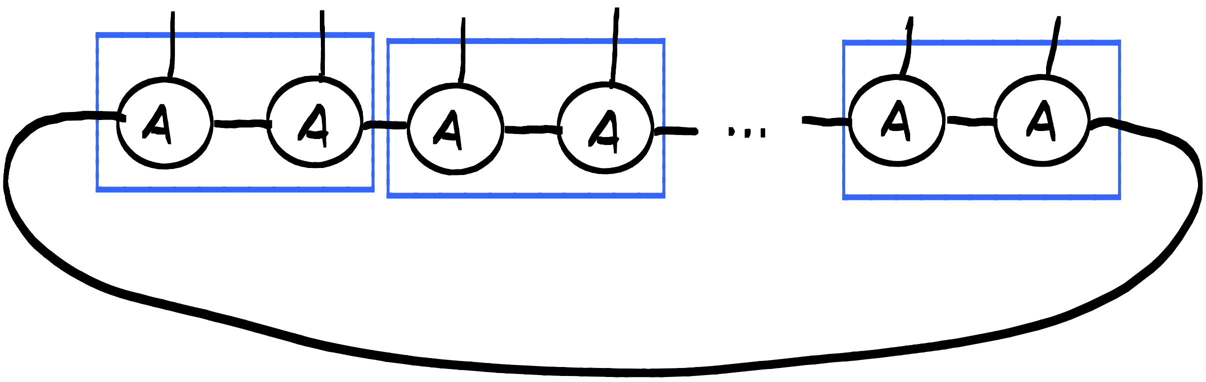
"MPS theory = CP map theory"

Thm Two sets of Kraus ops. $\{A_i\}$, $\{B_i\}$ define same CP map $\Leftrightarrow$ $\exists$ unitary U s.t.

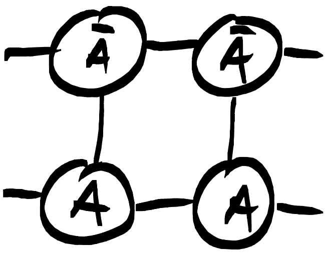
$$A_i = \sum_j U_{ij} B_j$$

$$\Updownarrow$$

Renormalisation in MPS



Associated CP map



$$= \mathcal{E}^2$$

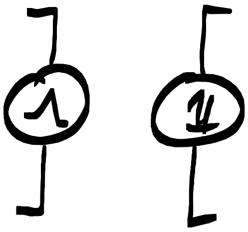
Renormalisation fixed points : $\lim_{n\to\infty} \mathcal{E}^n$

i.e. sol$^{\underline{ns}}$ of $\mathcal{E}^2 = \mathcal{E}$.

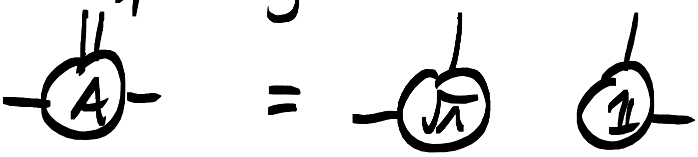
Assume $\mathcal{E}$ has

- unique eigval of max modulus (=1 wlog)
  i.e. spec $\mathcal{E} = \{1\} \cup D(0,\delta)$ $\delta<1$
- diagonal & full-rank fixed pt
- $\mathcal{E}$ is trace-preserving

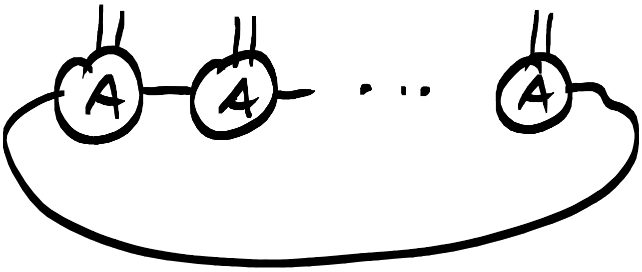
$\mathcal{E}^{\infty}(X) = \mathrm{tr}(X)\,\Lambda$ =



Corresponding A:

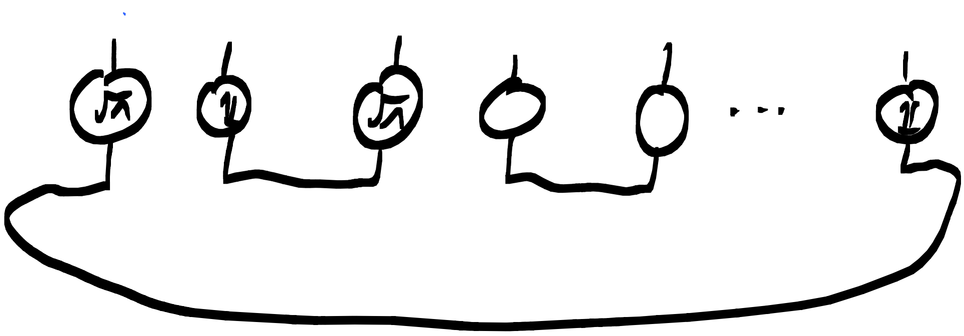


MPS for RG fixed pt:



$|\psi_\lambda\rangle = \sum_i \sqrt{\lambda_i}\,|ii\rangle$

=



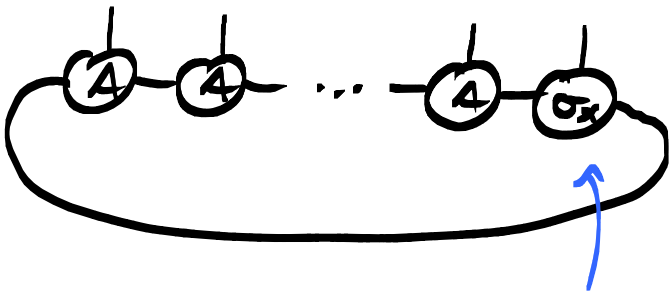
$= |\psi_\lambda\rangle^{\otimes n}$

Examples

- $A_0 = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}$ $\quad A_1 = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$

  $|MPS_A\rangle = |0\cdots0\rangle + |1\cdots1\rangle$ GHZ

- $A_0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \mathbb{1}$ $\quad A_1 = \begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}$



$= |W\rangle = |10\cdots0\rangle + |010\cdots0\rangle + \cdots + |0\cdots01\rangle.$

non-periodic b.c.

- AKLT

  $A_0 = \sigma_x \quad A_1 = \sigma_y \quad A_2 = \sigma_z$

Fundamental Thm

$$|MPS_A\rangle = |MPS_B\rangle \Leftrightarrow ??$$

Freedoms in A:

- A_i, $B_i = Y A_i Y^{-1}$, clearly $|MPS_A\rangle = |MPS_B\rangle$
- $A_i = \left(\begin{array}{c|c} B_i & D_i \\ \hline 0 & C_i \end{array}\right)$ $\quad \tilde{A}_i = \left(\begin{array}{c|c} B_i & 0 \\ \hline 0 & C_i \end{array}\right)$

$$|MPS_A\rangle = |MPS_{\tilde{A}}\rangle$$ (because of tr)

Exercise

Whenever have common invariant subspace S for all A_i, $\exists$ MPS representation of same state with $\tilde{A}_i = P_S A_i P_S + P_{S^\perp} A_i P_{S^\perp}$ block diagonal.

Now repeat this on each block
$\rightarrow$ canonical form:

$$\begin{pmatrix} \mu_1 \square & & & & 0 \\ & \mu_2 \square & & & \\ & & \square & & \\ & & & \ddots & \\ 0 & & & & \mu_n \square \end{pmatrix}$$

and no other inv. subspaces

μ's: normalisation so $\| \square \| = 1$.

What does this imply for CP-map?
For one block, CP map is <u>irreducible</u>, i.e. spec $\subseteq \{1\} \cup D(0,\delta) \cup \{\alpha_p\}$

$\{1\}$: always there

$\{\alpha_p\}$: simple eigvals, p^{th} roots of 1, p divisor of D

Now block sites (i.e. take powers of $\mathcal{E}^n$) to kill $\{\alpha_p\}$ part (i.e. $\alpha_p^n = 1$)

→ new inv. subspaces

→ block-decompose, rinse, repeat ...

$\vdots$

$$\rightarrow \begin{pmatrix} \square & & & \\ & \square & & \\ & & \ddots & \\ & & & \square \end{pmatrix}$$

CP map in each block is primitive

Only need to block <u>fixed</u> number of sites, dependent on matrix dimension.

<u>Def</u> (Primitive)

$$\operatorname{spec} \mathcal{E} \subseteq \underbrace{\{1\}}_{\text{simple}} \cup D(0,\delta) \qquad \delta < 1$$

& left & right fixed points full rank

If a MPS has a primitive transfer op. (i.e. single block in canonical form), call it "<u>injective</u>".

<u>Summary:</u> any MPS is a sum (with weights μ) of injective MPS.

Observation

$XX^\dagger$ fixed point of $\mathcal{E}^\dagger$ (X invertible)

$$XX^\dagger = \mathcal{E}^\dagger(XX^\dagger) = \sum_{i=1}^{d} A_i XX^\dagger A_i^\dagger$$

$$\Rightarrow \mathbb{1} = \sum_i \underbrace{X^{-1} A_i X}_{\tilde{A}_i} \underbrace{X^\dagger A_i^\dagger (X^\dagger)^{-1}}_{\tilde{A}_i^\dagger}$$

$$\tilde{\mathcal{E}}(Y) := \sum_{i=1}^{d} \tilde{A}_i^\dagger Y \tilde{A}_i \quad \text{is CPTP}$$

Since $X^{-1} A_i X$ defines same MPS as A_i, wlog can assume $\mathcal{E}$ is CPTP

If Q is fixed pt of $\mathcal{E}$,

$Q = U \Lambda U^\dagger$, can also assume fixed pt. is Λ (diagonal & full-rank).

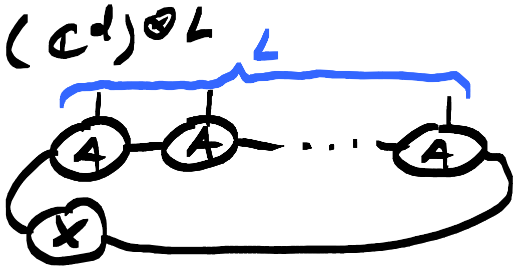
diagonal & full-rank

Thm

Let $|\Psi(A)\rangle$ be injective MPS.
Then $\exists L_0 \in \mathbb{N}$ s.t. $\forall L \ge L_0$ the map

injectivity length

$$\Gamma : M_D \longrightarrow (\mathbb{C}^d)^{\otimes L}$$
$$X \longmapsto$$



maps boundary conds. to states

$$= \sum_{i_1,\dots,i_L=1}^{d} \mathrm{tr}(X A_{i_1} \cdots A_{i_L}) \, |i_1 \dots i_L\rangle$$

is injective.

Furthermore, L_0 can be taken $\le D^4 - 1$ (quantum Wielandt Thm).

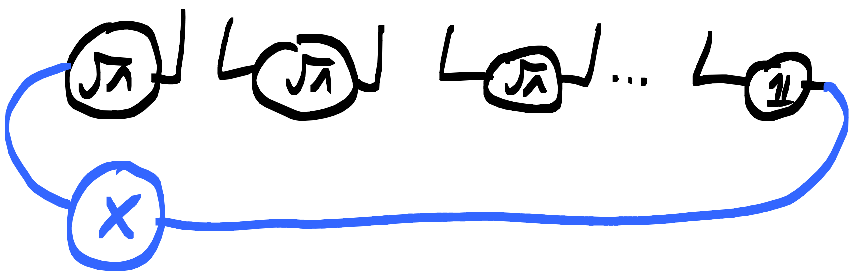
Proof idea:

primitivity: spec $= \{1\} \cup \{\le \delta\}$

L sites, CP map is $\mathcal{E}^L = \mathcal{E}^\infty + O(e^{-L})$

$\mathcal{E}^\infty = \mathrm{tr}(X)\Lambda$

Associated MPS is:



$X \longmapsto \sqrt{\Lambda}\, X \otimes \sim\!\sim$ clearly injective

But $\mathcal{E}^L$ is exp. close to this, & injectivity stable under small perturbations $\Rightarrow$ $\mathcal{E}^L$ injective.

For this argument, need $L \sim O(1/\delta)$.
To get L independent of δ much harder.

Note expect generic $\Gamma : \mathbb{C}^{d_1} \longrightarrow \mathbb{C}^{d_2}$ to be injective for $d_2 \geq d_1$

$\Rightarrow$ expect generic injectivity length $L_0 = O(\log D)$.

Can prove this (non-trivial).

Classical Wielandt:

A stochastic map

A primitive if $\exists \nu$: A^ν has strictly +ve coeff.

min of such $\nu = \nu(A)$ primitivity index

Wielandt Thm: $\nu(A) \leq D^2 - 2D - 1$.

Thm. already in CPTP form wlog

Two injective MPS $|\Psi(A)\rangle, |\Psi(B)\rangle$ with bond dimensions D_a, D_b satisfy

1. $\langle \Psi(A) | \Psi(A) \rangle \longrightarrow 1$ same for B

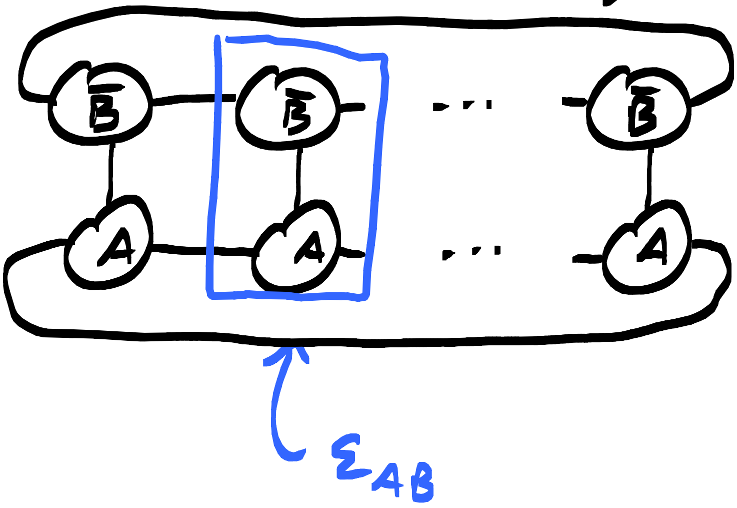
2. $$\lim_{N \to \infty} \langle \Psi(A) | \Psi(B) \rangle = \begin{cases} 1 & \text{or} \\ 0 \end{cases}$$

Moreover, in this case $D_a = D_b$ & $\exists \theta$, unitary U s.t. $A_i = e^{i\theta} U B_i U^\dagger$

Proof:

$$\langle \Psi(A) | \Psi(A) \rangle = \mathrm{tr}(\mathcal{E}^N) \longrightarrow 1$$

$$\langle \Psi(B) | \Psi(A) \rangle = \mathrm{tr}(\mathcal{E}^N_{AB})$$

$=$ 

$$\mathcal{E}_{AB}(X) = \sum_{i=1}^{d} B_i^\dagger X A_i$$

Let λ be eigval of $\mathcal{E}_{AB}$

X eigvect. s.t. $\sum_{i=1}^{d} B_i^\dagger X A_i = \lambda X$

fixed pt. of CP map for A

$$|\lambda \, \mathrm{tr}(X \Lambda_A X^\dagger)|^2 = \Big|\sum_{i=1}^{d} \mathrm{tr}(B_i^\dagger X A_i \Lambda_A X^\dagger)\Big|^2$$

$$= \Big|\sum_i \mathrm{tr}(\underbrace{X A \sqrt{\Lambda_A} \sqrt{\Lambda_A}}_{C} \underbrace{X^\dagger B_i^\dagger}_{D^\dagger})\Big|^2$$

$$\leq \Big(\sum_i \mathrm{tr}(X A_i \Lambda_A A_i^\dagger X^\dagger)^{1/2} \, \mathrm{tr}(B_i X \Lambda_A X^\dagger B_i^\dagger)^{1/2}\Big)^2$$

Cauchy-Schwartz $\quad \mathrm{tr}(C D^\dagger) \leq \mathrm{tr}(C C^\dagger)^{1/2} \, \mathrm{tr}(D D^\dagger)^{1/2}$

$$\leq \Big(\sum_i \mathrm{tr}(X A_i \Lambda_A A_i^\dagger X^\dagger)\Big)\Big(\sum_i \mathrm{tr}(B_i X \Lambda_A X^\dagger B_i^\dagger)\Big)$$

C.S. again for $\sum_i a_i b_i$

$$= \mathrm{tr}(X \Lambda_A X^\dagger)$$

choosing convention:

$$\sum_i A_i \Lambda_A A_i^\dagger = \Lambda_A$$

$$\sum_i B_i^\dagger B_i = \mathbb{1}$$

(opposite one to earlier — oops!)

$$\therefore |\lambda| \leq 1$$

If $\forall \lambda,\ |\lambda| < 1 \Rightarrow \langle \psi(A) | \psi(B) \rangle \xrightarrow[N\to\infty]{} 0$

$$\mathrm{tr}(\mathcal{E}_{AB}^N) \leq \lambda^N$$

If $\exists \lambda,\ |\lambda| = 1$

$\Rightarrow$ equality in Cauchy-Schwartz

$\Rightarrow \alpha X A_i = B_i X$ for some α $(*)$

$$\alpha \sum_i B_i^\dagger X A_i = \sum_i B_i^\dagger B_i X = X \Rightarrow \alpha = 1.$$

From $(*)$

$$|\alpha| \sum_i A_i^\dagger X^\dagger X A_i = \sum_i X^\dagger B_i^\dagger B_i X = X^\dagger X$$

$$\sum_i A_i^\dagger X^\dagger X A_i = \mathcal{E}_A(X^\dagger X)$$

$\Rightarrow X^\dagger X = \mathbb{1}$ since $\mathcal{E}_A$ has unique f.p.

Similar argument shows $D_A = D_B$

$\Rightarrow X$ unitary. $\square$

Recap:

$$|\Psi(A)\rangle = \sum_{i_1 \ldots i_N = 1}^{d} \mathrm{tr}(A_{i_1} \ldots A_{i_N}) \, |i_1 \ldots i_N\rangle$$

wlog
$$A_i = \begin{pmatrix} \mu_1 \boxed{A_i^1} & & & \\ & \mu_2 \boxed{A_i^2} & & \\ & & \ddots & \\ & & & \mu_b \boxed{A_i^b} \end{pmatrix}$$

with all A^b orthogonal: by Thm either identical or orthog. If identical, can just combine those blocks and sum μ's wlog $\leftarrow$ because of $\mathrm{tr}(A_{i_1} \cdots A_{i_N})$

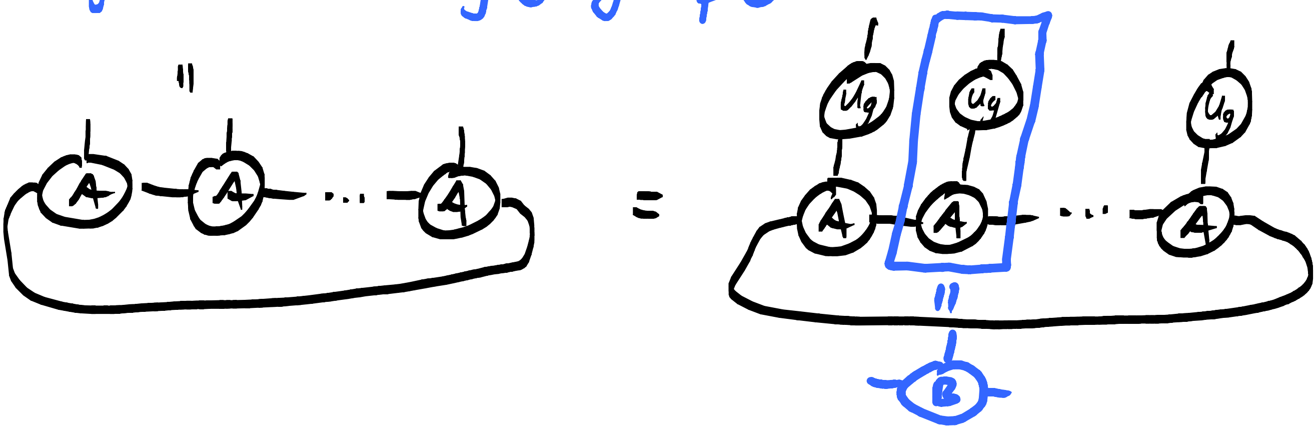
$$\mathcal{E}_j(X) = \sum_i A_i^{j\dagger} X A_i^j \quad \text{primitive } \forall j.$$

Application: Characterisation of symmetries

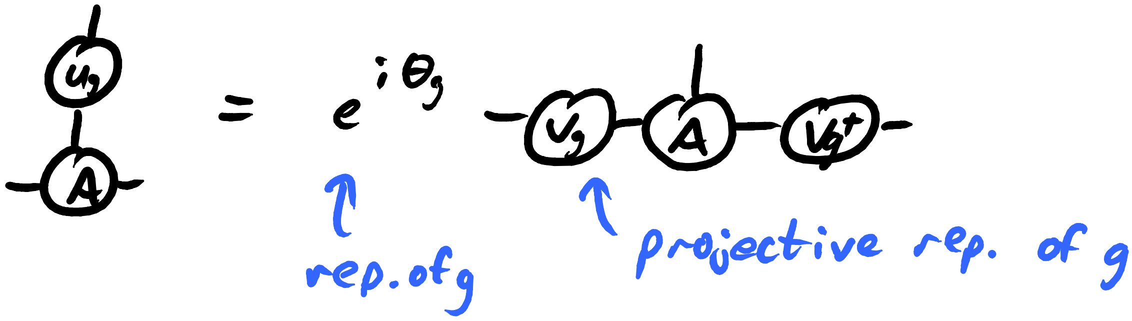
$$|\Psi(A)\rangle = U_g^{\otimes N} |\Psi(A)\rangle \quad \forall g, N$$

injective

$g \in$ group G



$\Rightarrow \forall g \ \exists V_g, \theta_g$ s.t.



Exercise

AKLT $\qquad A_{0,1,2} = \frac{1}{\sqrt{3}} \sigma_{z,x,y}$

$$G = \mathbb{Z}_2 \times \mathbb{Z}_2$$

$$U_{(1,0)} = \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix} \qquad U_{(1,1)} = \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix}$$

$$U_{(0,1)} = \begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix} \qquad U_{(0,0)} = \begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$$

$$\left.\begin{array}{ll} V_{(0,0)} = \mathbb{1}, & V_{(1,0)} = \sigma_z \\ V_{(0,1)} = \sigma_x, & V_{(1,1)} = \sigma_y \end{array}\right\} \text{projective rep.}$$

Hamiltonians in 1D

Hastings + Arad et al.:
g.s. of finite-range gapped Hamiltonians
$\approx |MPS\rangle$.

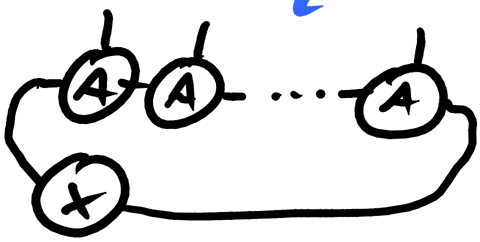
Want to show converse:
any $|MPS\rangle$ is g.s. of a gapped
finite-range H ("parent H").

Parent H

$|\psi(A)\rangle$ MPS (injective) can generalise

$G_L = \text{range}(\Gamma_L)$

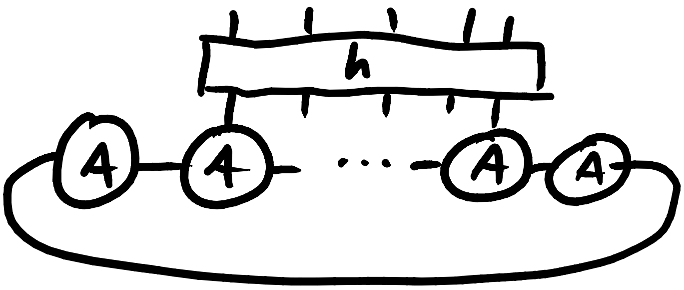
$\Gamma_L(X)$

$= \Big\{$  $: X \in M_D \Big\}$

vector space $\subset (\mathbb{C}^d)^{\otimes L_0}$
will be injectivity length $+1 \leq D^4$

$h := P^{\perp}_{G_{L_0+1}}$ Parent $H := \sum_i \tau_i(h) \otimes \mathbb{1}_{rest}$
translation by i

$h \geq 0$,

$h|\psi(A)\rangle =$  $= 0$

$\Rightarrow |\Psi(A)\rangle$ is g.s of H

& H is frustration-free.

<u>Def</u> Let $H = \sum_i h_i$ $\qquad h_i = \tau_i(h)$

H is called frust.-free if

$\forall$ g.s. $|\Psi\rangle$ of H, $\forall i$: $|\Psi\rangle$ is g.s. of h_i

<u>Thm</u>

If $L_0 \geq$ injectivity length $+1$, then parent H has $|\Psi(A)\rangle$ as unique g.s. & is gapped.

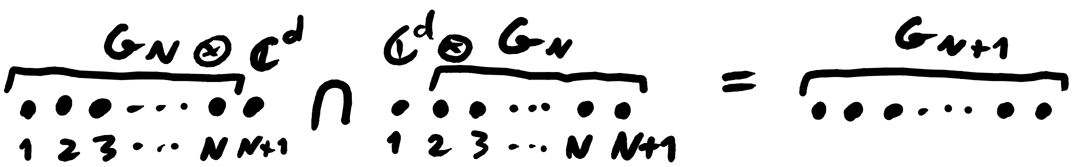
<u>Proof</u>

- Uniqueness of g.s.

  Step 1: <u>intersection property</u>

  $$G_N \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes G_N = G_{N+1}$$

  $$\left(\equiv G_{[1,N]} \otimes \mathbb{C}^d_{N+1} \cap \mathbb{C}^d_1 \otimes G_{[2,N+1]} = G_{[1,N+1]} \right)$$



$$G_N \otimes \mathbb{C}^d = \ker(h \otimes \mathbb{1})$$

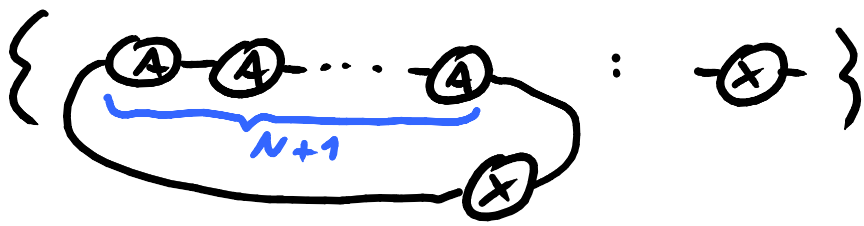
$$\mathbb{C}^d \otimes G_N = \ker(\mathbb{1} \otimes h)$$

$$G_N \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes G_N = \ker(h \otimes \mathbb{1} + \mathbb{1} \otimes h)$$

Proof of intersection property

$G_N \otimes \mathbb{C}^d =$ 

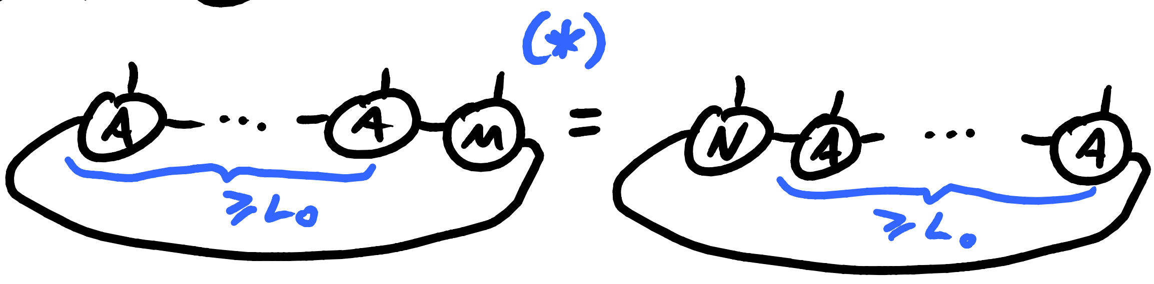
$\mathbb{C}^d \otimes G_N =$ 

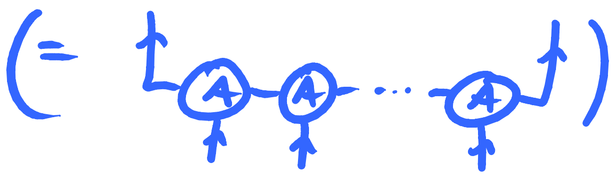
$G_{N+1} =$ 

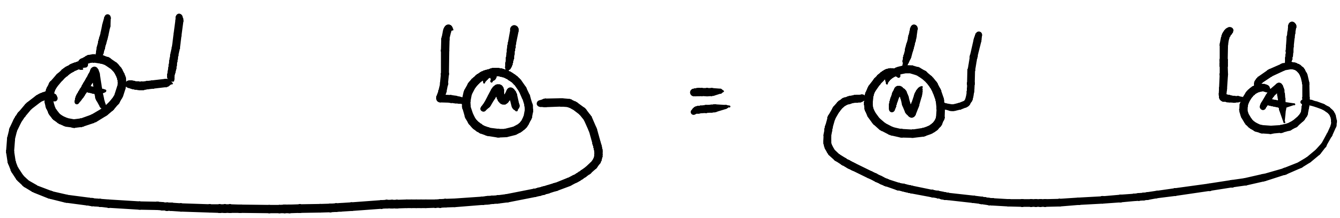
$\Rightarrow G_{N+1} \subseteq G_N \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes G_N$

Let $|\psi\rangle \in G_N \otimes \mathbb{C}^d \cap \mathbb{C}^d \otimes G_N$

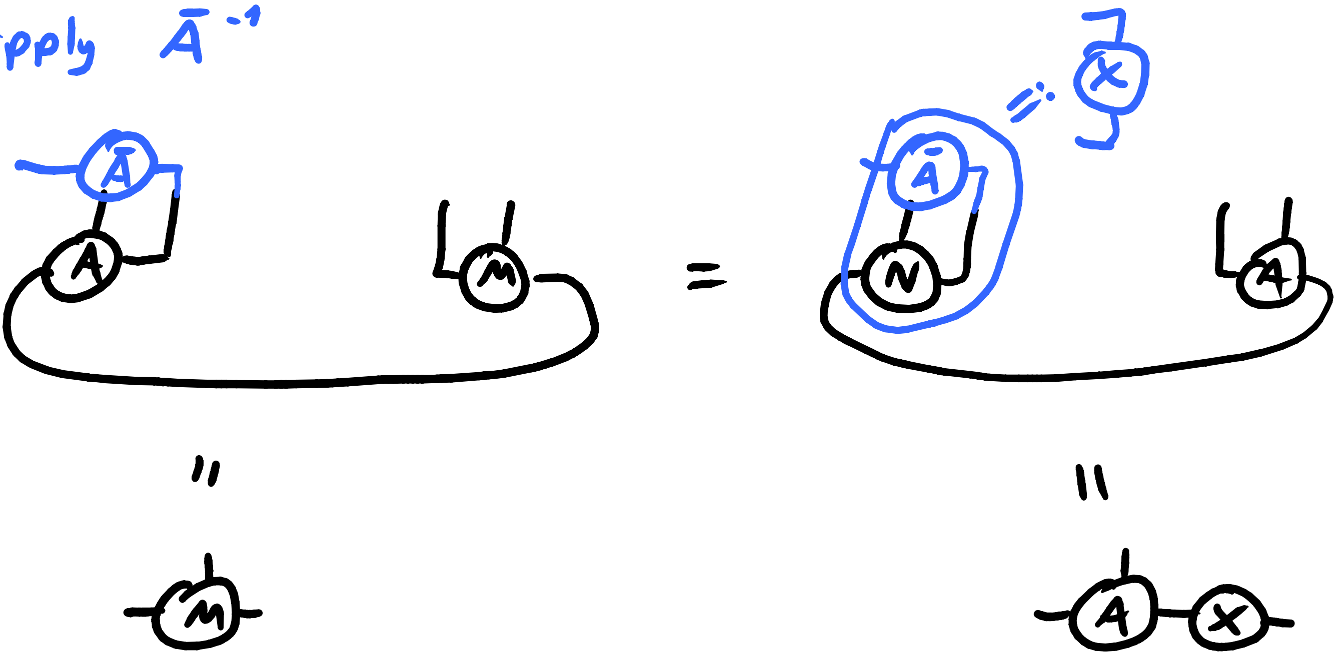
$\Rightarrow \exists$  ,  s.t.

$|\psi\rangle =$ 

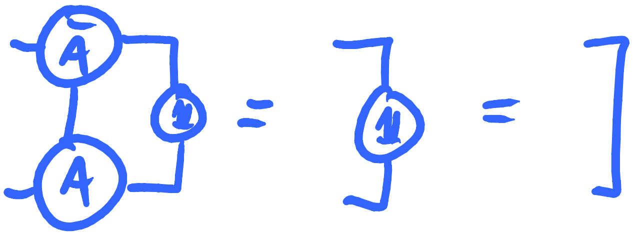
Apply Γ^{-1}  to A's.



Apply $\bar{A}^{-1}$



using



$\rightarrow$ plug this in $(*)$ $\Rightarrow$ $|\Psi\rangle \in G_{N+1}$.

After step 1:

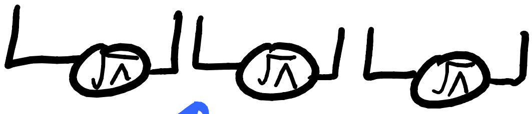
$$H_{[1,N]} = \sum_{i=1,\dots,N-(l_0+1)} \tau^i(h) \otimes \mathbb{1}_{rest}, \quad \ker(H_{[1,N]}) = G_N$$

$$\ker(H_{[1,N]}) = \text{g.s. } H_{[1,N]}$$

Step 2: similar tricks with periodic b.c. terms $\Rightarrow$ g.s. is unique $= |\Psi(A)\rangle$

Proof idea for gap:

By blocking r sites,

$|\psi(A)\rangle \underset{\varepsilon}{\approx}$  ...

unique g.s. of commuting Ham.

$h = \mathbb{1} - |\sqrt{\Lambda}\rangle\langle\sqrt{\Lambda}|$, $\quad H = \sum_i h_i$

(parent H of this product state)

Commuting $\Rightarrow$ gap ≥ 1.

Parent H of $|\psi(A)\rangle$ almost commuting

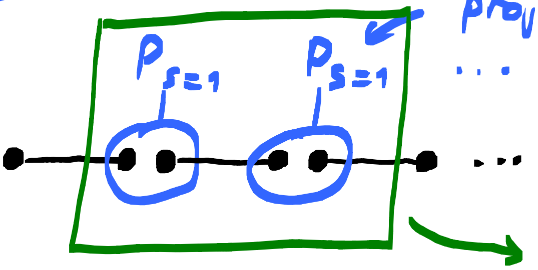
$\Rightarrow$ gapped $\square$

AKLT Hamiltonian

$\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$

$\frac{1}{2} \otimes \frac{1}{2} = 1 \oplus 0$

projector onto anti-sym. subspace



$2 \oplus \underbrace{1 \oplus 0}$

reduced state has full support here (not immediately obvious)

$h = P_{s=2}$

proj. onto spin 2 part is parent H

$$h = P_{s=2} = \vec{S}_i \cdot \vec{S}_{i+1} + (\vec{S}_i \cdot \vec{S}_{i+1})^2$$