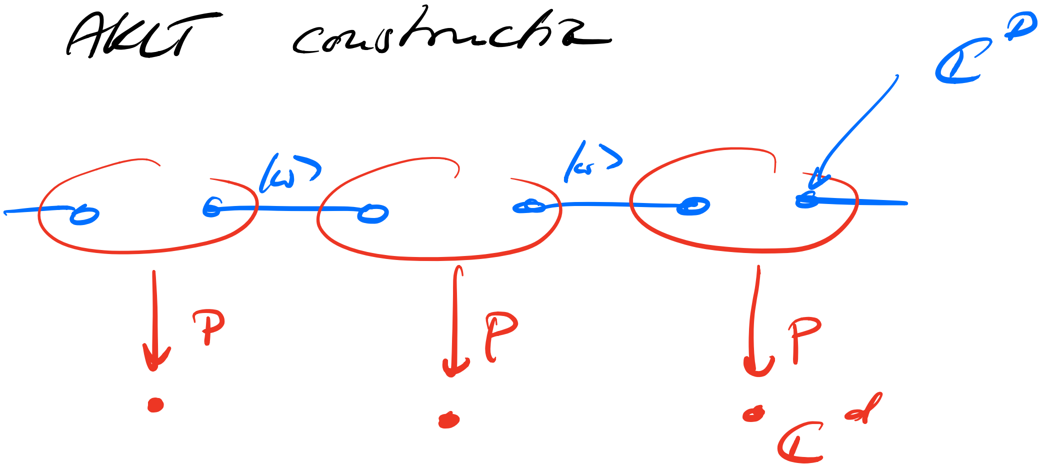
2. Solvable MPS models and classification of phases

a) Relation betw. AKLT construction and MPS

The AKLT construction



with arbitrary P and $|\omega\rangle$ is equivalent to MPS construction.

Step I:

Replace $|\omega\rangle$ by $|\Omega\rangle = \frac{1}{\sqrt{D}} |i,i\rangle$ by writing $|\omega\rangle = (\mathbb{1} \otimes T)|\Omega\rangle$ and replacing P by $P' = P(T \otimes \mathbb{1})$.

Step II:

Define A via $P' = \sum A^i_{\alpha\beta} |i\rangle\langle\alpha,\beta|$.

Then, the state equals

$$|\psi\rangle = \sum \mathrm{tr}[A^{i_1} A^{i_2} \cdots A^{i_N}] |i_1, \dots, i_N\rangle .$$

Proof / Details: see Exercise #12.

<u>Note</u>: This also works without trace.

b) Injective MPS

Definition: An MPS tensor $A \equiv A^i_{\alpha\beta}$ is called **injective** if the map

$$P(A) = \sum A^i_{\alpha\beta} |i\rangle\langle\alpha,\beta|$$

is injective.

An MPS tensor is called **normal** if it becomes injective after blocking some number k of sites,

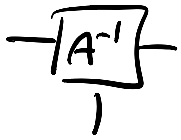
$$B^{i_1 \dots i_k} = A^{i_1} \cdot A^{i_2} \cdot \ldots \cdot A^{i_k} .$$

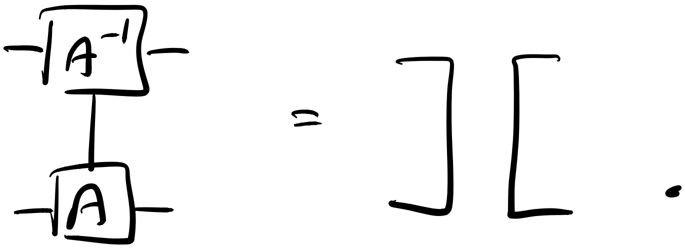
Correspondingly, we also talk of normal or injective MPS if it consists of normal or injective tensors.

(Note: Sometimes, MPS with normal tensors are also called "injective MPS".)

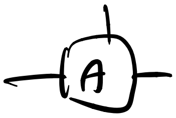
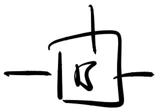
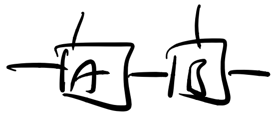
Remarks:

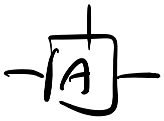
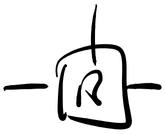
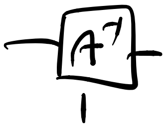
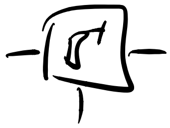
- There are bounds on how often one has to block to reach injectivity (quantum version of Wielandt's inequality).
- For a generic MPS, we expect that it is normal, and injectivity is reached rapidly.
- A PBC transl. inv. MPS without long-range order can be always brought into a form where the tensor $A^i_{\alpha\beta}$ is normal.

Observation: A is injective iff $P(A)$ has a left-inverse $P(A)^{-1}$, $P(A)^{-1}P(A) = \mathbb{1}$, or equivalently, there is a tensor  s.th.

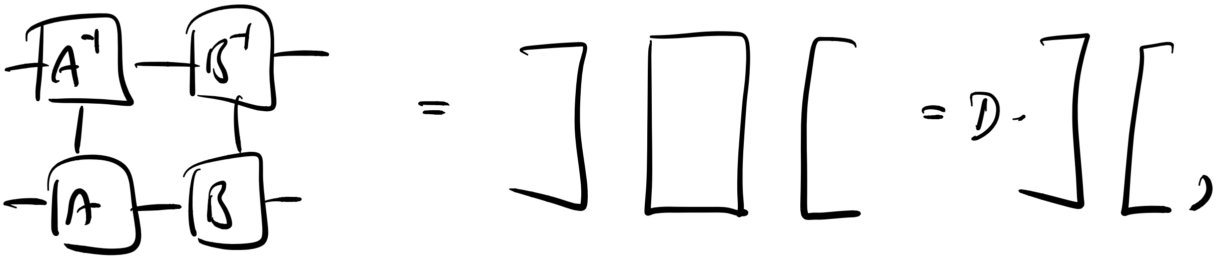


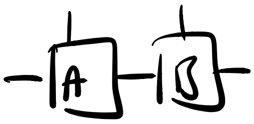
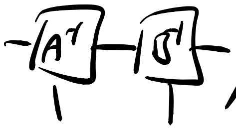
Lemma: Injectivity is stable under blocking, i.e.

,  injective $\Rightarrow$  injective.

Proof: ,  inj.: $\exists$ , .

Then:

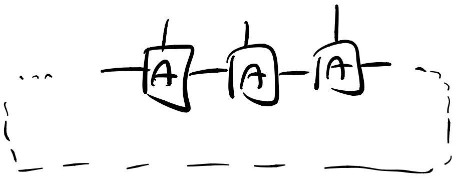
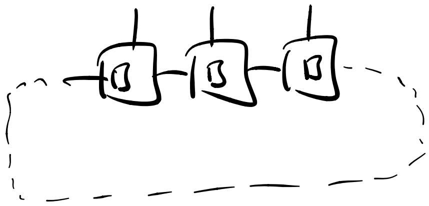


i.e.  injective (with left-inv. $\frac{1}{D}$ ).

$\blacksquare$

c) The fundamental theorem of MPS

Consider two injective MPS

$|\psi_N[A]\rangle =$  and $|\psi_N[B]\rangle =$ 

which describe the same state for all N,

$$|\psi_N[A]\rangle = |\psi_N[B]\rangle \quad \forall N.$$

What is the relation of A and B?

Observation: If $B^i = X A^i X^{-1}$ for some invertible (or left-invertible) X, then $|\psi_N[A]\rangle = |\psi_N[B]\rangle \ \forall N$.

Proof: $\mathrm{tr}[B^{i_1} B^{i_2} \dots B^{i_N}] =$

$$= \mathrm{tr}[X A^{i_1} \underbrace{X^{-1} X}_{= \mathbb{1}} A^{i_2} X^{-1} X^{i_3} \dots X A^{i_N} X^{-1}]$$

$$= \mathrm{tr}[A^{i_1} A^{i_2} \dots A^{i_N}].$$

$\boxtimes$

The fundamental theorem of MPS states that this is the only way in which $|\psi_N[A]\rangle = |\psi_N[B]\rangle$ th[...] can hold.

<u>Theorem (Fundamental Theorem of MPS):</u>

Let $\{A^{[s]}\}_{s=1}^{N}$ and $\{B^{[s]}\}_{s=1}^{N}$ be injective tensors which describe MPS $|\psi[\{X^{[s]}\}]\rangle$, $X = A, B$, and let $N \geq 3$.

Then,

$$|\psi[\{A^{[s]}\}]\rangle = |\psi[\{B^{[s]}\}]\rangle$$

if and only if there exist left-invertible $Z_1, \dots, Z_s$ such that

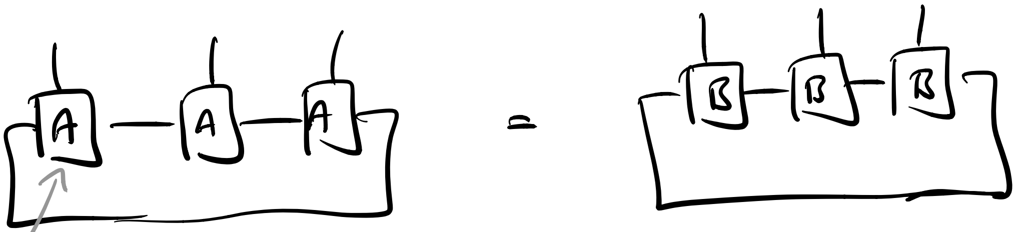
$$B^{[s],i} = Z_s \, A^{[s],i} \, Z_{s+1}^{-1}$$

$N+1 \equiv 1.$

We call the Z_s a gauge degree of freedom.

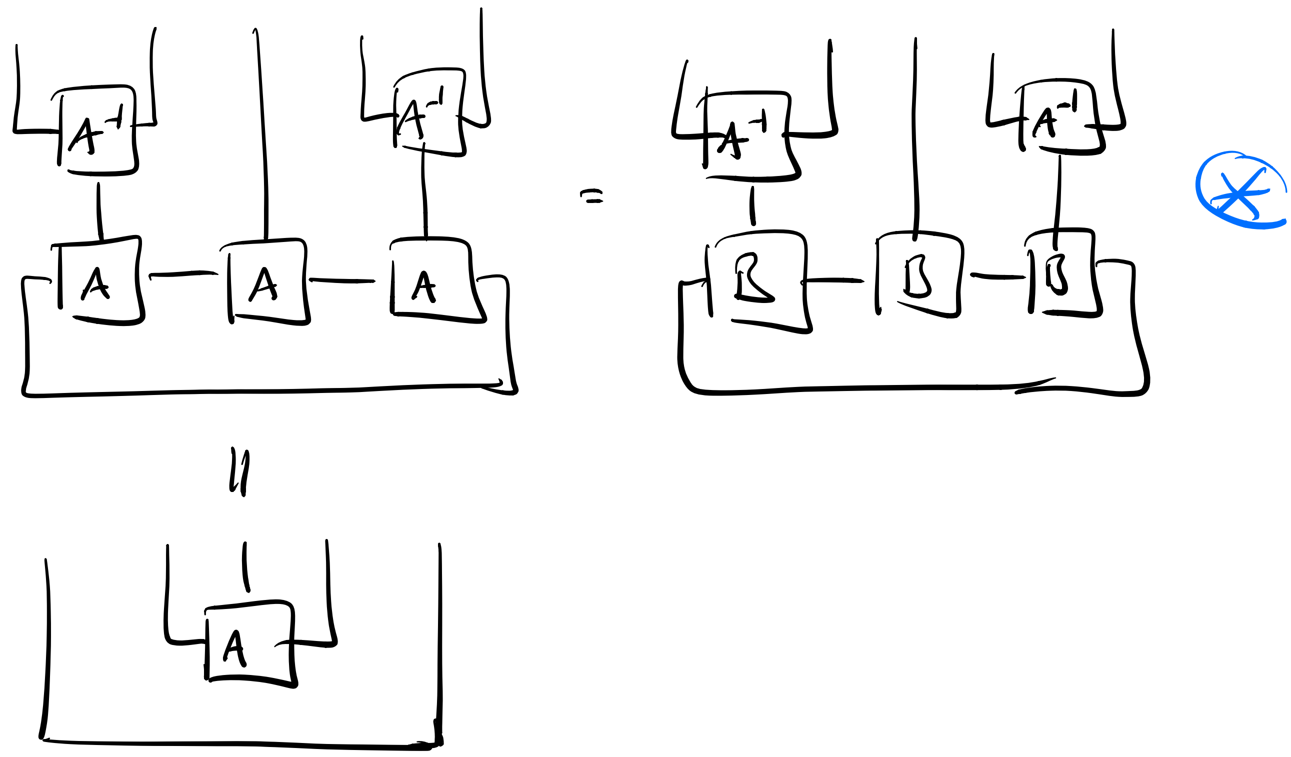
(Note that this implies $D_s(B) \geq D_s(A)$ (with $D(\cdot)$ the bond dimension at cut s; by symmetry $A \leftrightarrow B$, it must also hold that $D_s(A) \geq D_s(B)$ and thus $D_s(A) = D_s(B)$, and Z_s is square & invertible.

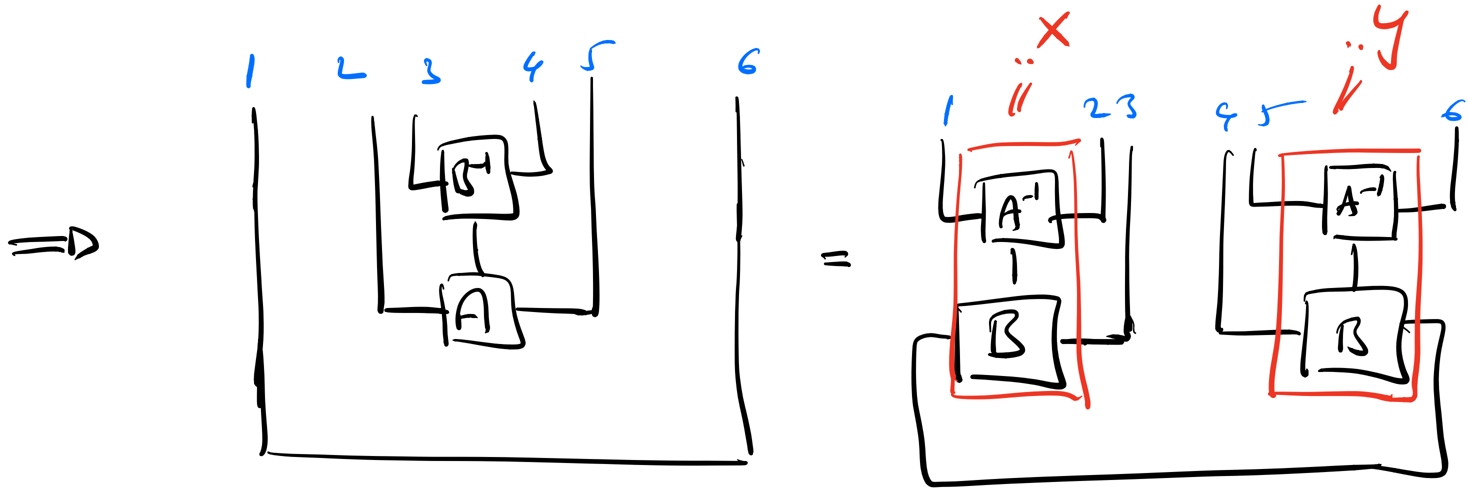
Proof: Let us wlog consider $s=2$. Block $A^{[3]}, \dots, A^{[N]}$ to one tensor $A^{[3]}$. Then,

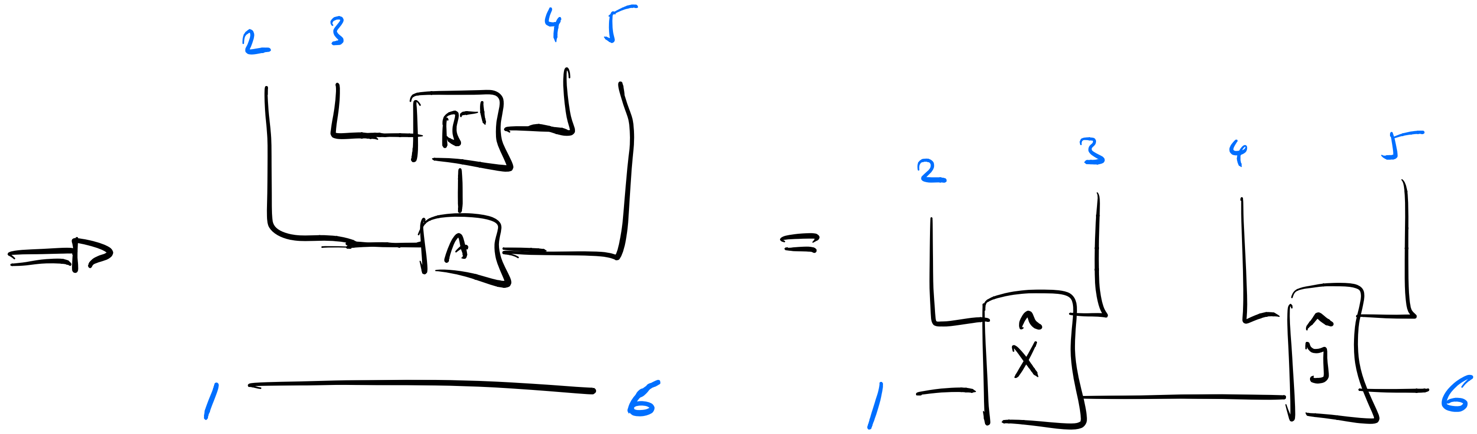


numbers [s] omitted for convenience – number = position!

$\Rightarrow$

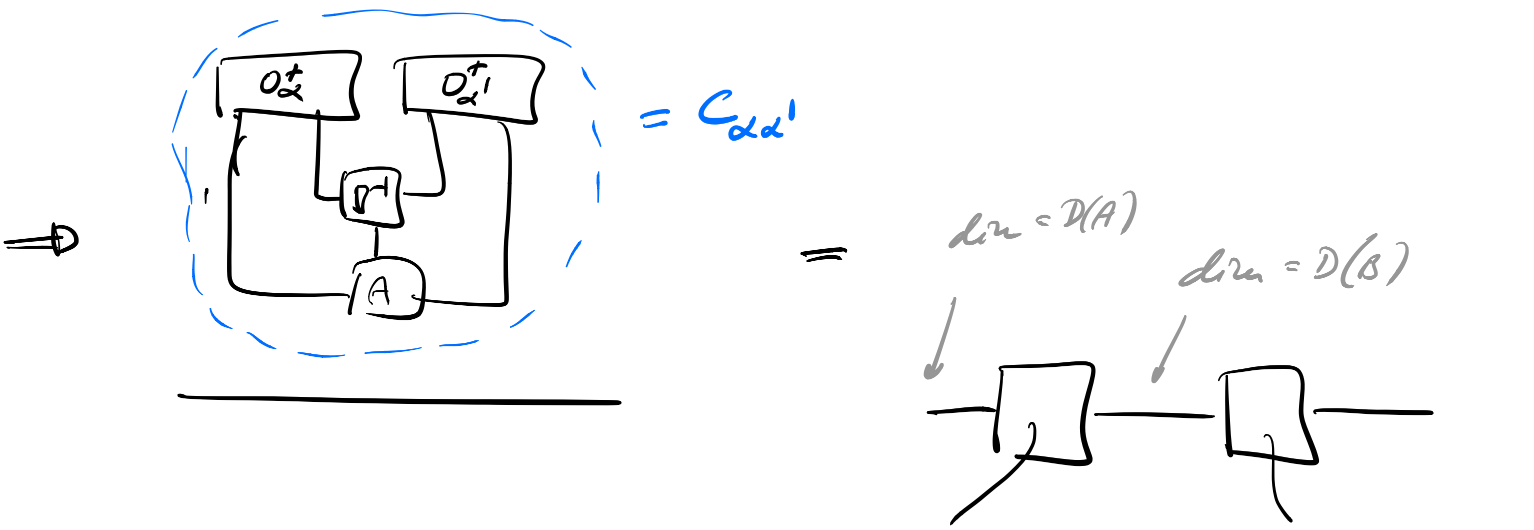






Now expand $\hat{X} = \sum x_{\alpha\beta}\, O_\alpha \otimes O_\beta$; $\hat{y} = \sum y_{\alpha\beta}\, O_\alpha \otimes O_\beta$,

with an ONB $\{O_\alpha\}$, $tr(O_\alpha^\dagger O_\beta) = \delta_{\alpha\beta}$.



$\sum x_{\alpha\beta} O_\beta =: X_\alpha$ $\qquad$ $\sum y_{\alpha'\beta} O_\beta = y_{\alpha'}$

$$\Longrightarrow X_\alpha Y_{\alpha'} = c_{\alpha\alpha'} \cdot \mathbb{1}$$

$$\Longrightarrow D(A) \leq D(B).$$

The inverse ($A \leftrightarrow B$) argument gives $D(B) \leq D(A)$,

and thus: $\Longrightarrow D(A) = D(B)$

(and this holds for every cut!)

As this holds for all α, α':

Fix α: $X_\alpha Y_{\alpha'} = c_{\alpha\alpha'} \mathbb{1}$

$\Longrightarrow Y_{\alpha'} \propto Y(\alpha)$, and since this

must hold $\forall \alpha$ (and $Y_{\alpha'}$ is indep. of α):

$$\Longrightarrow Y_{\alpha'} = c_{\alpha'} \tilde{Y}.$$

$$\Longrightarrow \hat{y} = \sum y_{\alpha'\beta}\, O_{\alpha'} \otimes O_\beta$$

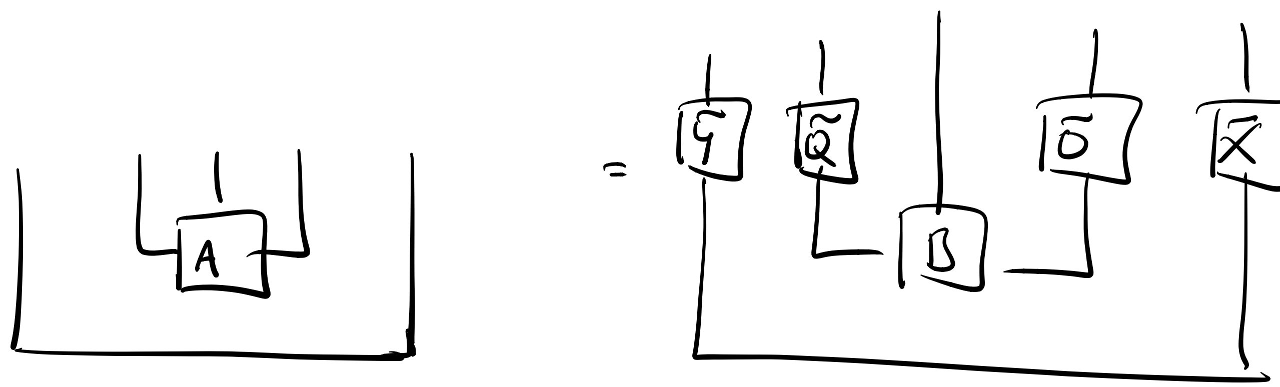
$$= \sum_{\alpha'} O_{\alpha'} \otimes \underbrace{\left(\sum y_{\alpha'\beta}\, O_\beta\right)}_{= c_{\alpha'} \tilde{Y}.}$$

$$= \sum_{\alpha'} c_{\alpha'} O_{\alpha'} \otimes \tilde{Y} = \tilde{O} \otimes \tilde{Y}$$

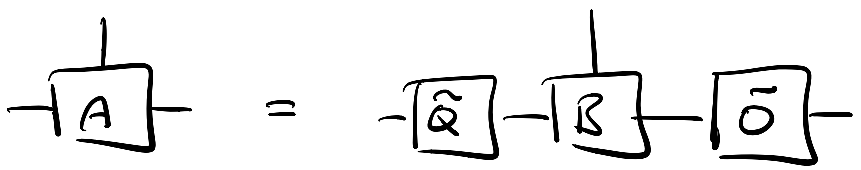
and similarly $\hat{X} = \tilde{Q} \otimes \tilde{X}$,

and $\tilde{X}\tilde{Y} = \mathbb{1}$.

$\xrightarrow{\text{substitute in } \circledast}$



$\Longrightarrow$



Also, we had seen that $D(A) = D(B)$ for all cuts,

and since A is injective, i.e., left-invertible, we have  ,

and thus $\tilde{Q}$ and $\tilde{O}$ must be full rank, i.e. invertible.

The fact that $\tilde{Q}$ and $\tilde{O}$ for adjacent cuts are inverses of each other follows from the fact that for two adjacent cuts, $\tilde{Q}$ and $\tilde{O}$ are constructed just as the pair $\tilde{X}$ and $\tilde{Y}$ above, for which $\tilde{X}\tilde{Y} = \mathbb{1}$.

$\boxtimes$

Note: The fundamental theorem still holds if $|\psi[A]\rangle = e^{i\phi}|\psi[B]\rangle$; then, the MPS tensors are related up to a phase:

$$B^{[s],i} = e^{i\phi_s} Z_s A^{[s],i} Z_{s+1}^{-1}$$

Note: If the MPS is transl. invariant, then the gauge transformations are also transl. invariant (by their construction).

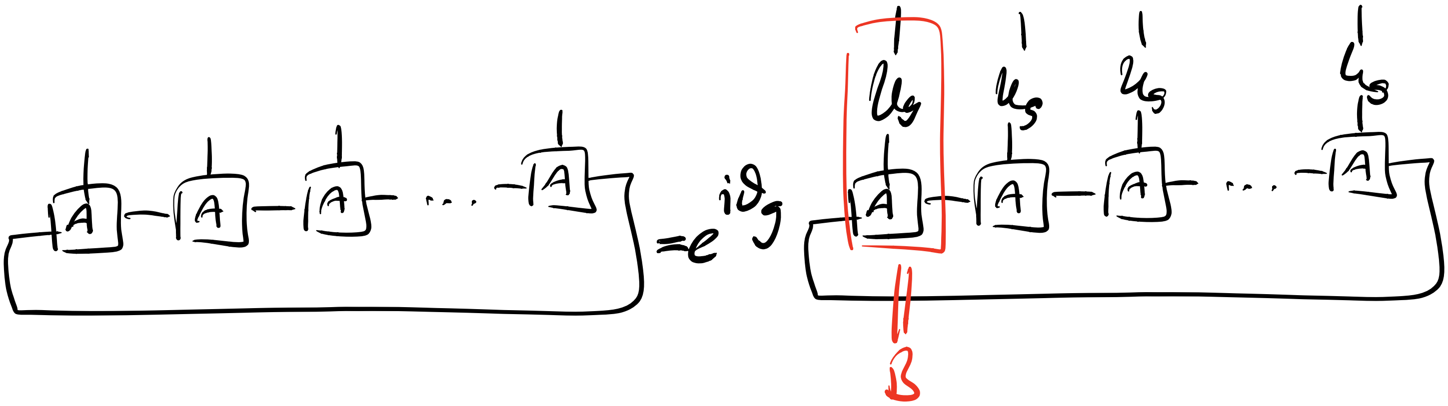
d) Symmetries in MPS & projective representations

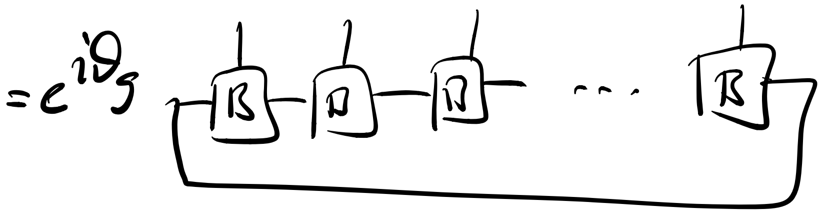
Consider Hamiltonian $H = \sum h_i$ with a symmetry $[H, U_g^{\otimes N}] = 0$, with U_g the representation of a symmetry group G, $U_g U_h = U_{gh}$, $g, h \in G$.

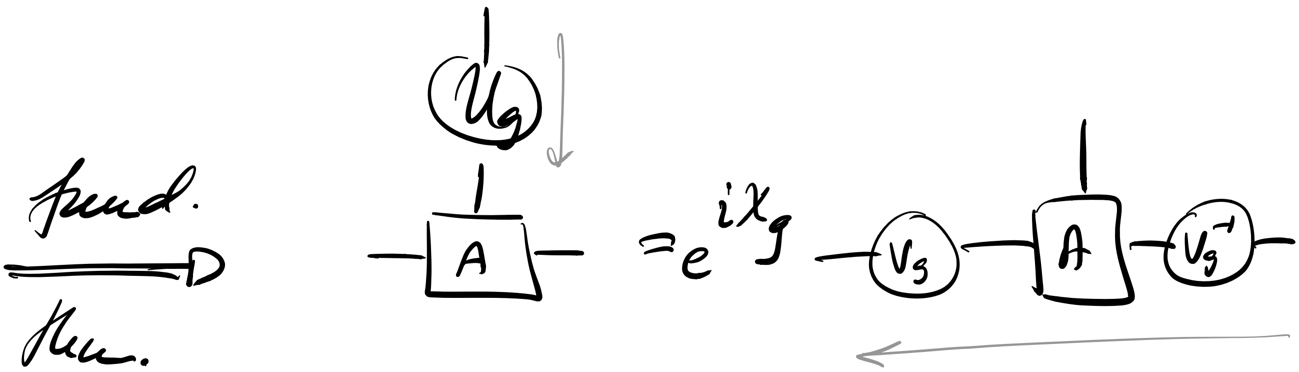
Let $|\psi\rangle$ be the unique ground state of H

$$\Longrightarrow \quad U_g^{\otimes N} |\psi\rangle = e^{i\vartheta_g} |\psi\rangle$$

If $|\psi\rangle$ is an MPS – or an (injective) MPS approximating the GS with the same symmetry – we have for this MPS

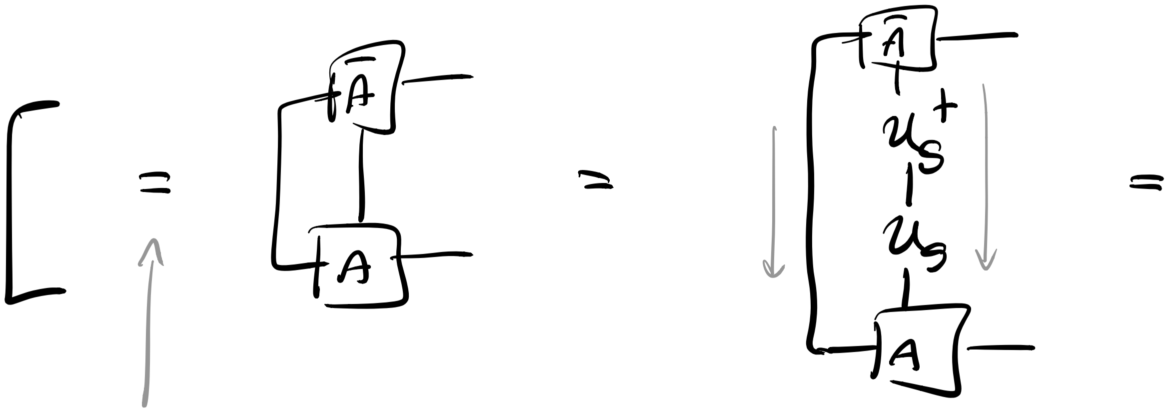




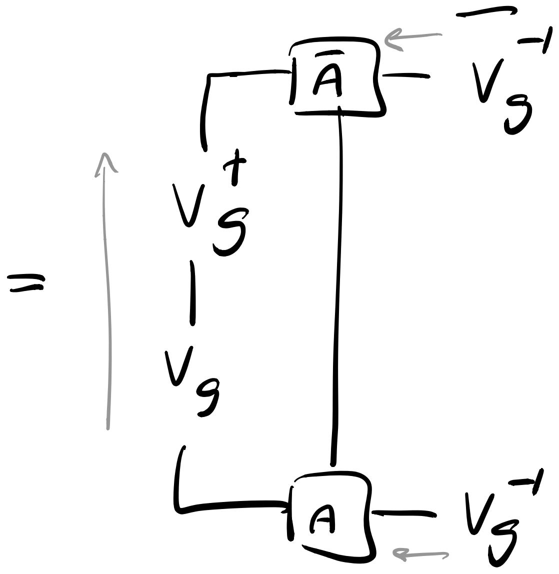


$(V_g \equiv Z_g^T)$

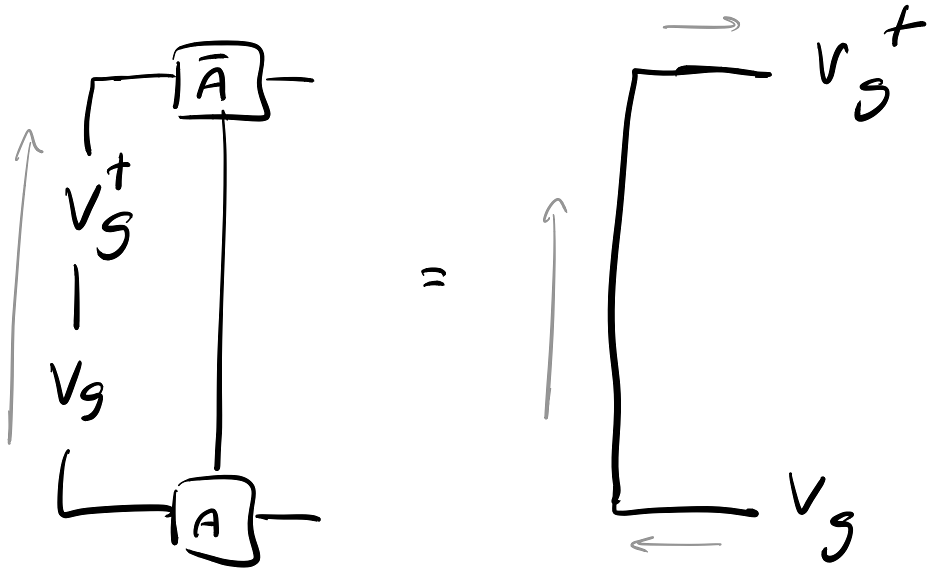
Now let A be in left-can. form:



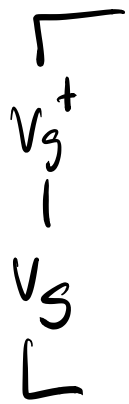
[leading eigenvector.



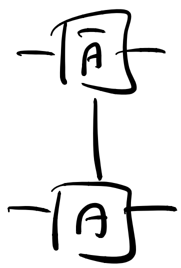
move $z_g^{-1}, \bar{z}_g^{-1}$ to other side $\Longrightarrow$



$\Longrightarrow$



is eigenvector of



with eigenvalue 1.

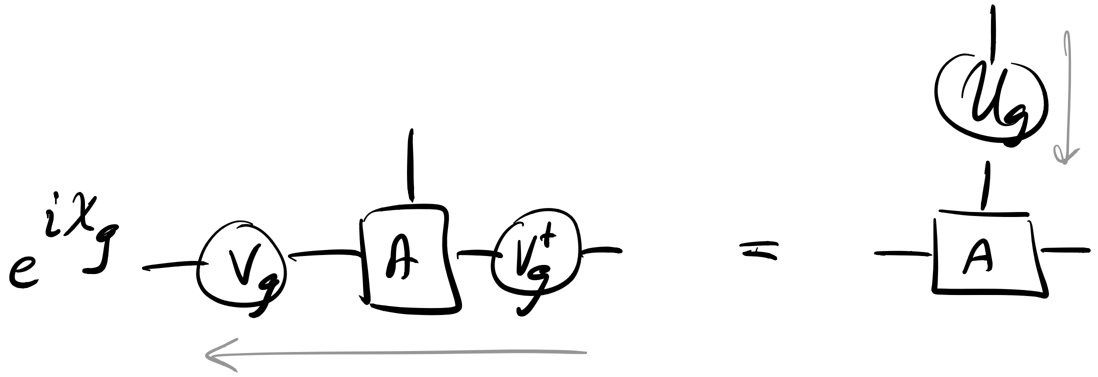
But: Injective MPS / ground state of gapped Ham. $\Longrightarrow$ no long-range order $\Longrightarrow$

$\Longrightarrow$ leading eigenvector <u>unique</u>!

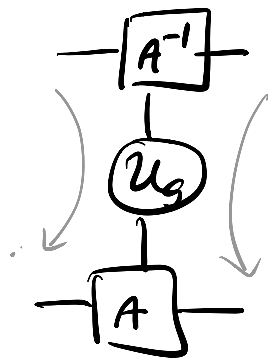
$$\Longrightarrow \quad V_g^{\dagger} V_g = \mathbb{1}$$

$\Longrightarrow$ V_g is unitary!

What else can we say about V_g?



$\Longrightarrow \quad V_g \otimes \bar{V}_g = e^{-i\chi_g}$

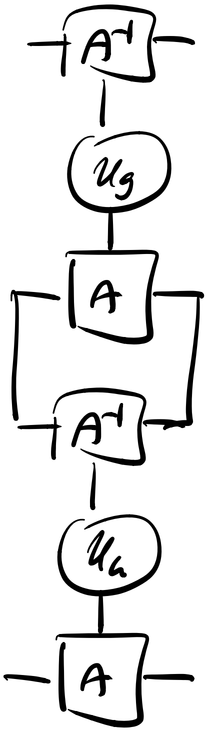


$(*)$

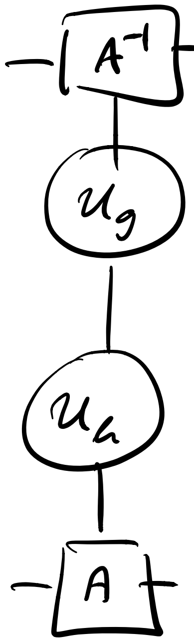
$\longrightarrow \quad (V_g V_h) \otimes (\overline{V_g V_h})$

$= (V_g \otimes \overline{V_g})(V_h \otimes \overline{V_h})$

$= e^{i(\chi_g+\chi_h)}$



$= e^{i(\chi_g+\chi_h)}$



$= e^{i(\chi_g+\chi_h)}$

$= e^{i(\chi_g+\chi_h-\chi_{gh})} \quad V_{gh} \otimes \overline{V_{gh}}$

$\Longrightarrow \quad \chi_g + \chi_h = \chi_{gh}$ (i.e., $\chi_\cdot$ is one-dimensional irreducible rep.), and thus:

$$(V_g \otimes \bar{V}_g)(V_h \otimes \bar{V}_h) = V_{gh} \otimes \bar{V}_{gh}$$

$$\Longrightarrow \quad V_g V_h = e^{i\omega(g,h)} V_{gh}$$

Furthermore, this is the best we can say, since V_g is only defined by $\circledast$ up to a phase — we have an equivalence relation $V_g \sim e^{i\phi_g} V_g$!

Definition: A set of unitaries V_g, $g \in G$, is called a projective representation of G if

$$V_g V_h = e^{i\omega(g,h)} V_{gh} \quad \forall g,h \in G.$$

From associativity, we get

$$V_g(V_h V_k) = V_g\, e^{i\omega(h,k)} V_{hk} = e^{i[\omega(g,hk)+\omega(h,k)]} V_{ghk}$$

$$\parallel$$

$$(V_g V_h) V_k = e^{i\omega(g,h)} V_{gh} V_k = e^{i[\omega(g,h)+\omega(gh,k)]} V_{ghk}.$$

$$\Longrightarrow \boxed{\omega(g,hk)+\omega(h,k) \overset{\text{mod } 2\pi}{=} \omega(g,h)+\omega(gh,k)}$$

This is called a 2-cocycle.

However, because $V_g \sim e^{i\phi_g} V_g$, we can also change

$$V_g V_h = e^{i\omega(g,h)} V_{gh}$$

$$\wr \qquad\qquad\qquad \wr$$

$$(e^{i\phi_g} V_g)(e^{i\phi_h} V_h) \qquad e^{i\phi_{gh}} e^{i\omega(g,h)} V_{gh}$$

$$\Longrightarrow \boxed{\omega(g,h) \overset{\text{mod } 2\pi}{\sim} \omega(g,h) + \phi_{gh} - \phi_g - \phi_h}$$

This is called a 2-coboundary.

We should thus consider equivalence classes $[\omega]$ of 2-cocycles modulo 2-coboundaries.

These are classified by the 2nd cohomology group

$H^2(G, U(1))$.

Example:

$G = SO(3)$, i.e. rotations in $\mathbb{R}^3$.

$$V_g = \exp[i\, \vec{S} \cdot \vec{\Theta}] \quad \text{for } \vec{\Theta} \in G,$$

vector $|\vec{\Theta}| \leq \pi$, identify opp. points w/ $|\vec{\Theta}| = \pi$.

or, simpler, the subgroup

$$H = \mathbb{Z}_2 \times \mathbb{Z}_2 \subset SO(3)$$

generated by π- rotations about x & z:

$$V_{(1,0)} = \exp[i\pi S_x]$$

$$V_{(0,1)} = \exp[i\pi S_z].$$

For integer spin, this is a normal (linear) representation. ($\rightarrow$ Proof: Homework)

For half-integer spin, however, it is impossible to make $\omega(g,h)$ trivial, regardless of the choice of the gauge degrees of freedom ϕ_g:

To this end, consider any gauge fixing, let $g=(1,0)$ (x-rot. by π), $h=(0,1)$ (z-rot. by π),

and look at

x & z-rot by π commute in $SO(3)$

$$V_{(1,0)} V_{(0,1)} = e^{i\omega(g,h)} V_{(1,1)}$$

$$= e^{i[\omega(g,h) - \omega(h,g)]} V_{(0,1)} V_{(1,0)}$$

Now consider e.g. spin-1/2:

$$V_{(1,0)} = \exp\left(i\pi \sigma_x/2\right) = i\sigma_x$$

$$V_{(0,1)} = \exp\left(i\pi \sigma_z/2\right) = i\sigma_z$$

$$\Rightarrow V_{(1,0)} V_{(0,1)} = (i\sigma_x)(i\sigma_z)$$

$$= -(i\sigma_z)(i\sigma_x)$$

$$= \underline{\underline{-}}\, V_{(0,1)} V_{(1,0)} \; !$$

$$\Rightarrow \omega(g,h) = \omega(h,g) + \pi \quad (\mathrm{mod}\ 2\pi),$$

i.e. ω <u>cannot be made trivial</u>!

Result: The integer and half-integer spin representations correspond to the two in-equivalent classes of projective representations of $SO(3)$ or $\mathbb{Z}_2 \times \mathbb{Z}_2$,

$$H^2(SO(3), U(1)) = H^2(\mathbb{Z}_2 \times \mathbb{Z}_2, U(1)) = \mathbb{Z}_2 .$$

Observations:

1) Two projective representations V_g, W_g in the same equivalence class $[\omega]$ can be combined, and they are in the same equivalence class:

$$V_g V_h = e^{i\nu(g,h)} V_{gh}$$

$$W_g W_h = e^{i\omega(g,h)} W_{gh}$$

Choose gauge $V_g \sim e^{i\varphi_g} V_g$, $W_g \sim e^{i\psi_g} W_g$

s.th. $\nu(g,h) = \omega(g,h)$.

Then,

$$(V_g \oplus W_g)(V_h \oplus W_h) =$$

$$= V_g V_h \oplus W_g W_h =$$

$$= e^{i\nu(g,h)} V_{gh} \oplus e^{i\omega(g,h)} W_{gh}$$

$$= e^{i\omega(g,h)} (V_{gh} \oplus W_{gh}). \quad \square$$

2) For two inequivalent proj. reps, $V_g \oplus W_g$ is

not a projective rep., since otherwise

$$V_g V_h \oplus W_g W_h = e^{i\omega(g,h)} V_{gh} \oplus e^{i\omega(g,h)} W_{gh},$$

i.e. there would be a gauge where

$$V_g V_h = e^{i\omega(g,h)} V_{gh},$$

$$W_g W_h = e^{i\omega(g,h)} W_{gh}.$$

3) The equivalence classes $[\omega] \in H^2(G, U(1))$ form a group under tensorizing representations:

$$(V_g \otimes W_g)(V_h \otimes W_h) = V_g V_h \otimes W_g W_h$$

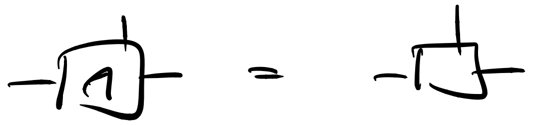
$$= e^{i\nu(g,h)} V_{gh} \otimes e^{i\omega(g,h)} W_{gh}$$

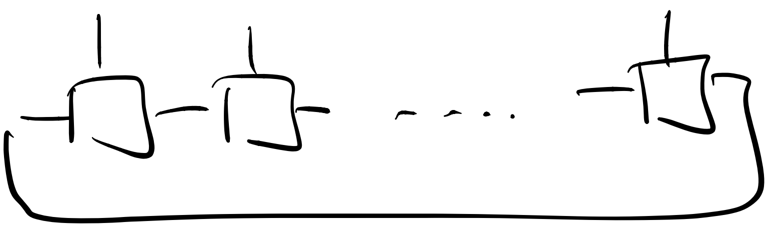
$$= e^{i[\nu(g,h) + \omega(g,h)]} (V_{gh} \oplus W_{gh})$$

e) Parent Hamiltonians

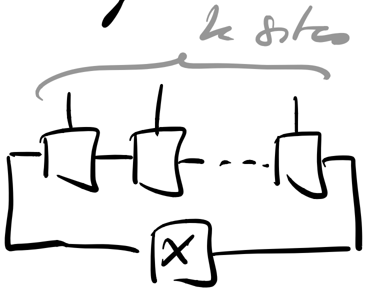
As for the AKLT model, we can construct parent Hamiltonians for any MPS:

Consider a tr.inv. PBC MPS $|\psi\rangle$ w/ tensor

$A =$  ,

$|\psi\rangle =$ 

Consider k contiguous sites, and define

$S_k := \Big\{$ 

$\Big|\ X\ D\times D$ matrix $\Big\}$

Then, $\dim S_k \leq D^2$, and $S_k \subset (\mathbb{C}^d)^{\otimes k}$.

$\Rightarrow$ For $d^k > D^2$, S_k is <u>not</u> the full space.

Define $h = \mathbb{1} - \Pi_{S_k}$

proj. onto S_k.

Then, $H = \sum h_i$ has the MPS $|\psi\rangle$

centered at i

as its ground state, $H|\psi\rangle = 0$; $H \geq 0$.

<u>Theorem:</u> If A is a normal tensor, with s the number of sites needed to reach injectivity, then the Hamiltonian $H = \sum h_i$,

with the h_i defined as $h_i = \mathbb{1} - \Pi_{S_k}$ for any $k \geq s+1$, has $|\psi\rangle$ as its <u>unique ground state</u> on any system size.

Such a Hamiltonian is called a <u>parent Hamiltonian</u>.

Stated here <u>without proof</u> — but note that the proof for the uniqueness of the AKLT ground state can be transferred if $k = 2s$.

<u>Theorem</u>: Under the conditions from the theorem above, <u>H is gapped</u>.

<u>Result (imprecise)</u>: Similar results also hold for MPS with $A^i = \bigoplus_{\alpha=1}^{\alpha_{max}} A^{i,\alpha}$, where every block α is injective:

The parent Hamiltonian has α_{max} ground states, and a gap above the ground state manifold.

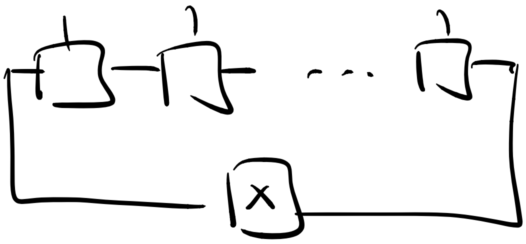
Furthermore, any transl. PBC MPS can be brought into such a form.

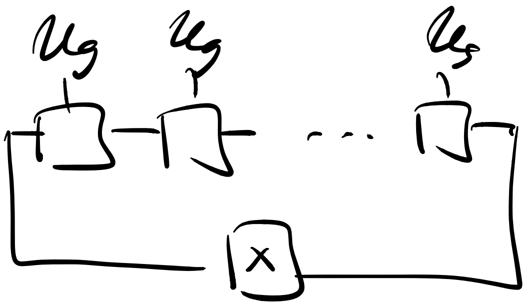
<u>Theorem:</u> If $|\psi\rangle$ has a symmetry,

$$u_g \cdot A = V_g \, A \, V_g^\dagger ,$$

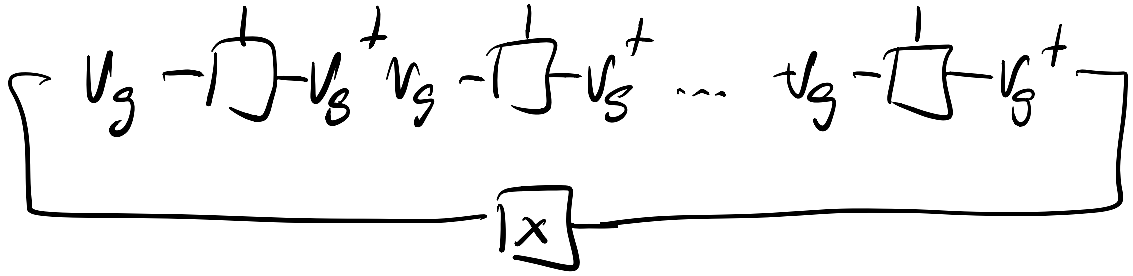
then the parent Hamiltonian inherits the symmetry, $[H, u_g^{\otimes n}] = 0$

<u>Proof:</u> Let $|\phi\rangle \in S_k$, i.e. $\exists X$:

$|\phi\rangle =$  .

Then, $u_g^{\otimes k} |\phi\rangle =$ 

$=$



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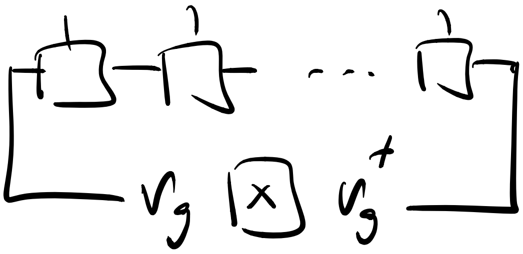

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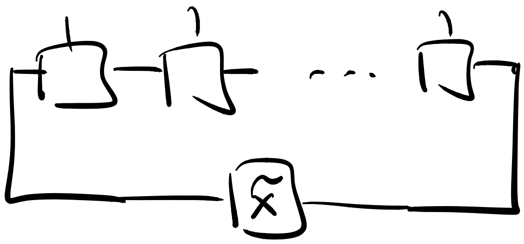


with $\tilde{X} = V_g X V_g^\dagger$

$\Longrightarrow \quad U_g^{\otimes k} |\phi\rangle \in S_k$

$\Longrightarrow \quad U_g^{\otimes k} \Pi_{S_k} (U_g^{\otimes k})^\dagger = \Pi_{S_k}$

$\Longrightarrow \quad [\Pi, U_g^{\otimes k}] = 0 .$ $\blacksquare$

1) Classification of 1D phases with symmetries

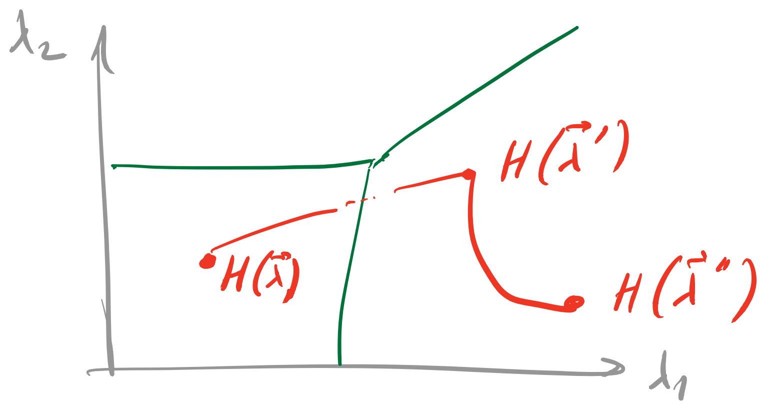
Quantum phases:

Consider $H(\vec{\lambda}) = \sum h_i(\vec{\lambda})$ local.

Phase = region in parameter space $\vec{\lambda}$ where properties of ground state don't change abruptly.

In particular, the correlation length should diverge exactly at the phase boundary.

Quantum phases are typically defined as regions where $H(\vec{\lambda})$ is gapped.



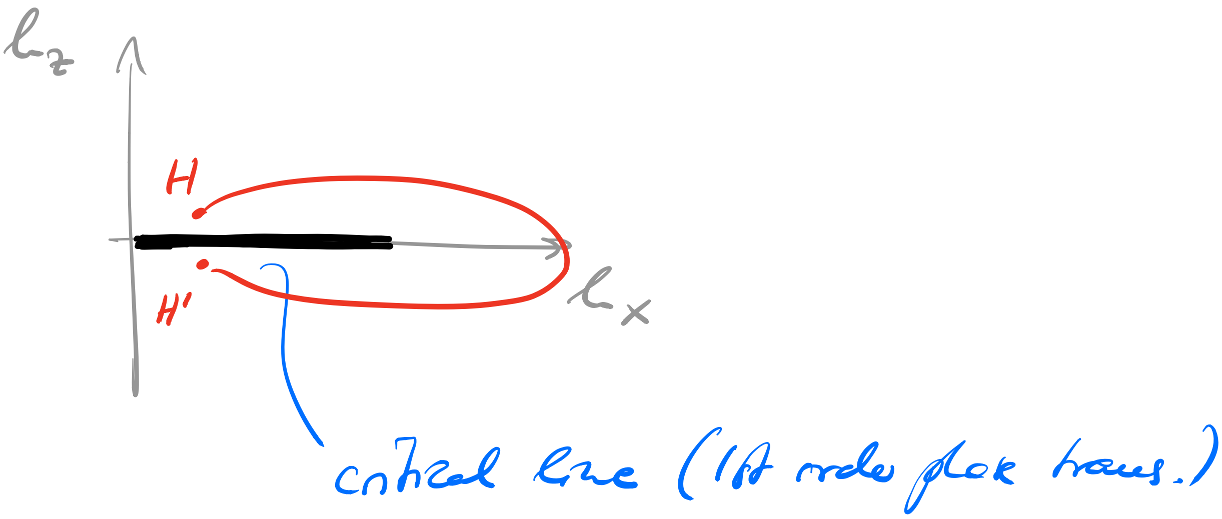
$H(\vec{\lambda})$ and $H(\vec{\lambda}')$ are defined to be in the same phase exactly if they can be connected by a gapped path.

In 1D, it is natural to restrict to $H(\vec{\lambda})$ with a symmetry,

$$[H(\vec{\lambda}), U_g^{\otimes N}] = 0.$$

E.g. Ising model in 1D:

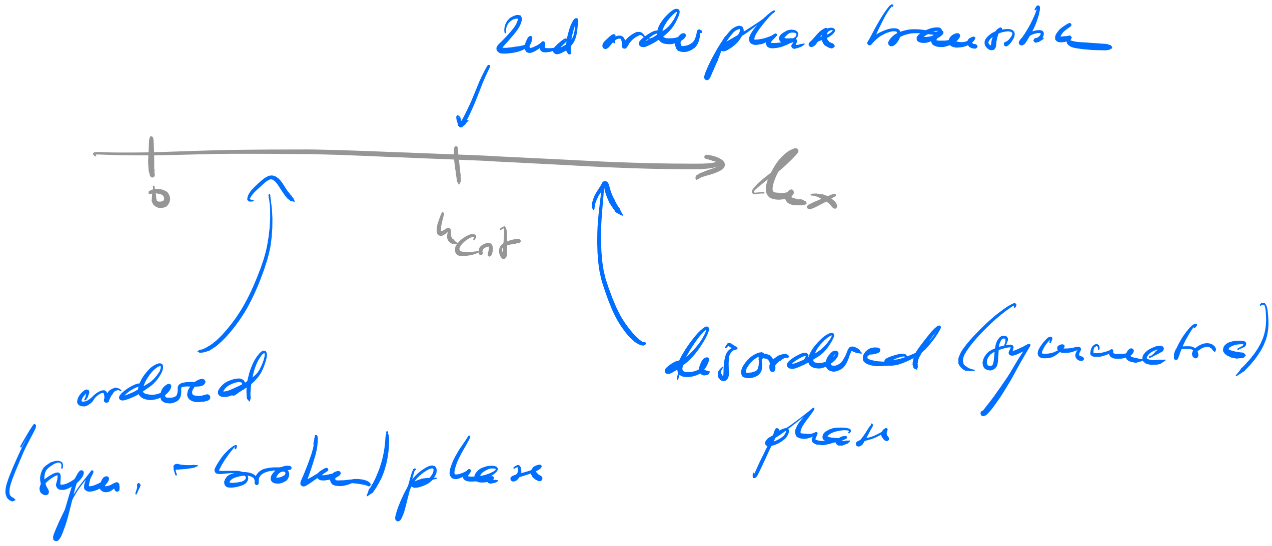
$$H = -\sum Z_i Z_{i+1} - h_x \sum X_i - h_z \sum Z_i$$



- Any two points (except meas. zero) can be connected.

- Impose $\mathbb{Z}_2$-sym $U_g^{\otimes N} = X^{\otimes N}$

$$\Rightarrow [Z_i, U_g^{\otimes N}] \neq 0 \Rightarrow h_z = 0.$$



Imposing symmetries makes phase diagram more interesting.

Observed: Symmetry breaking gives rise to different quantum phases.

Question: Can there be different phases even if we impose that the ground state is unique, i.e., no sym. breaking?

$$\boxed{\text{What is the quantum phase diagram of 1D systems w/ symmetry + unique g. state?}}$$

MPS form good approx. of ground states of (gapped) 1D systems & come with their parent Hamiltonian $\Rightarrow$ consider problem in family of MPS.

→ Starting / final point: given by injective ($\to$ unique g.s.!) MPS with tensors A^i, B^i.

→ interpolating path gapped / finite ξ: should also corresp. to path of MPS w/ inj. tensors $C^i(\lambda)$, $C^i(0) = A^i$; $C^i(1) = B^i$. In part., parent Ham. is continuous in C: Thus, cont. $C^i(\lambda)$ implies cont. interpolation

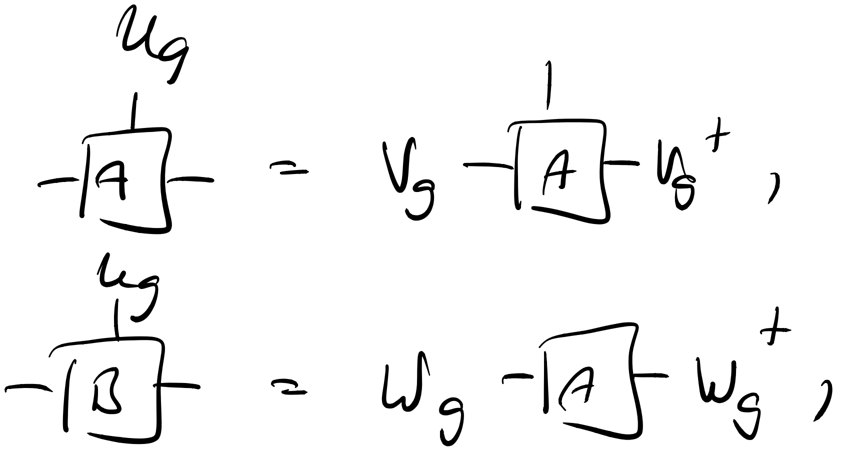
$$H_C(\lambda) = \sum h_i(\lambda).$$

<u>Problem setting</u>: Given two injective MPS with tensors A^i and B^i with a symmetry U_g^{ew}, when does there exist a path of

injective MPS $C^i(\lambda)$, $C^i(0) = A^i$, $C^i(1) = B^i$, with the same symmetry?

Consider e.g. $G = SO(3)$, u_g spin-1 representation.

Then,



where V_g, W_g are either sums $\oplus$ of only integer-spin reps. or only of half-integer spin reps.

<u>Claim</u>: A and B are in the same phase under $SO(3)$ symmetry – i.e. a path as above exists – if and only if V_g and W_g are in the same equiv. class.

(Note: This is a <u>general</u> result, not restricted to $SO(3)$!)

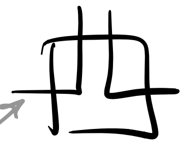
Proof idea:

If V_g & W_g are in the same equiv. class, build an interpolation $C(\lambda)$ with sym. $Z_g = V_g \oplus W_g$.

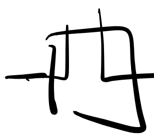
Naively: $C^i = (1-\lambda) A^i \oplus \lambda B^i$.

However, this is not good (since $\frac{\lambda^n}{(1-\lambda)^n} \longrightarrow 0$ or ∞).

Rather: First, interpolate to "fixed points" (possibly blocking sites)

$\tilde{A}$ =  with sym.

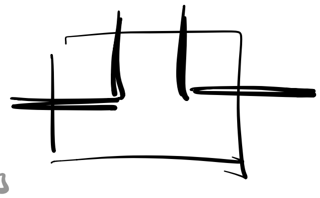
$\mathbb{C}^{d_A}$

V_g  $V_g^{\dagger}$ = 

,

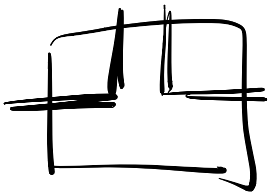
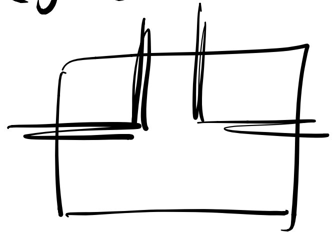
and same for $\tilde{B}$.

Then, we can interpolate locally:

$\tilde{C} =$  with

$\mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$

$(V_g \otimes W_g) \otimes (\overline{V_g \otimes W_g})$

$V_g \otimes W_g$  $V_g^{\dagger} \otimes W_g^{\dagger} =$ 

and $\tilde{C}(\lambda) = \left(\begin{array}{c|c} (1-\lambda)\mathbb{1} & \\ \hline & \lambda \mathbb{1} \end{array}\right) \tilde{C}$.

Conversely, any interpolation $\tilde{C}(\lambda)$ requires a symmetry action $Z_g = V_g \otimes W_g$ (since $[\omega]$ cannot be changed smoothly); however, this is impossible if V_g & W_g have diff. $[\omega]$.

<u>Result</u>: The classification of 1D phases with symmetries is given by the equivalence classes of the projective action of the symmetry on the entanglement degrees of freedom.