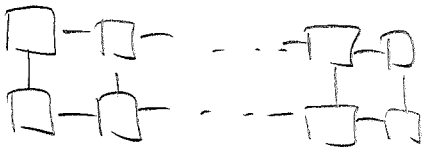
Numerical simulation with MPS

- Evaluation of expectation values is of the form



$= \langle e | \mathbb{E} \cdot \ldots \cdot \mathbb{E} | r \rangle$

$\mathbb{E}$: $D^2 \times D^2$ - matrices.

Start from left:

$(1 \times D^2) \cdot (D^2 \times D^2)$ - multiplications: D^4 steps

$\Rightarrow$ total $\sim N D^4$ steps $\Rightarrow$ efficient in N (as long as $D \doteq \text{poly}(N)$)

(Note: D^6 for PBC)

$\Rightarrow$ Efficient computation of exp. values etc.!

- Given local Hamiltonian $H = \sum h_{i,i}$, can we find the best MPS approx. to its ground state, i.e.

MPS $|\psi\rangle$ w/ some D s.th. $\langle \psi | H | \psi \rangle$ minimal?

(if gapped $\rightarrow$ area law $\rightarrow$ will be a good approx. of GS.)

Will present basic idea first. Several omissions / "bad practice" — will be fixed later!

Consider MPS $|\psi\rangle \equiv \sum_{i_1 \ldots i_N} \left(A^{[1]i_1} A^{[2]i_2} \cdots A^{[N]i_N} \right) |i_1 \ldots i_N\rangle$

$|\psi\rangle$ is a <u>linear function</u> $|\psi(A^{[s]})\rangle$ in <u>each $A^{[s]}$</u> individually.

Then, $\langle \psi(A^{[s]}) | H | \psi(A^{[s]}) \rangle$ is <u>quadratic</u> in $A^{[s]}$,

$$\langle \psi(A^{[s]}) | H | \psi(A^{[s]}) \rangle =: \vec{A}^{[s]\dagger} \cdot M \cdot \vec{A}^{[s]}$$

↑ "vectorized version" of $A^{[s]}$.

Can M be computed efficiently? — Yes (cf. later, but <u>using a matrix basis</u> would be (in principle) efficient.)

↑ don't do this...!

<u>Similarly</u>: $\langle \psi(A^{[s]}) | \psi(A^{[s]}) \rangle = \vec{A}^{[s]\dagger} \cdot N \cdot \vec{A}^{[s]}$.

Can we minimize $E(A^{[s]}) = \dfrac{\vec{A}^{[s]} M \vec{A}^{[s]}}{\vec{A}^{[s]} N \vec{A}^{[s]}}$

to find the <u>optimal $A^{[s]}$</u>?

→ Maps to an eigenvalue problem:

$$\min_{\vec{x}} \frac{\vec{x}^+ M \vec{x}}{\vec{x}^+ N \vec{x}} = \min_{\vec{x}} \frac{\left(\sqrt{N}\vec{x}\right)^+ \frac{1}{\sqrt{N}} M \frac{1}{\sqrt{N}} \left(\sqrt{N}\vec{x}\right)}{\underbrace{\left(\sqrt{N}\vec{x}\right)^+ \left(\sqrt{N}\vec{x}\right)}_{=|\vec{y}|^2}} = \min_{\vec{y}} \frac{\vec{y}^+ \frac{1}{\sqrt{N}} M \frac{1}{\sqrt{N}} \vec{y}}{|\vec{y}|^2}$$

$\Rightarrow$ solution is smallest eigenvalue $\lambda_{\min}\left(\frac{1}{\sqrt{N}} M \frac{1}{\sqrt{N}}\right)$.

(Corresponds to "generalized eigenvalue problem" $M\vec{y} = \lambda N \vec{y}$.)

$\Rightarrow$ Efficiently yields optimal $A^{[s]}$ for a fixed configuration of the other $A^{[k]}$.

- Iterative algorithm:
  - Start w. some state (random, good guess, other meth.)
  - Start at site $s=1$. Optimize $A^{[1]}$.
  - Repeat for $s = 2, 3, \ldots, N$. ("sweep")
  - Repeat for $s = N-1, \ldots, 1$,
  - and so on ...

  → energy will always decrease

  → monitor energy, stop when sufficiently converged.

Core idea of the Density Matrix Renormalization Group algorithm (DMRG, White '92)

- Is this provably convergent?

→ No. Counterexamples exist!

→ But: Works extremely well in practice (w/ well-chosen initial state...)

→ Provably conv. efficient algorithm recently found (very different approach & not (yet?) practical, Landau, Vazirani, Vidick '13)

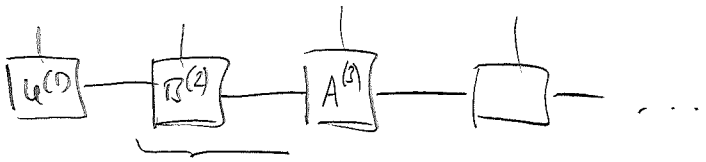
Improvements / implementation issues to keep track:

① $\frac{\vec{A}\cdot\Pi\vec{A}}{\vec{A}\cdot N\cdot\vec{A}}$ can be ill-conditioned if N has small eigenvalues.

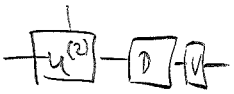
Can we resolve that / get rid of N?

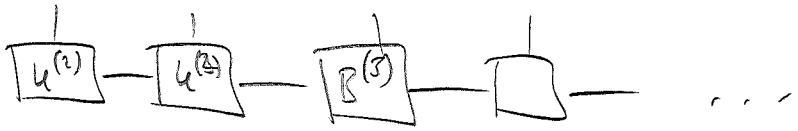
→ Restrict to ORC. Then we can choose an "isometric gauge" (cf. the MPS construction from an arbitrary state in Lecture 10, pg. 71-74):

SVD:



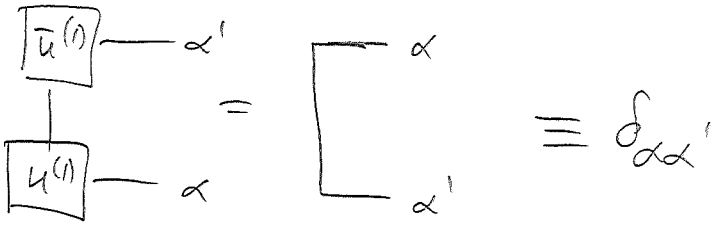
SVD



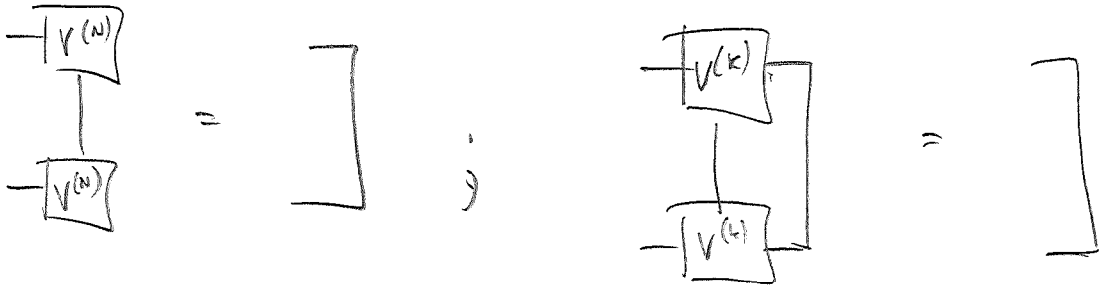


etc.

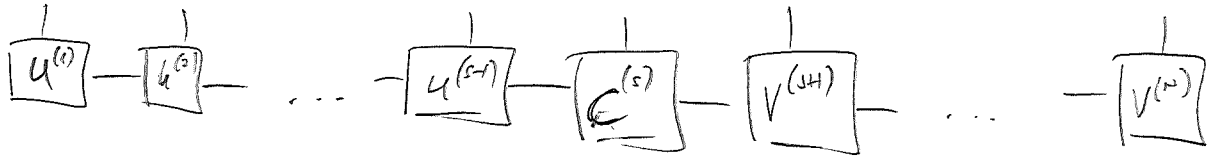
Properties: $U^{(1)}$ isometry:



We can do this also from the right end:

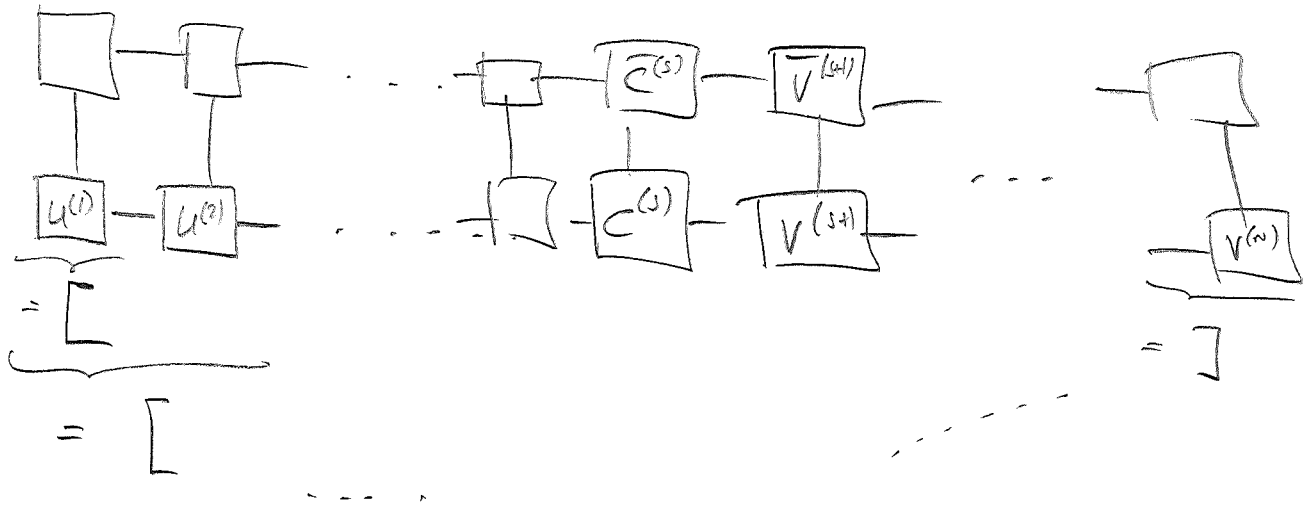


Perform gauge around site s:

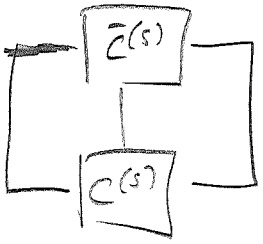


(Note: $C^{(s)}$ contains same info as $A^{(s)}$ – we can as well optimize $C^{(s)}$)

Now what is $\langle \psi(C^{(s)}) | \psi(C^{(s)}) \rangle$?



$=$



$= |\vec{C}^{(s)}|^2 = 1$.

$\Rightarrow$ Have removed $N \rightarrow$ optimization problem

$$\min \frac{\langle \psi(C^{(s)}) | H | \psi(C^{(s)}) \rangle}{\langle \psi(C^{(s)}) | \psi(C^{(s)}) \rangle} = \min_{|C^{(s)}|=1} \vec{C}^{(s)\dagger} \tilde{M} \vec{C}^{(s)}$$

is a normal eigenvalue problem (well-cond.!)

- Saves computational effort (no N needed, + see later)
- When sweeping, updating gauge only requires to update <u>one site</u>!

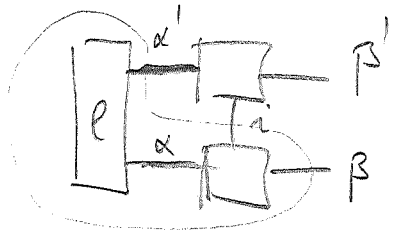
<u>Further optimizations:</u>

(2) <u>Tensor contraction:</u>

<u>Recall:</u> $\langle\psi|O|\psi\rangle = \langle\psi|\cdot E\cdot E\cdot\ldots$ etc.

$\Rightarrow (1\times D^4)\cdot(D^2\times D^2) = D^4$.

<u>But:</u>



can be summed in different orders, and typ.

$D \gg d$ (since large $D \Rightarrow$ good approx.)

Eg.: first sum <u>α</u>: $(D\times D)\cdot(D\times dD) \longrightarrow dD^3$ ops.

<u>then sum α'&i</u>: $D\times dD)\cdot(dD\times D) \longrightarrow dD^3$ ops.

$\Rightarrow dD^3$ ops. $\ll D^4$ ops!

$\Rightarrow$ Scaling of method is <u>D^3N</u>!

③ Optimization in computation of Hamiltonian:

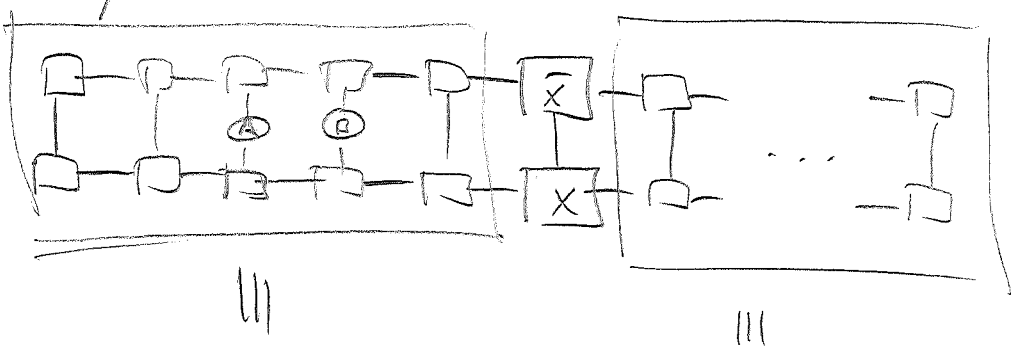
(Different approaches exist, ...)

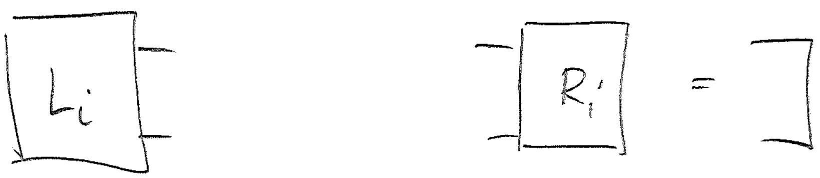
$$\langle\psi(A^{[s]})|H|\psi(A^{[s]})\rangle = \vec{A}^{[s]\dagger} M \vec{A}^{[s]} \Longrightarrow M = ?$$

Use $H = \sum h_i \Longrightarrow M = \sum M_i$.

Assume wlog $h_i = A \otimes B$.

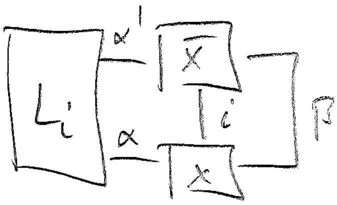
Different types of terms: $(X \equiv A^{[s]})$





(iso. gauge!)

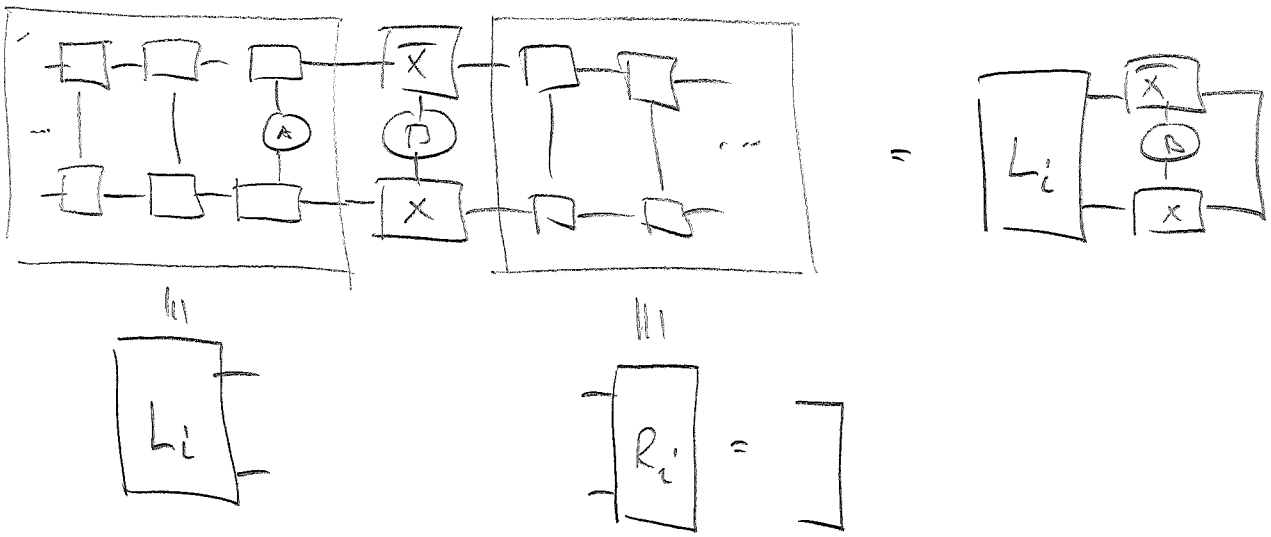
=



$$\Longrightarrow M_i = \mathbb{1} \otimes L_i \otimes \mathbb{1}$$

(arrows under the factors: i, α,α', β.)

... similar for A, B right of s.



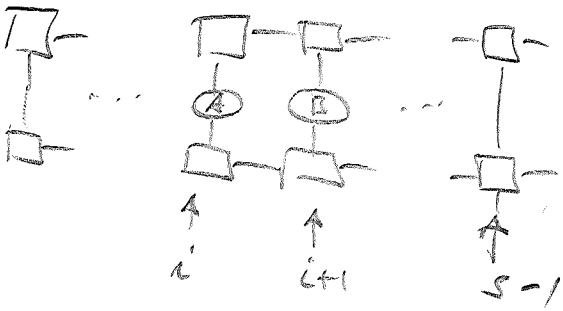
$$\Rightarrow \Pi_i = \mathbb{1} \otimes L_i \otimes \mathbb{1} .$$

$\Pi = \sum \Pi_i$ over all Ham. terms.

Optimizations for Π:

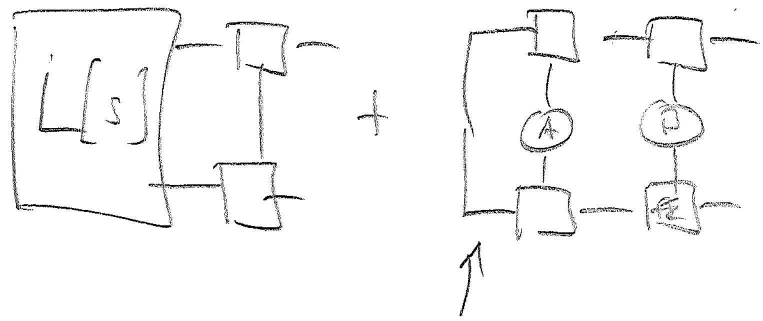
- The whole influence of all Ham. terms left of a position s can be summed up in

$$L[s] = \sum_{i+1<s}$$



- ~~When moving $s \to s+1$, $L[s+1]$ can be computed from $L[s]$~~

- When moving from $s \to s+1$, $L[s+1]$ can be computed from $L[s]$ as

$L[s+1] =$ 

Bruckner gauge!

- By storing all $L[k]$ for $k \leq s$, we already know $L[s]$ when moving $s \to s-1$.

- Correspondingly for right!

$\Longrightarrow$ Effort to determine M during sweep is <u>independent of N!</u>

④ For large D, use Krylov methods (Lanczos/Arnoldi) to minimize $A^{[s]}$!