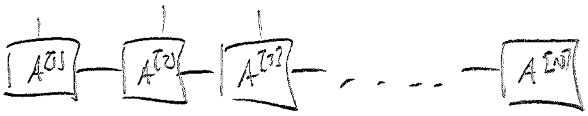
Wrap-up of last lecture:

Variational optimization over MPS — the DMRG method

OBC MPS:



1. Initialize tensors (randomly)
2. Sweep through lattice:

   $s = 1, 2, \ldots, N-1, N, N-1, \ldots, 2, 1, 2, \ldots$ etc.

   For each s, optimize energy

$$E[A^{[s]}] = \frac{\langle \psi[A^{[s]}] | H | \psi[A^{[s]}] \rangle}{\langle \psi[A^{[s]}] | \psi[A^{[s]}] \rangle} \qquad (*)$$

   as a function of s until convergence.

The optimization $(*)$:

With isometric gauge around site s,

$$\langle \psi[A^{[s]}] | \psi[A^{[s]}] \rangle = \vec{A}^{[s]} \cdot \vec{A}^{[s]} = |\vec{A}^{[s]}|^2$$

↑ vectorized form of $A^{[s]}$

and $\langle \psi[A^{[s]}] | H | \psi[A^{[s]}] \rangle = \vec{A}^{[s]} \cdot M \vec{A}^{[s]}$

(since $|\psi[A^{[s]}]\rangle$ is linear in $A^{[s]}$).

$$\min_{|\vec{A}^{[s]}|=1} \vec{A}^{[s]} \cdot \Pi \vec{A}^{[s]}$$ is the smallest eigenvalue of Π and can be solved efficiently.

The D^3-trick:

Π can be determined efficiently using the transfer operator

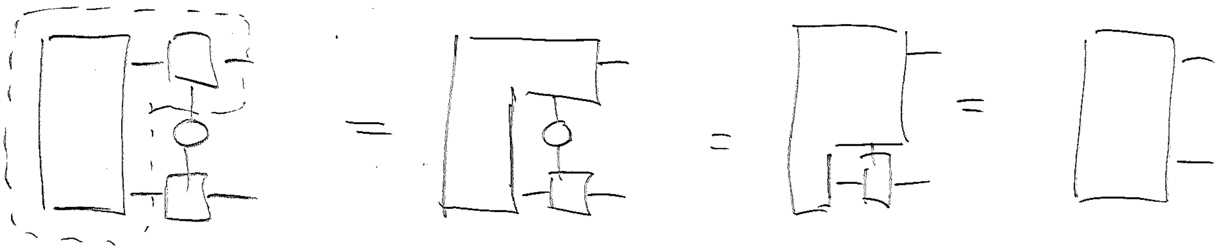
$$E_O = \sum A^i \otimes \bar{A}^j \langle j|O|i\rangle$$

vector E_O E_1 E_1

: multiply left/right bnd. vector with transfer operator.

This scales like D^4.

However: We only need to apply TOp to vector, and this can be done in $O(D^3)$ operations:



$\Longrightarrow$ Scales like D^3!

DMRG & periodic boundary conditions:

Can we extend this to periodic boundary conditions?

Central question: Can we still minimize

$$E[A^{[s]}] = \frac{\langle \psi[A^{[s]}] | H | \psi[A^{[s]}] \rangle}{\langle \psi[A^{[s]}] | \psi[A^{[s]}] \rangle} \quad ?$$

Problem: We cannot impose the isometric gauge any more (recall that there we had to start from the end of the chain!)

Of course, $|\psi[A^{[s]}]\rangle$ is still linear in $A^{[s]}$

$$\Longrightarrow \quad E[A^{[s]}] = \frac{\vec{A}^{[s]} \cdot M \vec{A}^{[s]}}{\vec{A}^{[s]} \cdot N \vec{A}^{[s]}}$$

(M, N can be computed as M before for OBC)

$\Longrightarrow$ This can be minimized by solving the generalized eigenvalue problem

$$M \vec{A}^{[s]} = \lambda \cdot N \vec{A}^{[s]}$$

(E.g., you can substitute $\vec{Y} := N^{1/2} \vec{A}^{[s]}$, then

$$E[\vec{Y}] = \frac{\vec{Y} \cdot N^{-1/2} M N^{-1/2} \vec{Y}}{\vec{Y} \cdot \vec{Y}}$$, which is a normal eigenvalue problem equiv. to the generalized e.v. problem!

Caveats: 1) N could have zero eigenvalues.

For those: i) the states is not well-defined,

ii) M must have a 0 eigenvalue with the same eigenvector (otherwise the energy diverges: ↯)

$\Rightarrow$ we can exclude those subspaces.

2) N can have very small eigenvectors. This can be problematic, since the system is very sensitive to numerical inaccuracies in N & M in that subspace!

$\Rightarrow$ be careful!

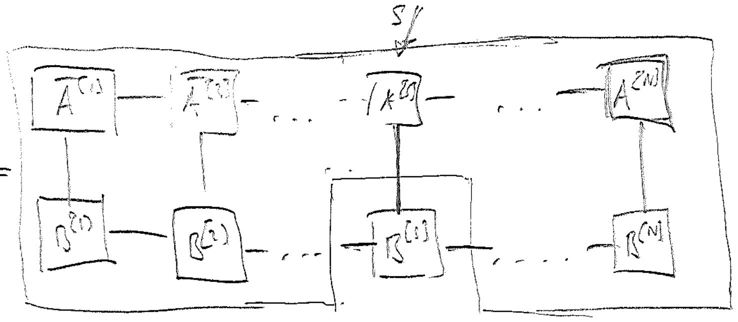
MPS & excited states:

How can we find excited states? (E.g., to compute gaps etc.!)
(W.l.o.g. we discuss OBC).

1. Find the ground state MPS (tensors $A^{[1]}, \ldots, A^{[N]}$)
2. Do another DMRG run with tensors $B^{[1]}, \ldots, B^{[N]}$, and minimize
$$\frac{\langle \psi[B^{[1]},\ldots,B^{[N]}] | H | \psi[B^{[1]},\ldots,B^{[N]}]\rangle}{\langle \psi[B^{[1]},\ldots,B^{[N]}] | \psi[B^{[1]},\ldots,B^{[N]}]\rangle},$$

subject to the constraint $\langle \psi[B^{[1]},\ldots,B^{[N]}] | \psi[A^{[1]},\ldots,A^{[N]}]\rangle = 0$.

The minimization works again by sweeping through the lattice, and for a given $B^{[s]}$, the constraints is linear in $B^{[s]}$:

$\vec{K} :=$ 

$= \vec{K} \cdot \vec{B}^{[s]}$

$\Rightarrow$ we have to solve the <u>eigenvalue problem</u> in the <u>subspace orthogonal to $\vec{K}$!</u>

(i.e.: minimize $\min_{|\vec{A}^{[s]}|=1} \vec{A}^{[s]} \cdot P_\perp M P_\perp \vec{A}^{[s]}$

Proj. on orth. subspace!

$\Rightarrow$ This way, we can sequentially build a hierarchy of excited states!

(<u>Note</u>: low-lying excited states still satisfy area law $\Rightarrow$ MPS approximation still valid. High-lying states are anyways impractical since we need to build them one by one.)

MPS & time evolution:

How can we simulate time evolution?

* $H = \sum h_{i,i+1}$

+ $|\psi(t=0)\rangle$ = some simple state (product, MPS, ground state, ...)

$\Rightarrow$ What is $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ and/or its properties?

---

1. The Trotter (Lie-Trotter, Suzuki-Trotter) decomposition:

$$\boxed{e^{\epsilon(A+B)} = e^{\epsilon A} e^{\epsilon B} + O(\epsilon^2)}$$

Use this to rewrite:

$$H = \overbrace{\sum_{i \text{ even}} h_{i,i+1}}^{H_{even}} + \overbrace{\sum_{i \text{ odd}} h_{i,i+1}}^{H_{odd}}$$

terms within each sum mutually commute

$$e^{-iHt} = \left(e^{-iHt/K}\right)^K = \left(e^{-i(H_{even}+H_{odd})t/K}\right)^K$$

$$= \left(e^{-iH_{even}t/K} e^{-iH_{odd}/K} + O\left(\frac{1}{K^2}\right)\right)^K$$

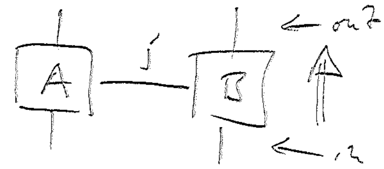
$$= \underbrace{\left(\left(\prod_{i \text{ even}} e^{-ih_{i,i+1}t/K}\right)\left(\prod_{i \text{ odd}} e^{-ih_{i,i+1}t/K}\right)\right)^K}_{\text{good approx. to } e^{-iHt} \text{ for } K \gg t!} + O\left(\frac{1}{K}\right).$$

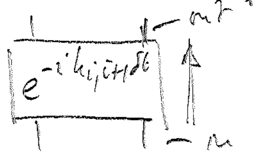
$$t/K =: \delta t$$

2. Simulation w/ MPS:

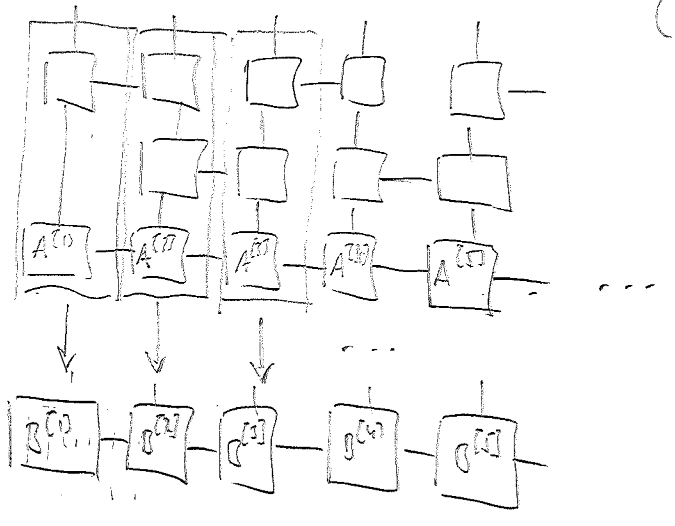
* $|\psi(t=0)\rangle$ is MPS w/ tensors $A^{[1]}, \dots, A^{[N]}$, bond-dim. D.

* Determine MPS for $|\psi(\delta t)\rangle = \left(\prod_{\text{even}} e^{-ih_{i,i+1}\delta t}\right)\left(\prod_{\text{odd}} e^{-ih_{i,i+1}\delta t}\right)|\psi(t=0)\rangle$

Write $\underbrace{e^{-ih_{i,i+1}\delta t}}$ $= \sum_{j=1}^{d^2 \text{ at most}} A_j \otimes B_j \equiv$ 



This is again a singular value decomposition. (→ exercise)

$|\psi(\delta t)\rangle =$ 

$\Rightarrow |\psi(\delta t)\rangle$ is MPS w/ $D' \leq d^4 D$

↑ dep. on Ham.!

If we continue like that, D grows exponentially in time!
However, $e^{-ih_{i,i+1}\delta t} \approx \mathbb{1} \Rightarrow$ it should add little entanglement, so a smaller D should be enough

$\Rightarrow$ truncate D to some D_{max}!

Truncating $D' \to D_{max}$:

We want to find the MPS $A^{[1]}, \dots, A^{[N]}$ w/ D_{max} closest to MPS $B^{[1]}, \dots, B^{[N]}$ w/ D'.

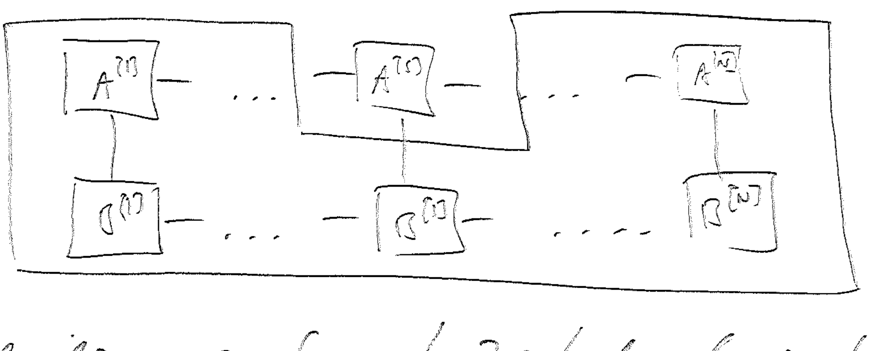
⇒ maximize overlap
$$\frac{|\langle\psi[A^{[1]},\dots,A^{[N]}]|\psi[B^{[1]},\dots,B^{[N]}]\rangle|^2}{\langle\psi[A^{[1]},\dots]|\psi[A^{[1]},\dots]\rangle \underbrace{\langle\psi[B^{[1]},\dots]|\psi[B^{[1]},\dots]\rangle}_{\text{constant } N_B}}$$

⇒ this can be done again as DMRG: sweep and <u>maximize</u>

$$O[\vec{A}^{[s]}] = \frac{|\overbrace{\langle\psi[A^{[1]},\dots,A^{[s]}]|\psi[B^{[1]},\dots]\rangle}^{\text{linear in } \vec{A}^{[s]}}|^2}{\underbrace{\langle\psi[A^{[1]},\dots,A^{[s]}]|\psi[A^{[1]},\dots,A^{[s]},\dots]\rangle}_{\text{w/ gauge: } |\vec{A}^{[s]}|^2}}$$

$$= \frac{(\vec{A}^{[s]} \cdot \vec{L}) \cdot (\vec{L} \cdot A^{[s]})}{|\vec{A}^{[s]}|^2}$$

⇒ same as before in DMRG, w/ $M = \vec{L}\vec{L}^{\dagger}$



$=: \vec{L}$

⇒ bond dim. can be truncated efficiently!

⇒ Algorithm for simulating time evolution!