Introduction to DMRG

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References:
White PRL 69, 2863 (1992)
JH, Pollmann arXiv:1805.0055 (follow here)
Schollwoeck arXiv:1008.3477

Recap

e.g. Spin-$\frac{1}{2}$ $j_n = |\uparrow\rangle, |\downarrow\rangle$

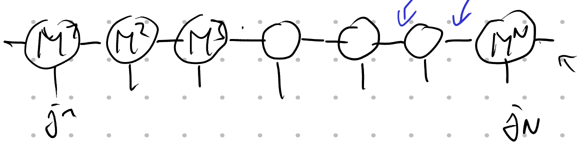
$\downarrow$

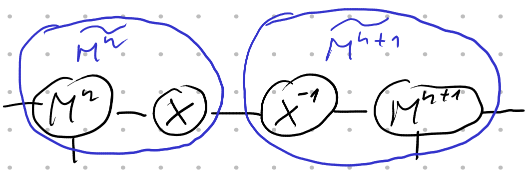
$|j_1 \ldots j_N\rangle$

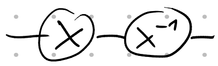
$|\psi\rangle = \sum_{\{j_n\}}$ 

MPS ansatz:

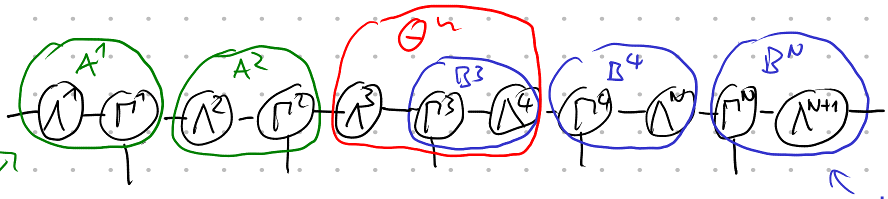
virtual bonds, bond dimension χ



Gauge freedom 

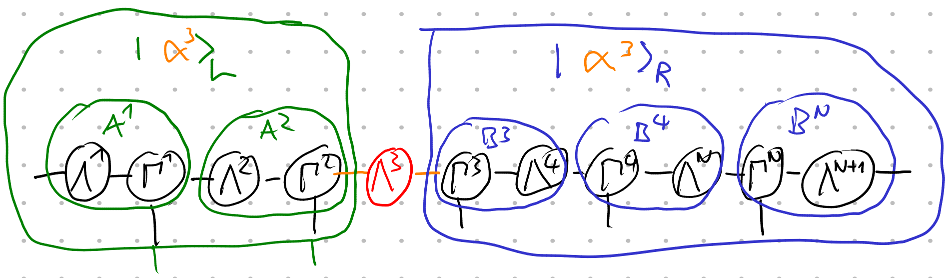
yields same state for  $= \mathbb{1} =$ —

can be used to bring MPS into canonical form defined by Schmidt decomposition

$\psi =$ 

left-canonical

right-canonical

$=$ 

$$= \sum_{\alpha^3} |\alpha^3\rangle_L \quad \lambda_{\alpha^3} \quad |\alpha^3\rangle_R$$

on each virtual bond!

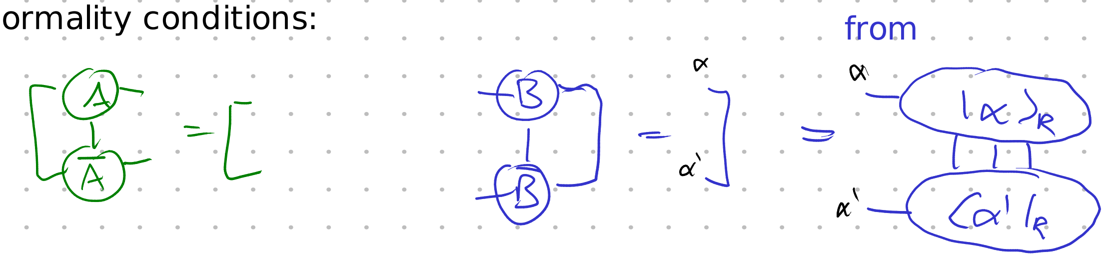
Schmidt states form orthonormal basis on left/right part

Identify virtual bond indices with Schmidt states!

$|\alpha^n_R\rangle$ 

$|j^n\rangle \otimes \cdots \otimes |j^N\rangle$

Orthonormality conditions:



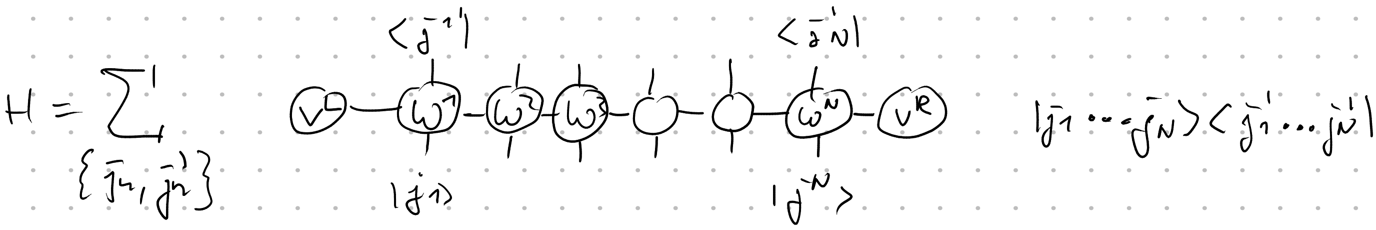
Note:

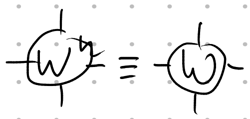
numerically ill conditioned

Matrix product operators

= generalization of MPS to operators

convenient for Hamiltonians beyond nearest neighbors



for translation invariant H (often)  same W for all n

$$W_n = \begin{pmatrix} \mathbb{1}_n & Z_n & -gX_n \\ 0 & 0 & -JZ_n \\ 0 & 0 & \mathbb{1}_n \end{pmatrix}, \quad v_L = (1 \quad 0 \quad 0), \quad v_R = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

entries: local operators

$$\underset{N=2}{\leadsto} \quad v_L W_1 W_2 v_R = (\mathbb{1}_1 \quad Z_1 \quad -gX_1) \begin{pmatrix} -gX_2 \\ -JZ_2 \\ \mathbb{1}_2 \end{pmatrix}$$

$$= -g\,\mathbb{1}_1 X_2 - J Z_1 Z_2 - g X_1 \mathbb{1}_2$$

$$N=3: \quad v_L W_1 W_2 W_3 v_R = (\mathbb{1}_1 \quad Z_1 \quad -gX_1) \underbrace{\begin{pmatrix} \mathbb{1}_2 & Z_2 & -gX_2 \\ & & -JZ_2 \\ & & \mathbb{1}_2 \end{pmatrix} \begin{pmatrix} -gX_3 \\ -JZ_3 \\ \mathbb{1}_3 \end{pmatrix}}_{\begin{pmatrix} -g\mathbb{1}_2 X_3 - J Z_2 Z_3 - g X_2 \mathbb{1}_3 \\ -J Z_2 \mathbb{1}_3 \\ \mathbb{1}_2 \mathbb{1}_3 \end{pmatrix}}$$

$$\rightsquigarrow \quad H = \sum_n -g X_n - J Z_n Z_{n+1} \quad = \text{ transverse field Ising model}$$

General block structure of W

$$W = \left(\begin{array}{c|c|c} \mathbb{1} & C & D \\ \hline & A & B \\ \hline & & \mathbb{1} \end{array}\right), \quad v_L = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \end{pmatrix}, \quad v_R = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$$

yields $H = \sum_n D_n + C_n B_{n+1} + C_n A_{n+1} B_{n+2} + C_n A_{n+1} A_{n+2} B_{n+3} + \dots$

D onsite term
C B nearest neighbors
C A...A B long-range terms

Further examples

$$W^n = \begin{pmatrix} \mathbb{1} & X^n & Y^n & -hZ^n \\ & & & JX^n \\ & & & JY^n \\ & & & \mathbb{1} \end{pmatrix} \quad \rightsquigarrow \quad H = \sum_n J\left(X^n X^{n+1} + Y^n Y^{n+1}\right) - h Z^n$$

$$W^n = \begin{pmatrix} \mathbb{1} & P^n & 0 & 0 \\ & & X^n & 0 \\ & & & P^n \\ & & & \mathbb{1} \end{pmatrix} \quad \rightsquigarrow \quad H = \sum_n P^n X^{n+1} P^{n+2}$$

One can formalize this to auto-generate MPOs given the terms in H!

Side-note: W is not diagonalizable, it has a Jordan block structure:

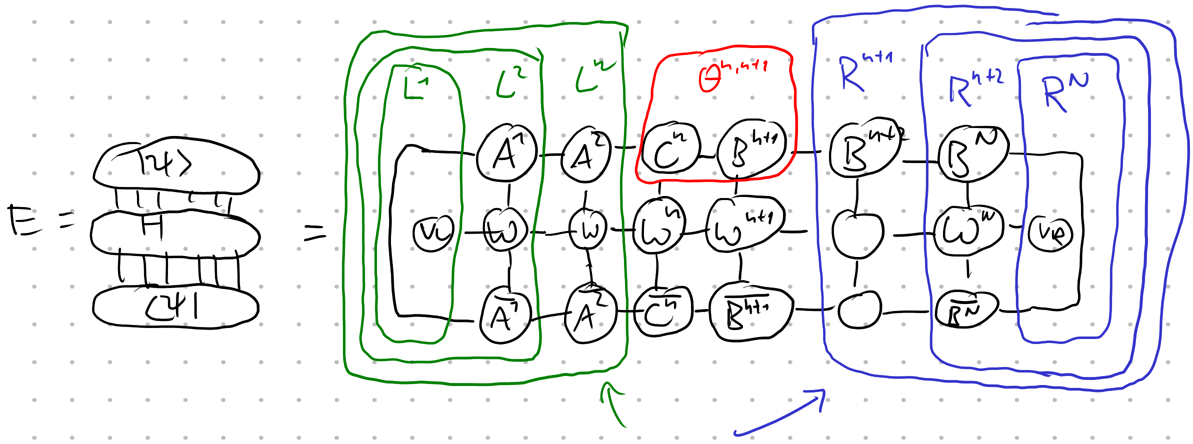
$$H = \begin{pmatrix} 1 & \varepsilon \\ & 1 \end{pmatrix} \rightsquigarrow \quad \begin{pmatrix} 1 & \varepsilon \\ & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \varepsilon \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\begin{pmatrix} 1 & \varepsilon \\ & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

H is extensive; applying transfer matrix adds energy density.

Density Matrix Renormalization Group (DMRG) algorithm

goal: variational minimzation of energy $E = \langle \psi | H | \psi \rangle$



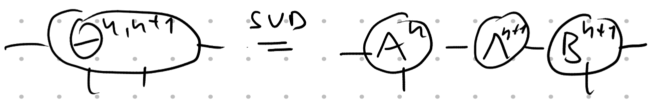
left/right environments,
contain only left/right-canonical MPS tensors!

Finite DMRG:

Start with MPS in right canonical form

for n in {1, 2, ..., N-1}: sweep left to right

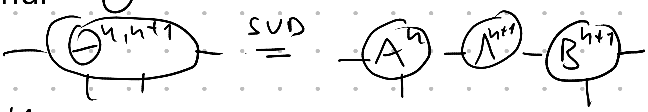
find optimal $\Theta^{n,n+1}$ keeping other tensors fix explained below

split  and truncate

use A^n to calculate updated L^{n+1}

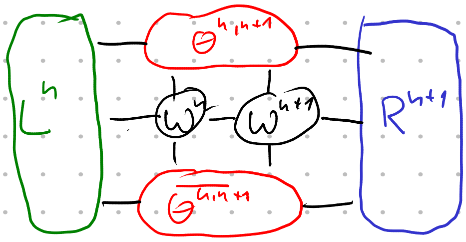
for n in {N-1, ... , 2, 1}: sweep right to left

find optimal $\Theta^{n,n+1}$

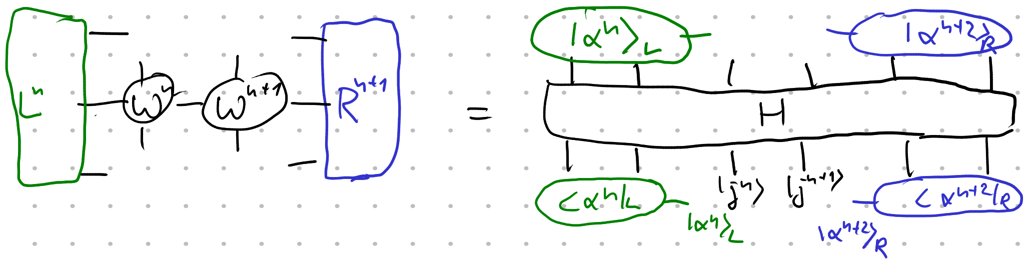
split  and truncate

use B^{n+1} to calculate updated R^{n+1}

How to find optimal $\Theta^{n,n+1}$?

$E =$ 

define $H_{eff}^{n,n+1} =$

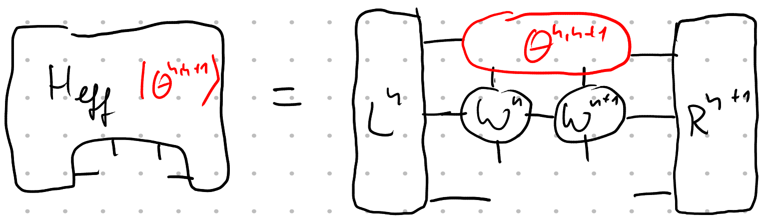


This is H (projected) in the basis $|\alpha^n\rangle_L \otimes |j^n\rangle \otimes |j^{n+1}\rangle \otimes |\alpha^{n+2}\rangle_R$

This is an orthonormal basis!

Hence, the optimal  can be found by diagonalizing $H_{eff}^{n,n+1}$

viewed as a matrix acting on the top indices



Note: contraction order matters for efficiency:

$\mathcal{O}(\chi^3 D d^3)$ vs $\mathcal{O}(\chi^4 d^4)$

Using the Lanczos Algorithm, we can find optimal  with $\mathcal{O}(\chi^3 D + \chi^2 D^2)$

Infinite DMRG

consider system which is translation invariant by with unit cells with N sites

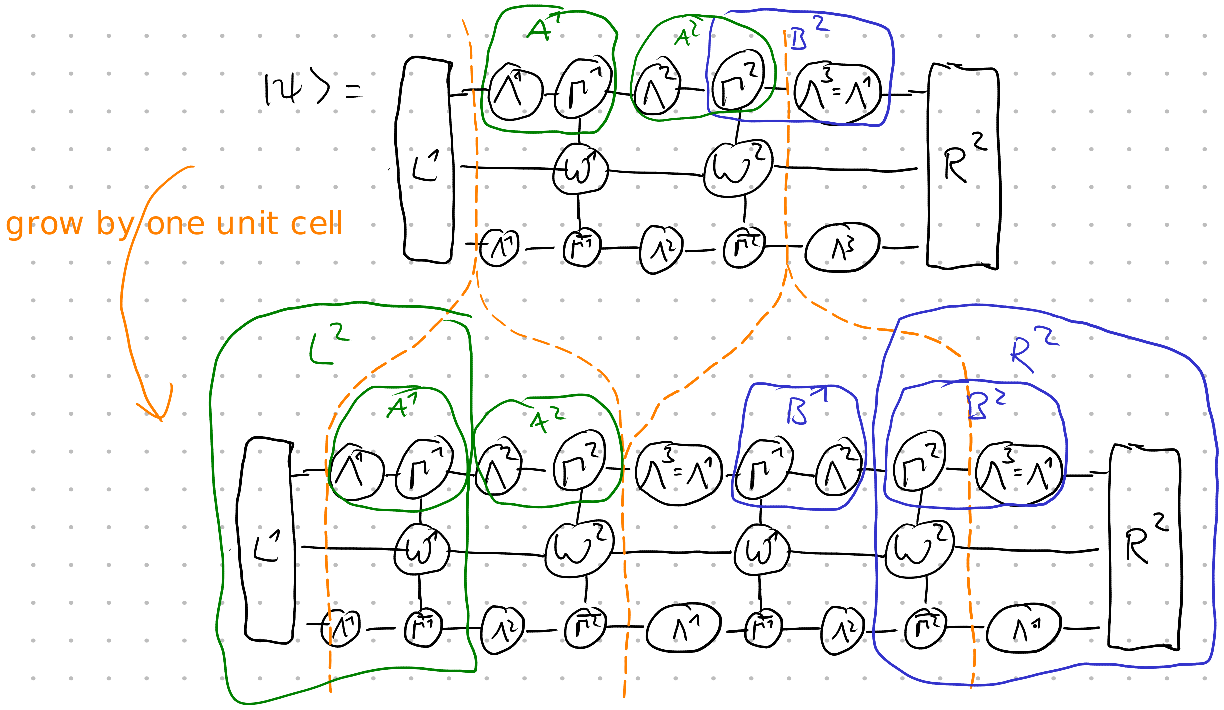
Start with a small system of just one unit cell

Sweep left-right-left in a single unit cell (as in finite DMRG)
    include the bond between the unit cells (which is trivial for finite DMRG)

During each sweep, grow left/right environments by one unit cell
    assuming translation invariance

Repeat sweeps until actual translation invariance is reached

Example: N=2



towards 2D: DMRG on a cylinder

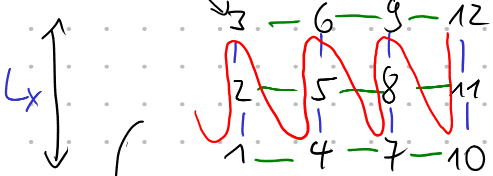
MPS = 1D ansatz, but: MPO allows long-range hopping

idea: map 2D system to a 1D chain

physical sites

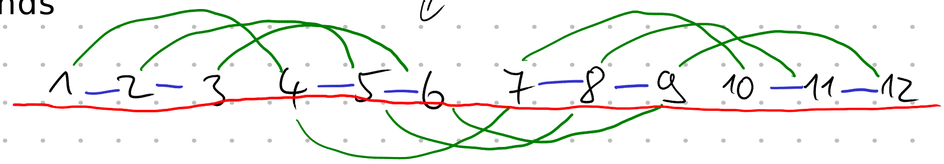
MPS "snake"

hopping in x and y



long range hopping!

pull on MPS ends



price: area law predicts $S = \text{const} \cdot L_y \leq \log \chi$

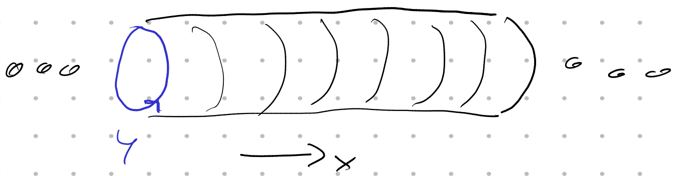
$$\Leftrightarrow \quad \chi \geq \exp(\text{const} \cdot L_y)$$

$\Rightarrow$ L_y needs to be small, but L_x can be big

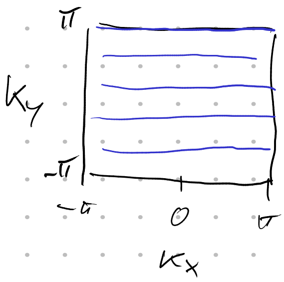
need to study scaling/dependence on L_y, often severe finite-size effects!

periodic boundary conditions in y-direction often reduce finite-width effect

$\rightsquigarrow$ infinite, narrow cylinder



allowed momenta in
Brillouin zone: Ly cuts



can shift cuts by
"threading flux through the cylinder"
= particles hopping around the cylinder
pick up a phase.