Introduction to MPS

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ETN Summer school, Padua 05/2024

(Some) Reviews / lecture notes:
JH, Pollmann arXiv:1805.00055
Schollwoeck arXiv:1008.3477
Vanderstaten et al. arXiv:1810.07006
Paeckel et al. arXiv:1901.05824
Cirac et al. arXiv:2011.12127

See also
https://tenpy.readthedocs.io/en/latest/literature.html

Motivation

Interested in (strongly correlated) quantum many body systems

many interesting phenomena, e.g.
- (high-Tc) superconductivity
- quantum Hall effect
- moire phyiscs on TMDs, twisted bilayer Graphene
- many body localization
- constrained dynamics, Hilbert space fragmentation
- ultracold atoms
- relations to quantum information / computing
- ...

Goal: solve Schrödinger equation

$$H\,|\psi_0\rangle = E_0\,|\psi_0\rangle$$

$$i\hbar\,\partial_t\,|\psi(t)\rangle = H\,|\psi(t)\rangle$$

Models

are usually local: $H = \sum_x h_x$ $\quad x$ on lattice

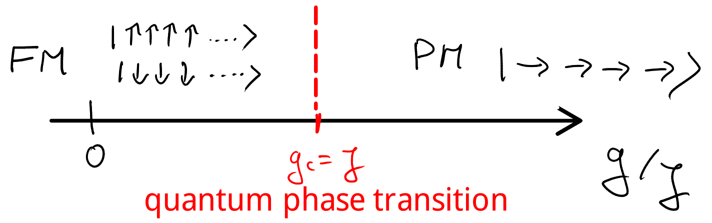
e.g. Hubbard model $H = -t \sum_{\langle i,j\rangle} \left(c_{i\sigma}^{\dagger} c_{j\sigma} + h.c.\right) + U \sum_i n_{i\uparrow} n_{i\downarrow}$

Heisenberg model $H = J \sum_{\langle i,j\rangle} \vec{S}_i \cdot \vec{S}_j$

1D Transverse field Ising model
(focus today)

$$H = -J \sum_{i=1}^{N-1} Z_i Z_{i+1} - g \sum_i^N X_i$$

ground state phase diagram:



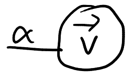
Challenge: exponentially large Hilbert space $\mathcal{H} = \bigotimes_{i=1}^{N} \mathbb{C}^d$

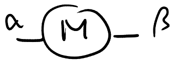
here: $d=2$ $\quad |\uparrow\rangle$, $|\downarrow\rangle$

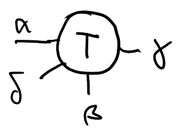
$\dim \mathcal{H} = d^N$ way too big to represent $|\psi\rangle$ exactly!

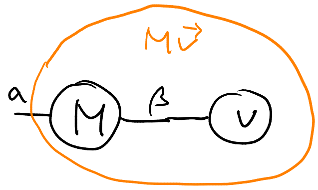
=> decompose wave function into tensor networks, with almost no error

Notation

vector $\vec{v} = (v_\alpha) =$ 

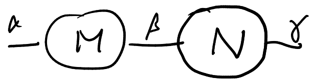
matrix $M = (M_{\alpha\beta}) =$ 

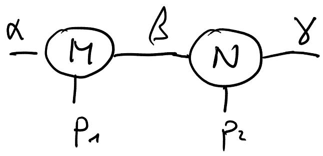
tensor $T = T_{\alpha\beta\gamma}^{\delta} =$ 

contraction $M\vec{v} = \sum_\beta M_{\alpha\beta} v_\beta =$ 

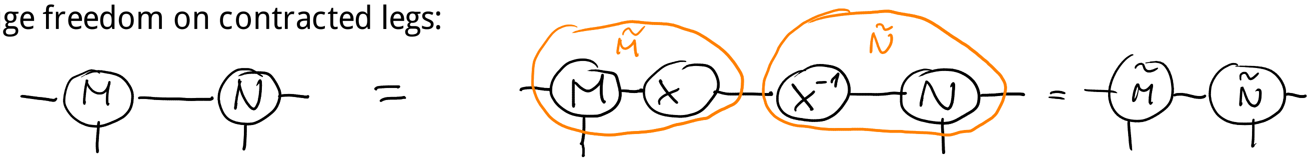
identity: $\mathbb{1} = \delta_{\alpha\beta} =$ 

computational cost of contraction: $\approx \mathcal{O}(\prod \text{leg dims})$ FLOPS

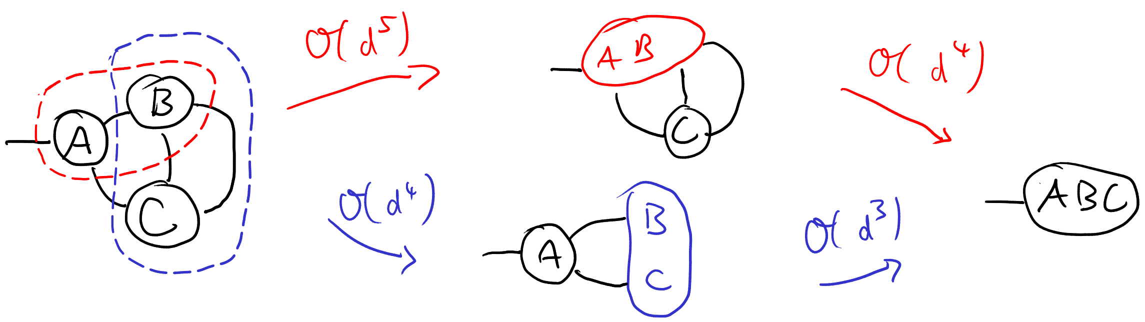
e.g. $\alpha, \beta, \gamma = 1 \dots \chi$,  $\to \mathcal{O}(\chi^3)$

$p_1, p_2 = 1, \dots d$  $\to \mathcal{O}(\chi^3 d^2)$

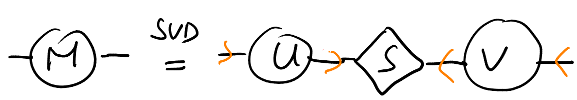
Note: gauge freedom on contracted legs:



Note: contraction order matters!

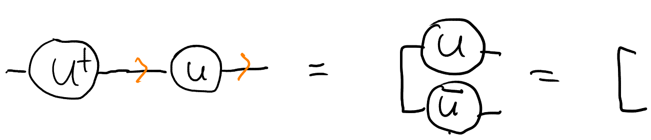


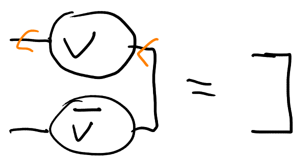
Singular Value Decomposition (SVD)

Theorem: for any matrix $M \overset{SVD}{=} U S V$ 

with diagonal S and $U^\dagger U = \mathbb{1}$, $V V^\dagger = \mathbb{1}$

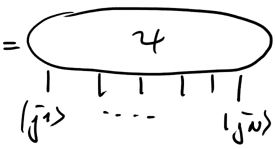
arrow notation: contracting incoming legs of U with $U^\dagger$ yields identity on outgoing legs:





Tensor network states: overview

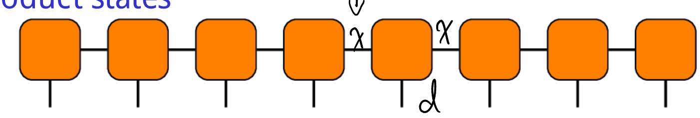
$|\psi\rangle = \sum_{j_1 \dots j_N}$ 

$|j_1 \dots j_N\rangle$ = 

different classes are different ansätze how to decompose ψ

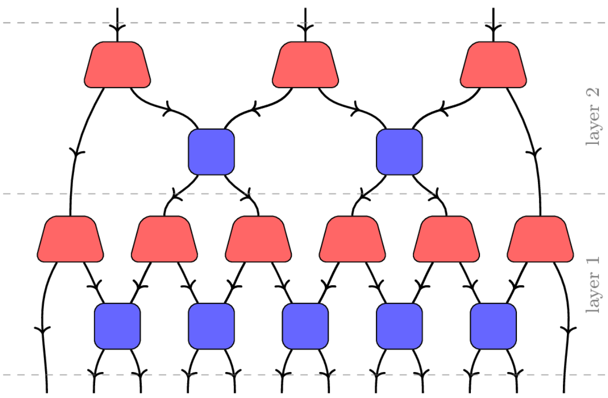
maximal "bond" dimension χ on "virtual" (contracted) legs $\rightsquigarrow$ number of free parameters $\mathcal{O}(N \cdot d \cdot \chi^2) \ll \mathcal{O}(d^N)$

MPS
matrix product states

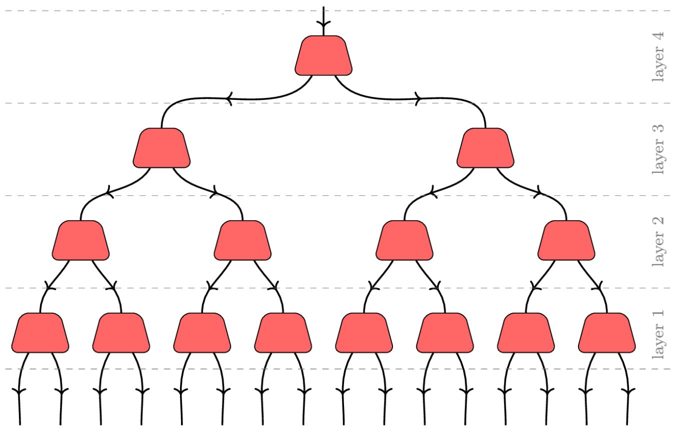


MERA
Multiscale entanglement renormalization ansatz

Tree TNS

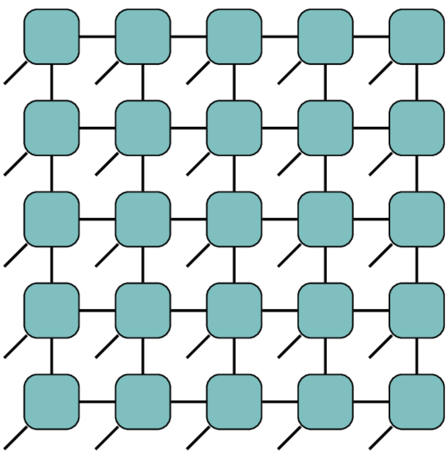


$\cong$

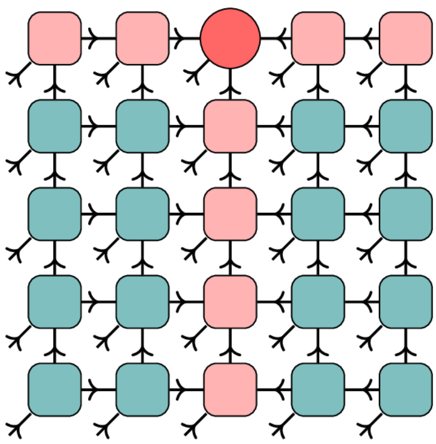


2D (or 3D) PEPS
Projected entangled pair states

isoTNS
isometric TNS



$\cong$

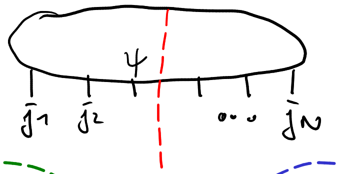


Why does this work??? "Area law of entanglement"

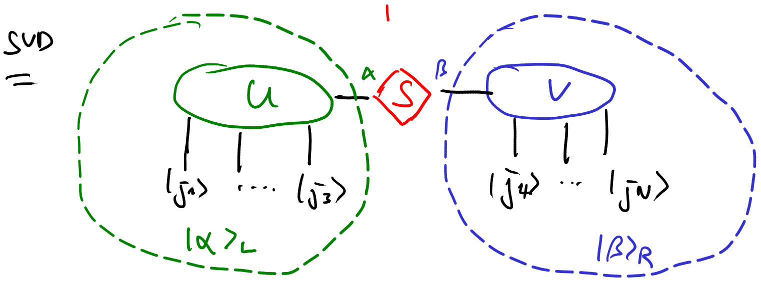
Schmidt decomposition

= apply SVD to wave function $|\psi\rangle$

$$|\psi\rangle = \sum_{j_1 \dots j_N}$$



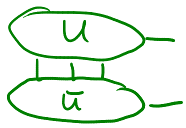
$|j_1 \dots j_N\rangle$



$$= \sum_\alpha |\alpha_L\rangle \, S_\alpha \, |\alpha\rangle_R$$

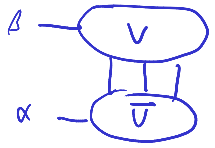
with orthonormal Schmidt basis (ONB)

$_L\langle \alpha | \beta \rangle_L =$

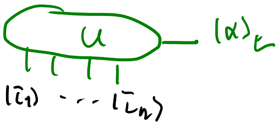


$= \Big[^{\beta}_{\alpha} = \delta_{\alpha\beta}$

$_R\langle \alpha | \beta \rangle_R =$



$= {}^{\beta}_{\alpha}\Big]$

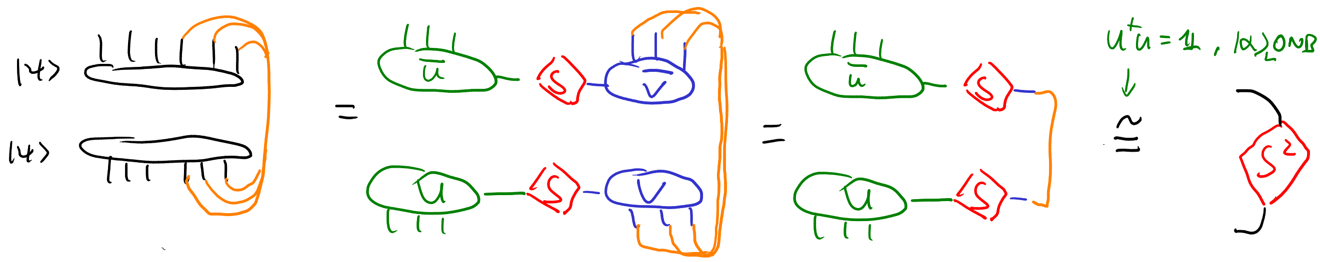


is basis transformation from $|i_1\rangle \otimes \dots |i_n\rangle$ into Schmidt basis!

Entanglement entropy

$$S = -\mathrm{Tr}\left(\rho_A \log \rho_A\right), \quad \rho_A = \mathrm{Tr}_B |\psi\rangle\langle\psi|$$

$\rho_A =$



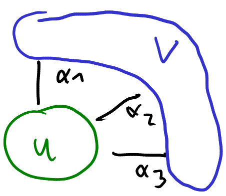
⇝ S_α^2 are eigenvalues of ρ_A (and ρ_B) ⇝ $\boxed{S = -\sum_\alpha S_\alpha^2 \log S_\alpha^2}$

normalization: $\mathrm{Tr}\, \rho_A = \sum_\alpha S_\alpha^2 \overset{!}{=} 1$

with bond dimension χ maximal for $S_\alpha^2 = \frac{1}{\chi}$ ⇝ $S \leq -\sum_\alpha \frac{1}{\chi} \log \frac{1}{\chi} = \log \chi$

⇝ too represent state with S, we need a (MPS) bond dimension $\boxed{\log \chi \geq S \text{ or } \chi \geq \exp(S)}$

for general cuts in a tensor network:



effectively group leg indices

$\alpha = (\alpha_1, \alpha_2, \alpha_3)$

α runs from 1 to $\chi^{(\#\text{legs cut})}$ ⇝ $\log\left[\chi^{(\#\text{legs cut})}\right] = (\#\text{legs cut}) \cdot \log \chi \geq S$

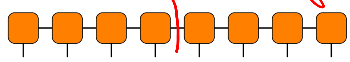
Area law of entanglement — Hastings 2007

For ground states of local, gapped H:

$S \sim$ length of cut

in 1D: length of cut = const

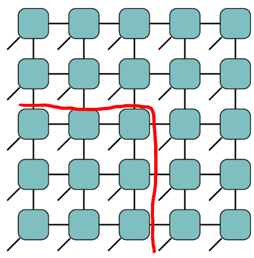
cut: 1 leg $\rightsquigarrow$ $\log \chi \geq S$



$\rightsquigarrow$ area law captured by MPS!

in 2D: number of legs cut ~ length of cut

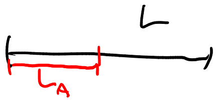
$\rightsquigarrow$ captured by PEPS!



in contrast: conformal field theory prediction for critical (non-gapped) systems in 1D:

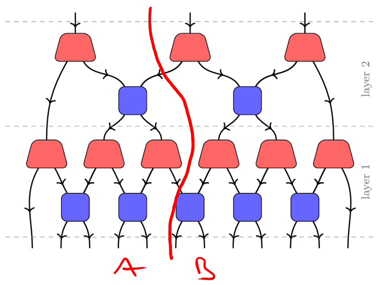
Calabrese, Cardy 2004

$$S = \frac{c}{6} \log\left(\frac{L_A}{\pi a} \sin\left(\frac{\pi L_A}{L}\right)\right) + \text{const} \underset{L_A = \frac{L}{2}}{=} \frac{c}{6} \log(L_A) + \text{const}$$



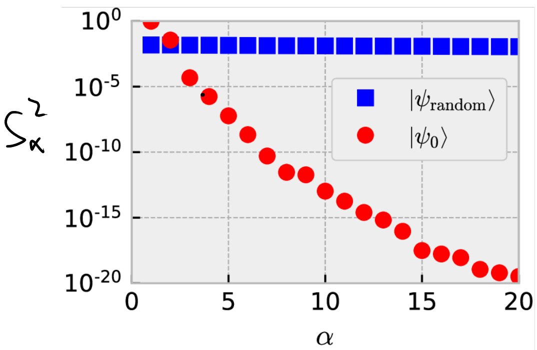
$\rightsquigarrow$ can be used to extract central charge c

captured by MERA:

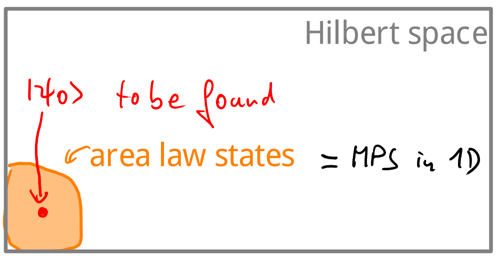


legs cut ~ # layers ~ log L

The area law explains why we can use tensor networks:



ground states are in a small corner of the Hilbert space, which we can represent and search with TNS

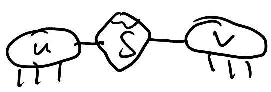


$= MPS$ in 1D

$\Rightarrow$ we can truncate in the Schmidt spectrum

keep only χ_{max} rows/columns of U/S/V

$$|\psi\rangle = \sum_{\alpha=1}^{2^{L_A}} |\alpha_L\rangle\, S_\alpha\, |\alpha_R\rangle \approx \sum_{\alpha=1}^{\chi_{max}} |\alpha_L\rangle\, \tilde{S}_\alpha\, |\alpha_R\rangle =$$



renormalize $\quad \tilde{S}_\alpha = S_\alpha \Big/ \sqrt{\sum_{\alpha<\chi}' S_\alpha^2}$

truncation error:

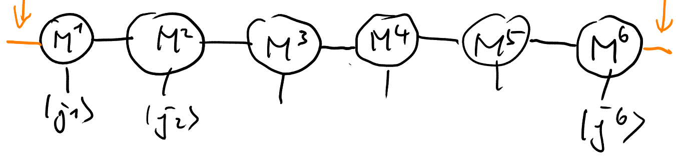
$$\left\| |\psi\rangle - |\psi^{tr}\rangle \right\|^2 = 2\left(1 - \sqrt{\sum_{\alpha<\chi} S_\alpha^2}\right) \approx \sum_{\alpha>\chi} S_\alpha^2$$

In the following, we focus on MPS

Canonical Form

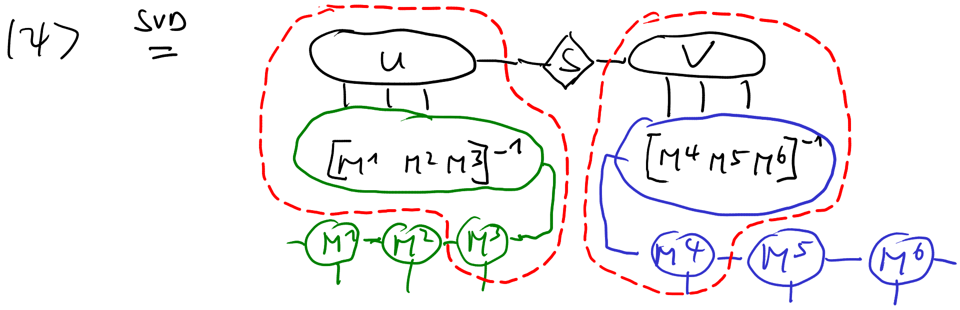
trick: introduce dummy indices $\alpha=1$, $\beta=1$ on the boundaries to make tensors look like bulk

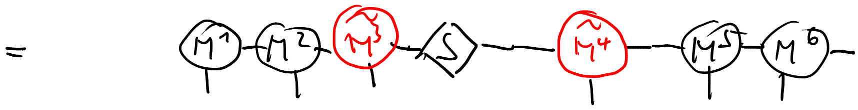
General MPS: $|\psi\rangle =$



no isometry conditions

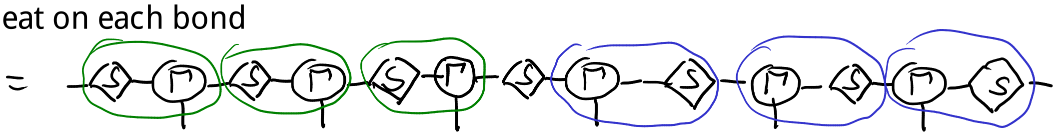
Canonical form: use gauge freedom of inserting XX^{-1} on the virtual bonds to bring MPS into Orthonormal form corresponding to Schmidt states on each bond:





drop site indices from tensors to simplify notation

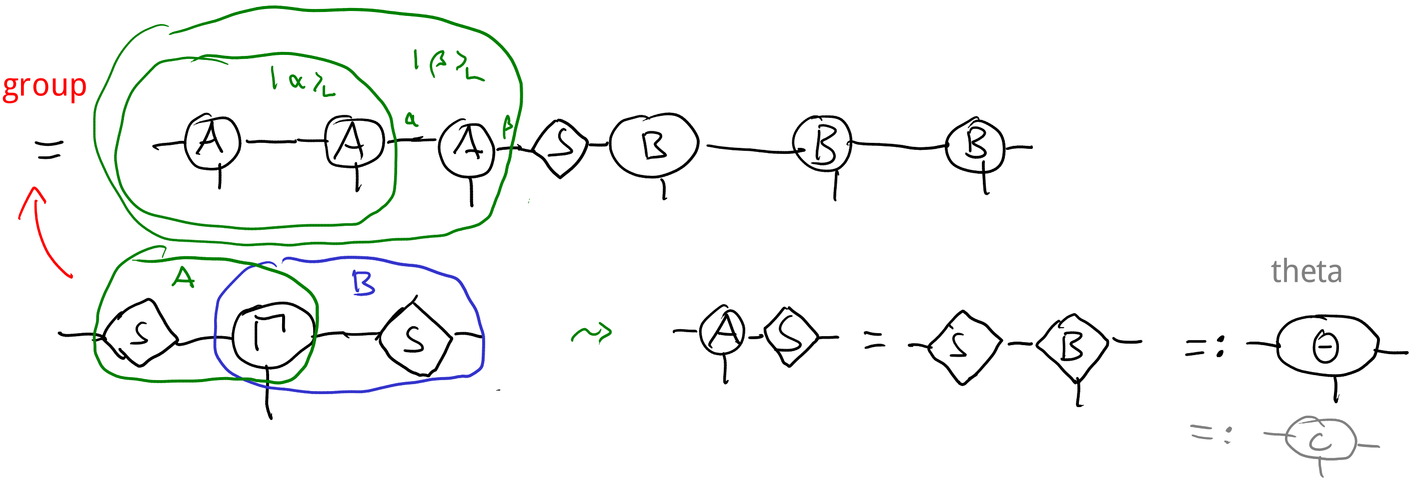
repeat on each bond



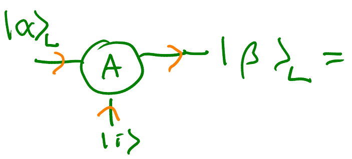
this is Vidal's Gamma-Lambda notation

here S instead of Lambda

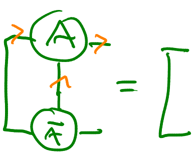
group

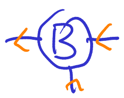


The A / B tensors are basis transformations of Schmidt vectors and hence isometries!

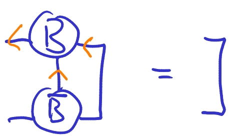


$= \sum_{i,\alpha} A^{i}_{\alpha\beta} |\alpha\rangle_L |i\rangle$



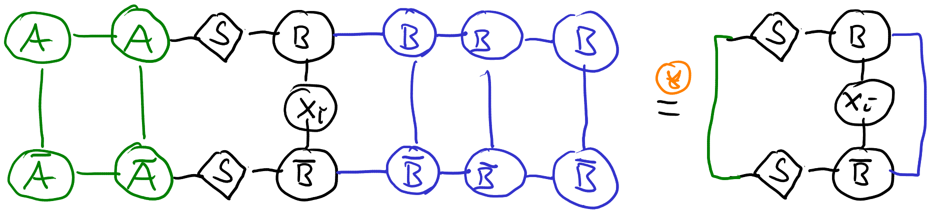


similarly:



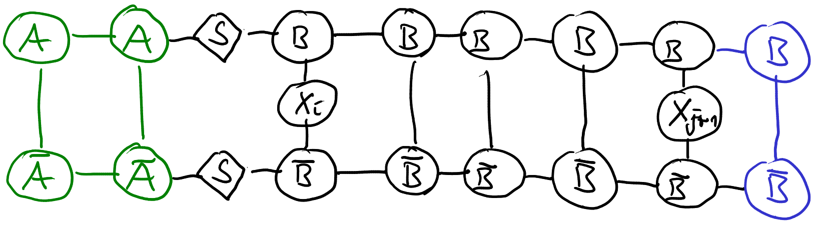
Expectation values

$\langle X_i \rangle \equiv \langle \psi | X_i | \psi \rangle =$

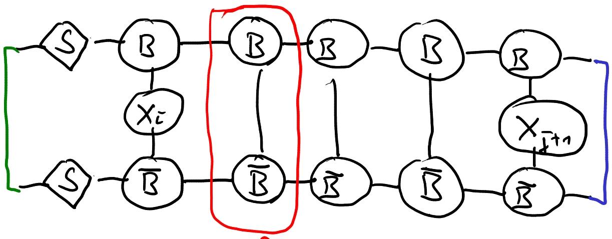


Correlation function

$\langle X_i \, X_{j+1} \rangle =$



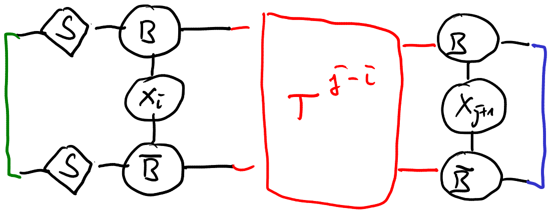
$=$



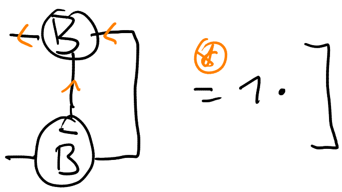
Transfermatrix T

for translation invariant MPS

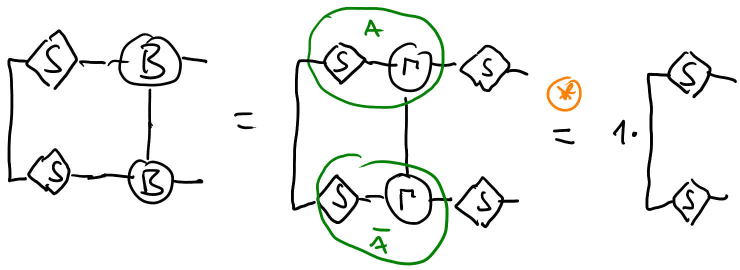
$=$



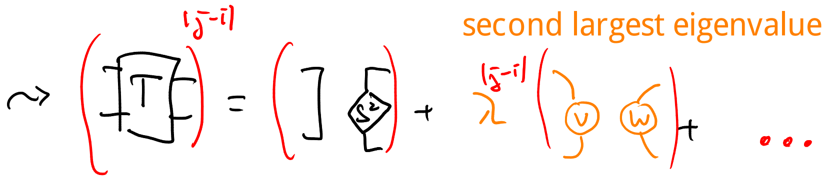
T (as matrix from left to right) is not hermitian: left/right eigenvectors are not the same.
Dominant eigenvectors with eigenvalue 1 are:



and



second largest eigenvalue / -vectors $|\lambda| < 1$

$\rightsquigarrow$  subleading

$\rightsquigarrow$ $\langle X_i X_j \rangle \overset{\sim}{=}$ 

$j-i \gg 1$

$= \langle X_i \rangle \underbrace{}_{\langle X_{j+1}\rangle} + e^{-\frac{1}{\xi}|j-i|} \underbrace{}_{\text{const}}$

correlations decay exponentially in MPS!
powerlaw correlations in critical states are approximated by sums of exponentials