TENSOR NETWORKS FOR QUANTUM MANY-BODY SYSTEMS

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MCQST

DFG FOR 5522

DFG TRR 360

T-NiSQ

Benasque, 17.4.2024
NTQC2024

In this talks…

NOTES:

introducing Tensor Network States

basic numerical algorithms

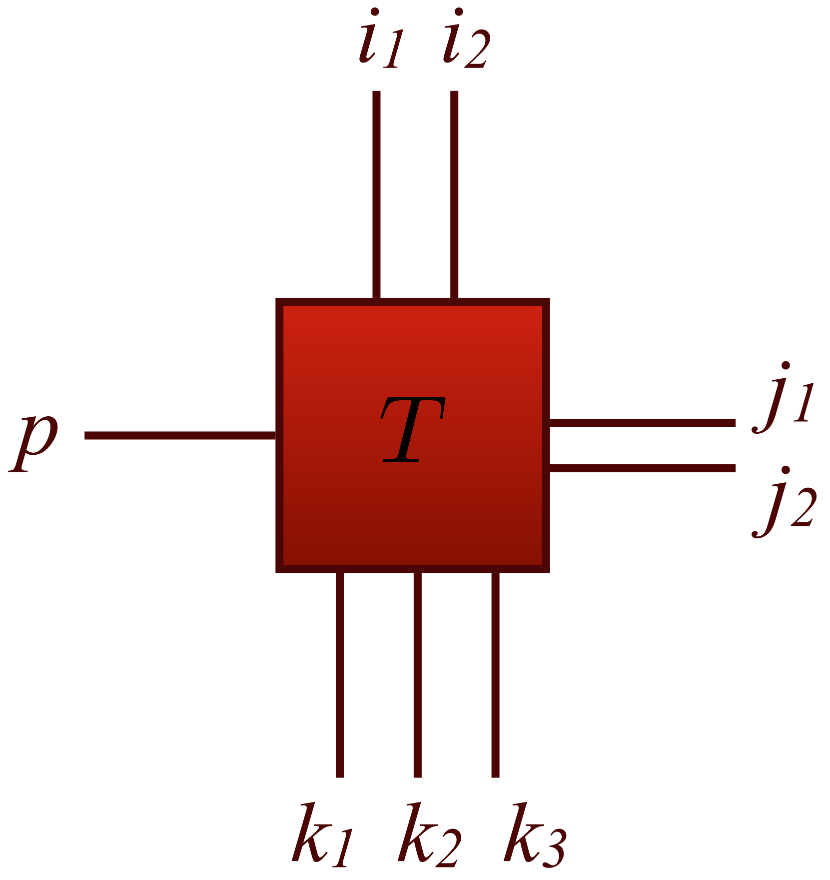
unguided TUTORIAL:

What are tensor networks?

a graphical language ( )

pictorial representation

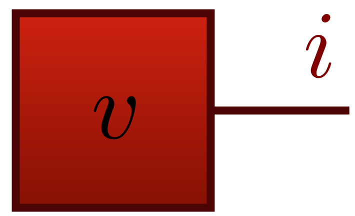
tensor = multidimensional array



$$\{T_{i_1 i_2, j_1 j_2, k_1 k_2 k_3, p}\}_{\{i,j,k,p\}}$$

pictorial representation

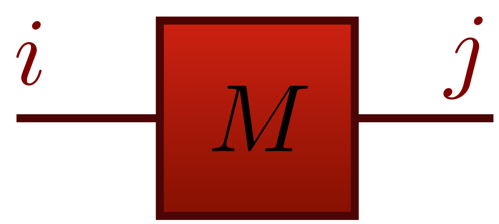
vector



v_i

$i = 1, \ldots D$

matrix

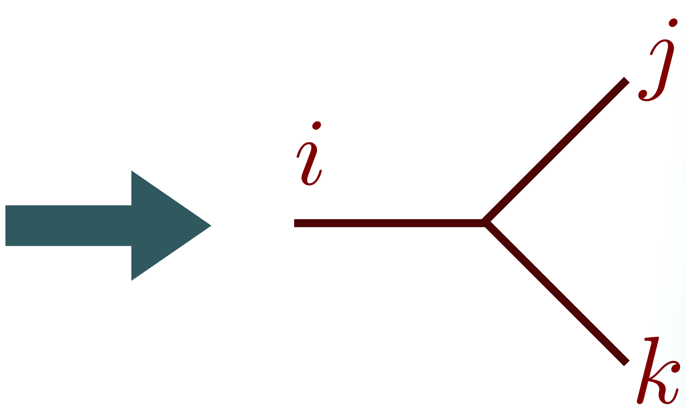


M_{ij}

$i = 1, \ldots D_1$
$j = 1, \ldots D_2$

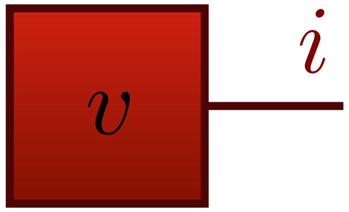
a special case

δ_{ij}

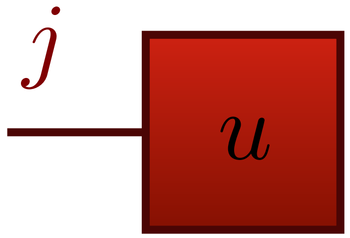


contractions

vector

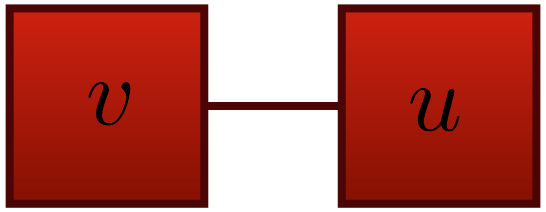


v_i $\quad i = 1, \ldots D$



u_j $\quad j = 1, \ldots D$

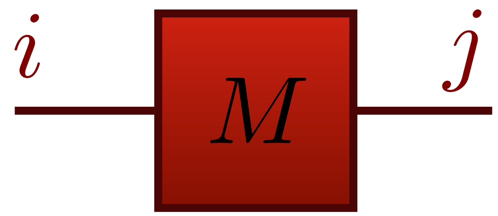
vector-vector



$$v \cdot u = \sum_i v_i u_i$$

contractions

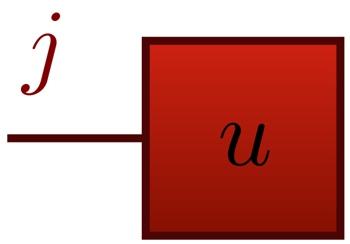
matrix



M_{ij}

$i = 1, \ldots D_1$
$j = 1, \ldots D_2$

vector



u_j

$j = 1, \ldots D_2$

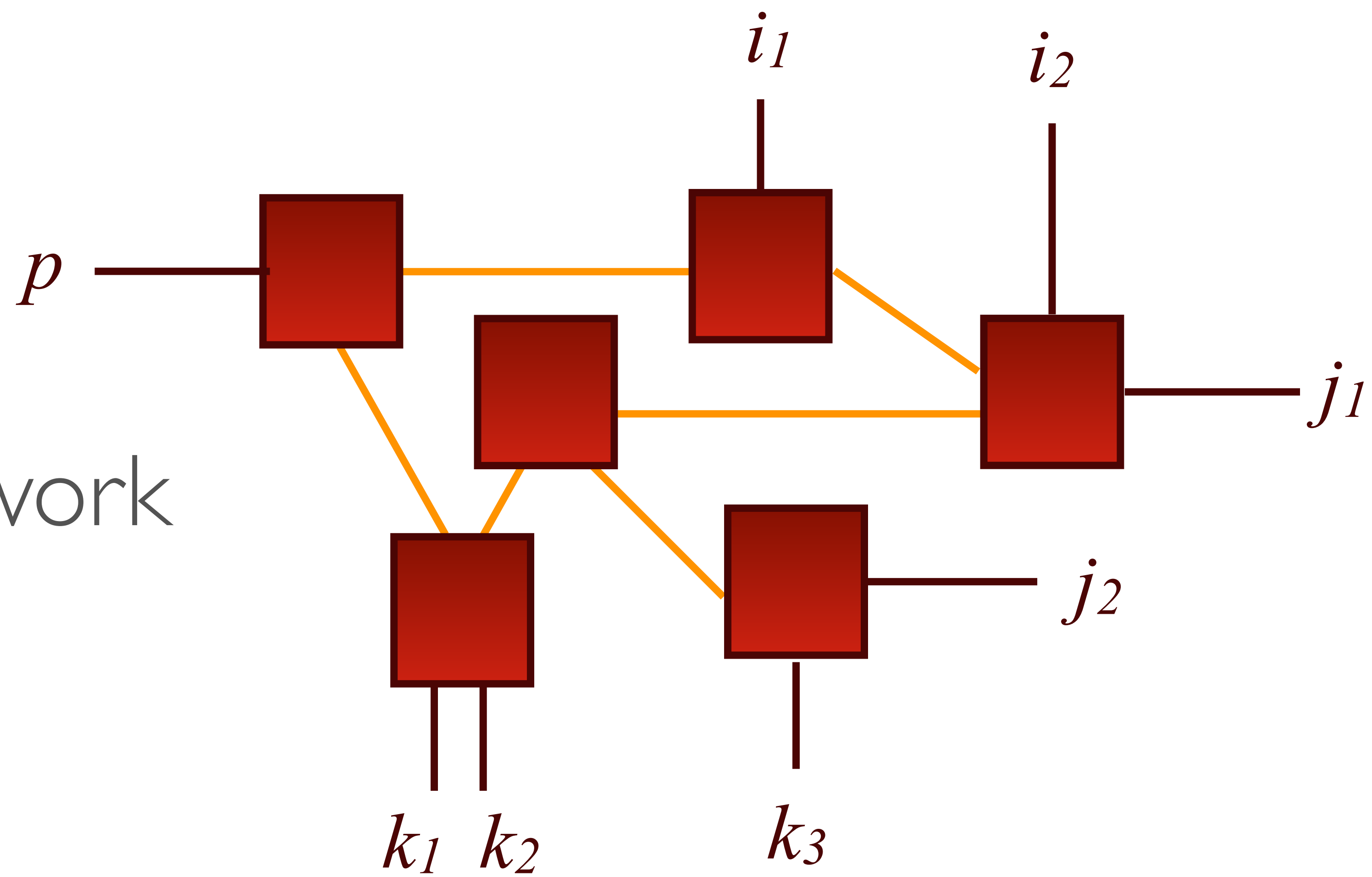
matrix-vector

$$v = M \cdot u = \sum_j M_{ij} u_j$$

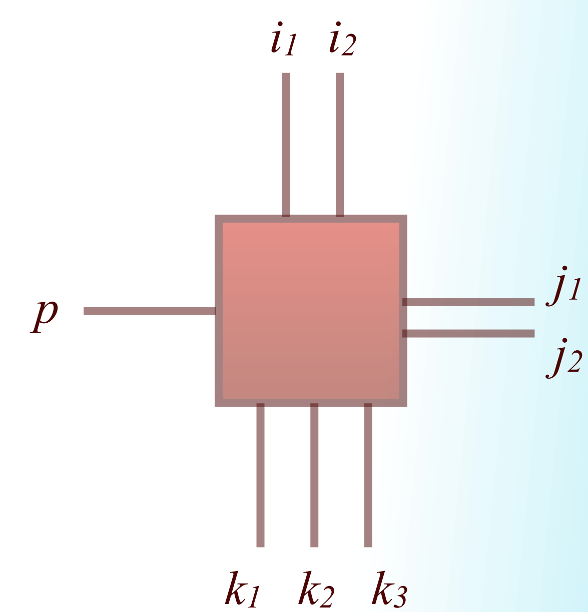
tensor network

tensor = multidimensional array

tensor network
(TN)

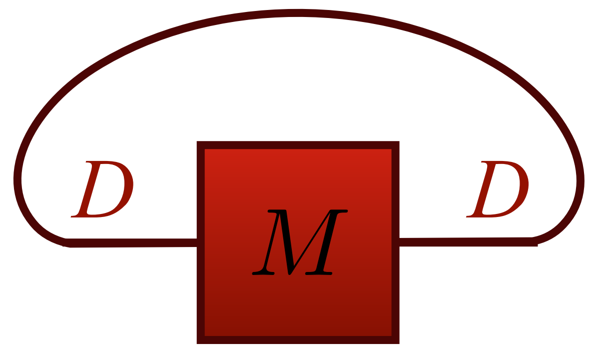


$$\{T_{i_1 i_2, j_1 j_2, k_1 k_2 k_3, p}\}_{\{i,j,k,p\}}$$



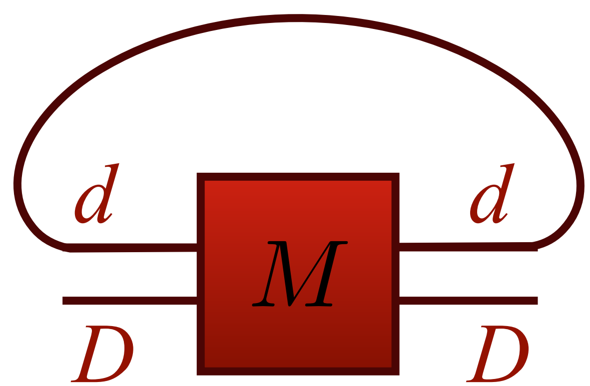
basic routines

trace ?



$$M_{ij}$$

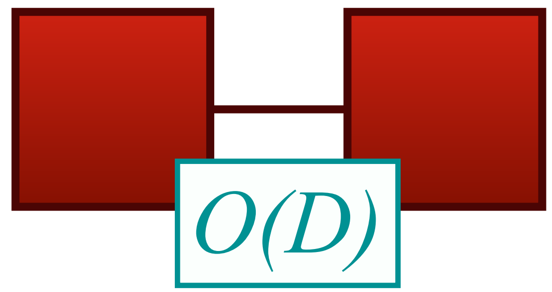
partial trace



$$\sum_{ij} M_{ia,jb}\delta_{ij} = \sum_{i} M_{ia,ib}$$

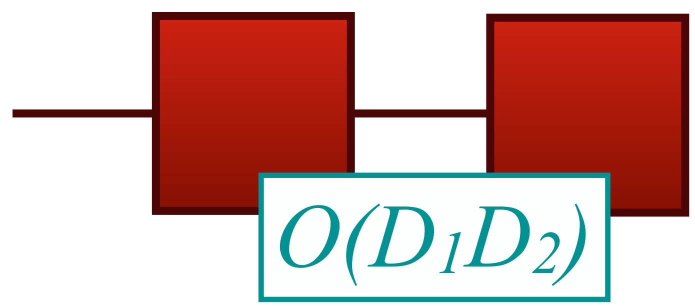
computational costs

vector-vector



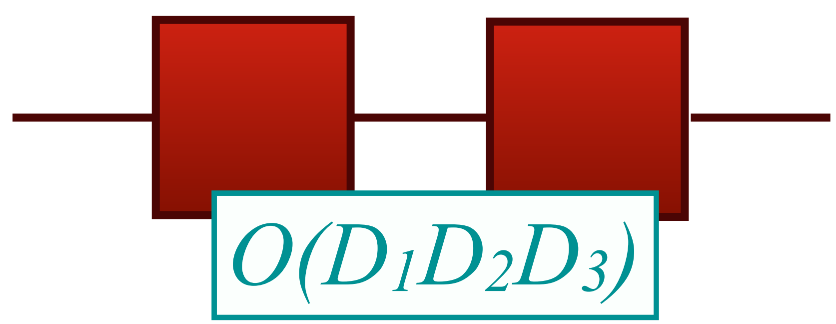
$$v \cdot u = \sum_i v_i u_i$$

matrix-vector



$$v = M \cdot u = \sum_j M_{ij} u_j$$

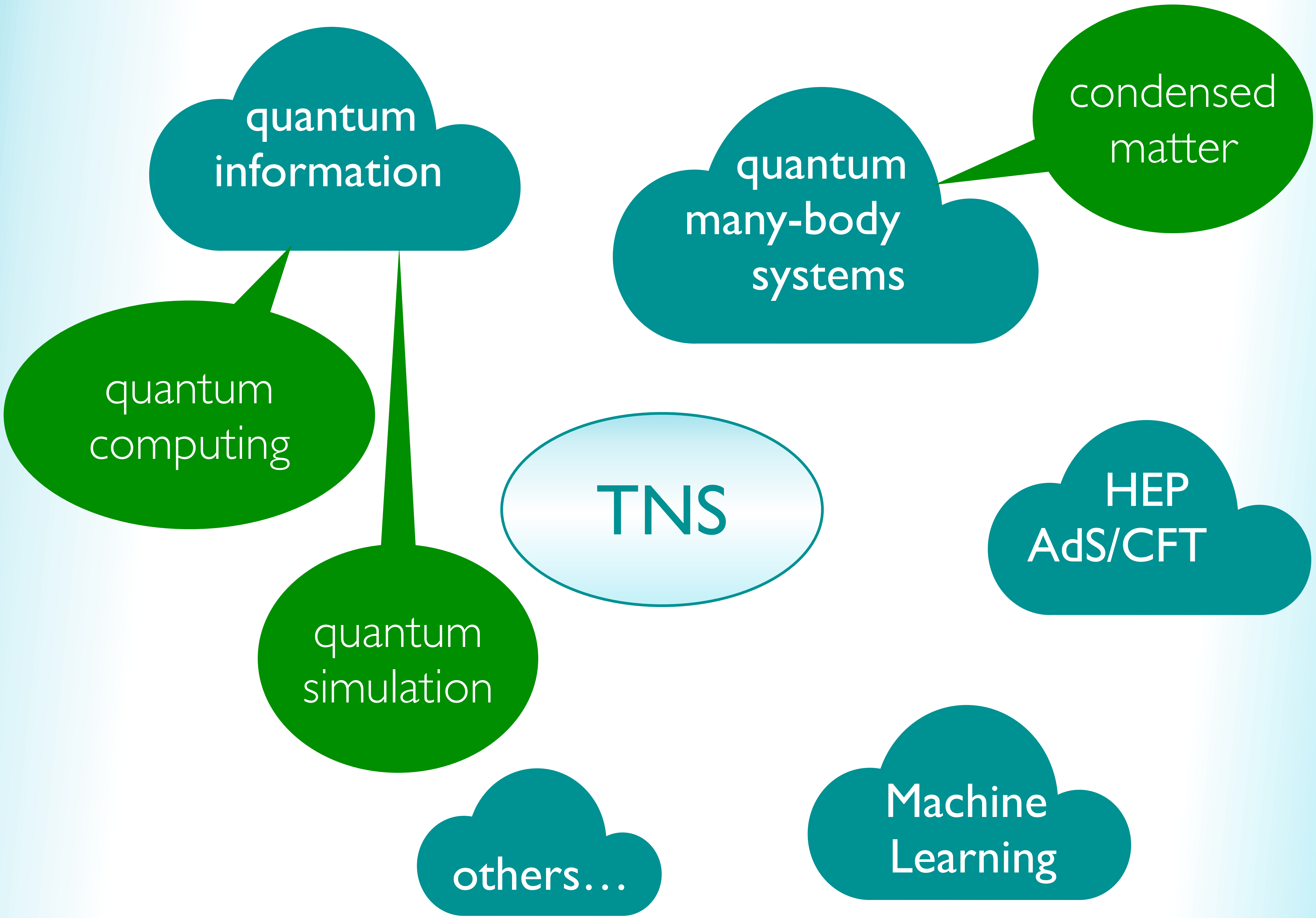
matrix-matrix



$$M \cdot N = \sum_j M_{ij} N_{jk}$$

in general: product of open and contracted dimensions pictorial representation

Why are they interesting?

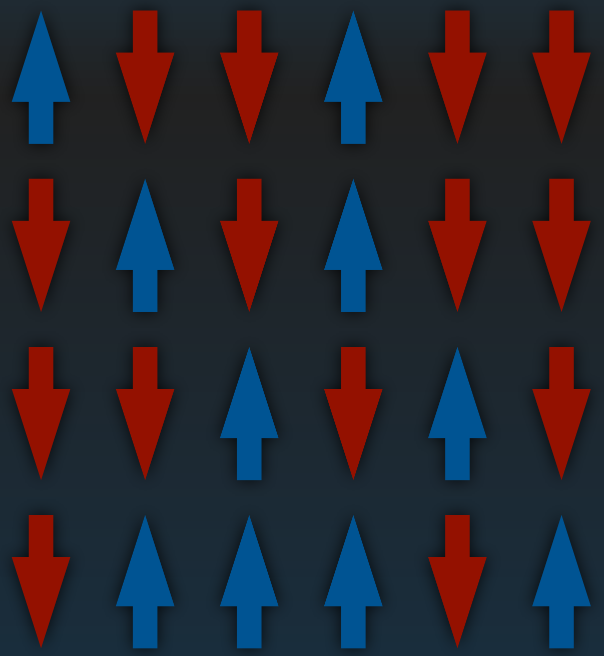

quantum information
quantum computing
quantum simulation
TNS
quantum many-body systems
condensed matter
HEP AdS/CFT
Machine Learning
others…

many-body problems are hard…

classical *vs* quantum systems

classical spin system

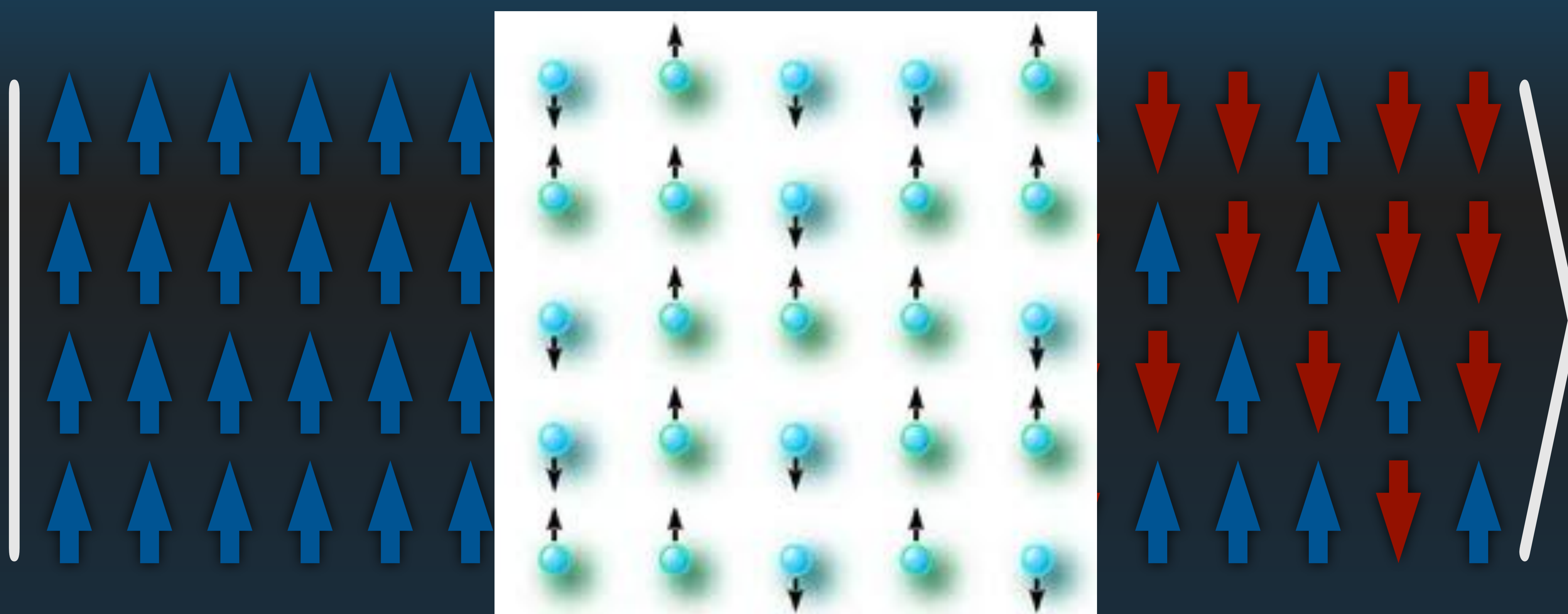
$$H = \sum_{<ij>} h_{ij}$$



2^n possibilities

quantum systems are more difficult to simulate

classical *vs quantum* systems

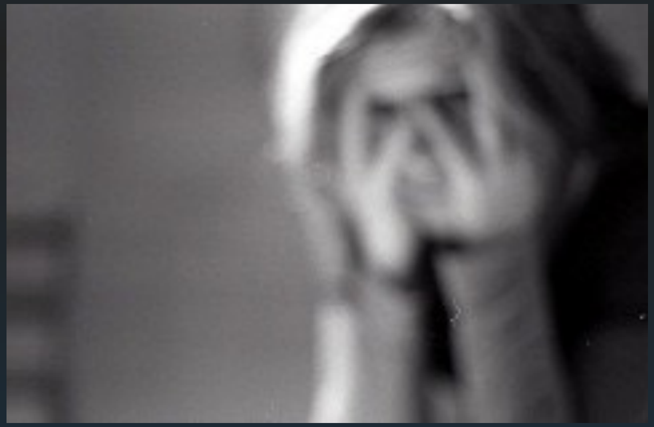
c_1  $\dots$

2^n basis dimension

quantum spin system

$$H = \sum_{\langle ij \rangle} h_{ij}$$

Classical simulation of quantum problems?



in general, impossible

but quantum information gives us useful tools for some cases

TNS: quantum inspired tools for the classical simulation of quantum many-body problems

WHAT ARE TNS?

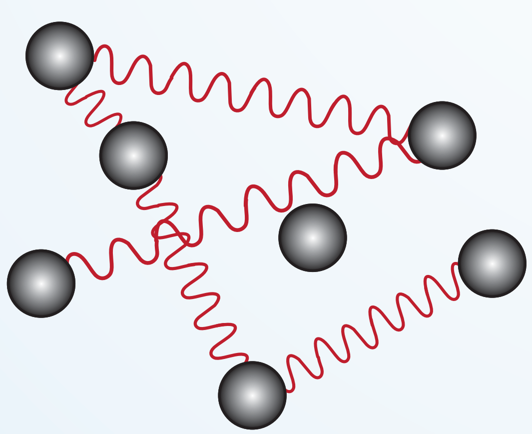
- TNS = Tensor Network States

Context: quantum many body systems

interacting with each other

$\{|i\rangle\}_{i=0}^{d-1}$

N



Goal: describe

interesting states

equilibrium states

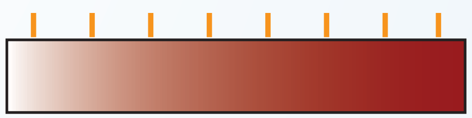
ground, thermal states

WHAT ARE TNS?

- TNS = Tensor Network States

A general state of the N-body Hilbert space has exponentially many coefficients

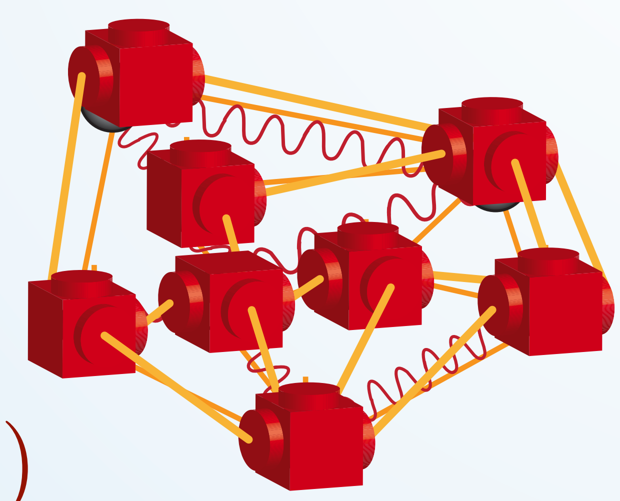
$$|\Psi\rangle = \sum_{i_j} \boxed{c_{i_1 \dots i_N}} |i_1 \dots i_N\rangle$$



N-legged tensor

d^N

N



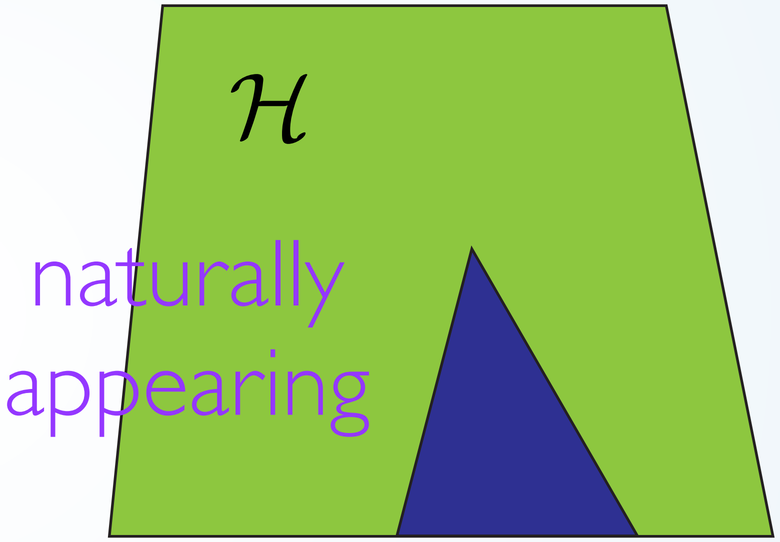
$\text{poly}(N)$

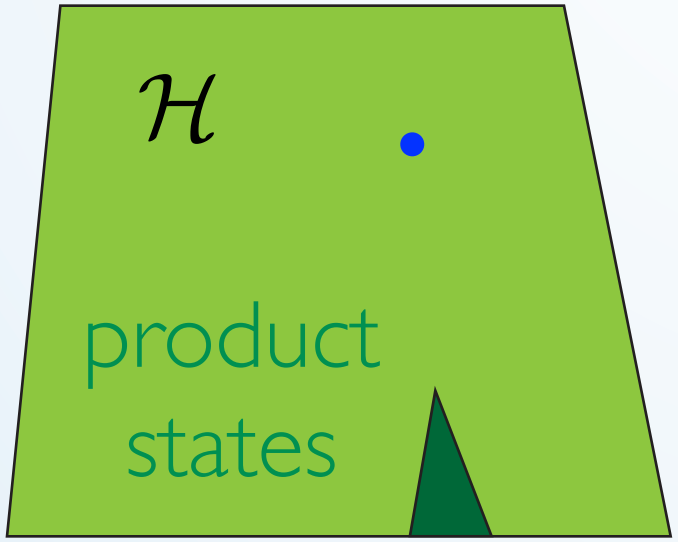
A TNS has only a polynomial number of parameters

WHY SHOULD TNS BE USEFUL?

States appearing in Nature are peculiar

State at random from Hilbert space is not close to product





We look for the particular "*corner*" of the Hilbert space

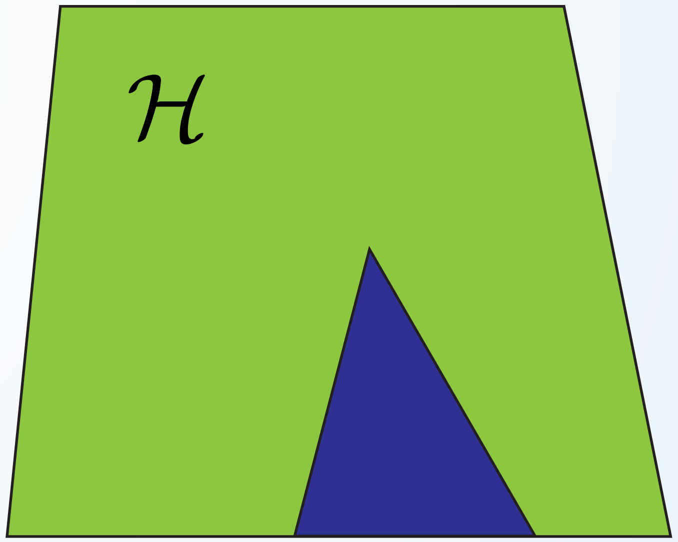
- TNS = Tensor Network States

WHY SHOULD TNS BE USEFUL?

The goal is to find good descriptions of physical states

WANTED

- ➡ efficient representation
- ➡ computable observables
- ➡ (variational) algorithms



entanglement is a good criterion

entanglement in TNS picture

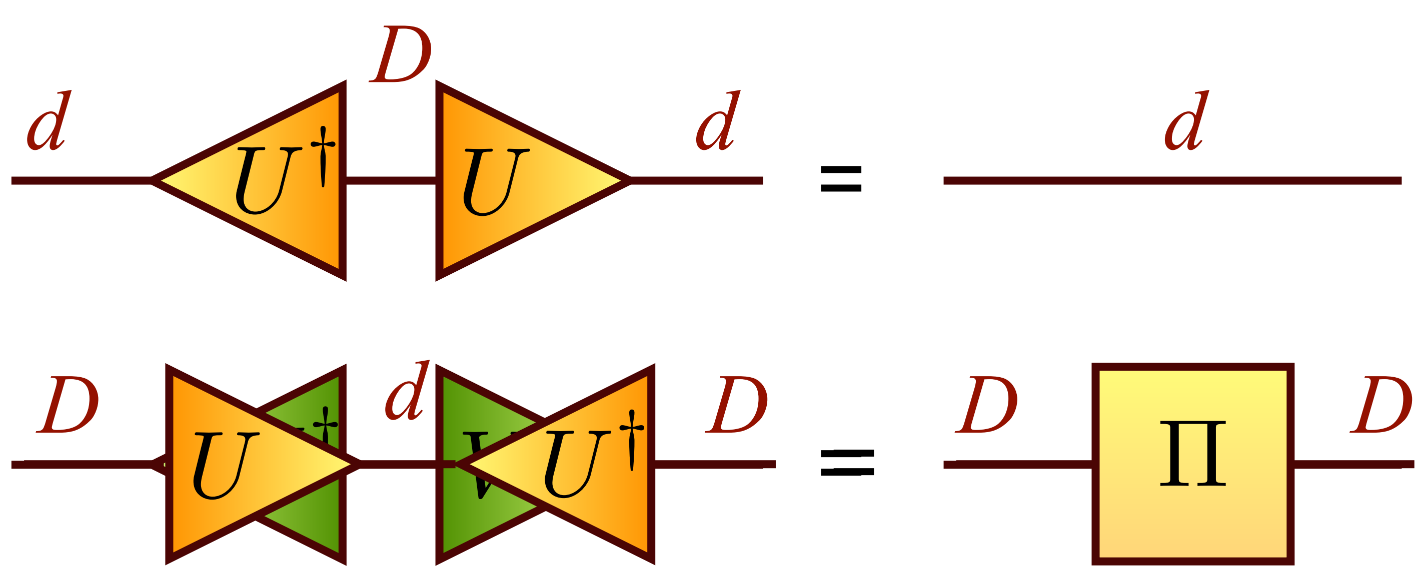
recall: any matrix admits a singular value decomposition (SVD)

$$A = USV^\dagger$$

diagonal

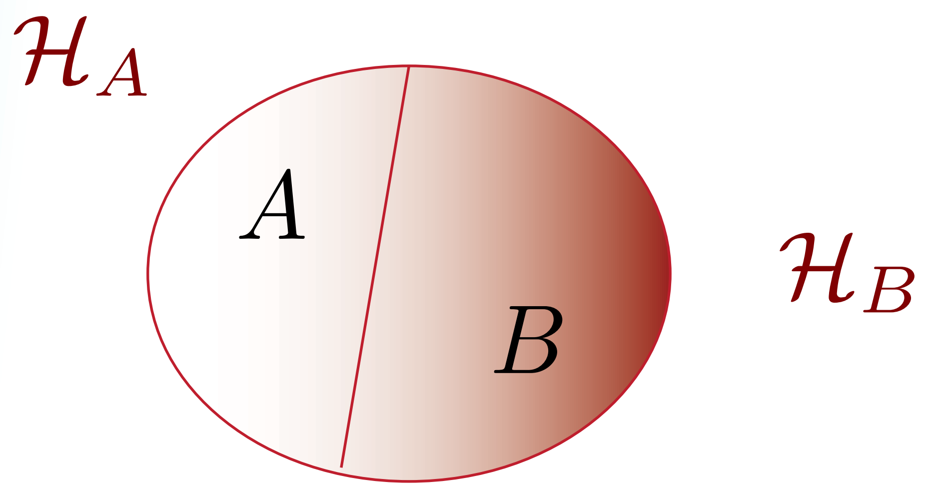
isometries

isometry



entanglement in TNS picture

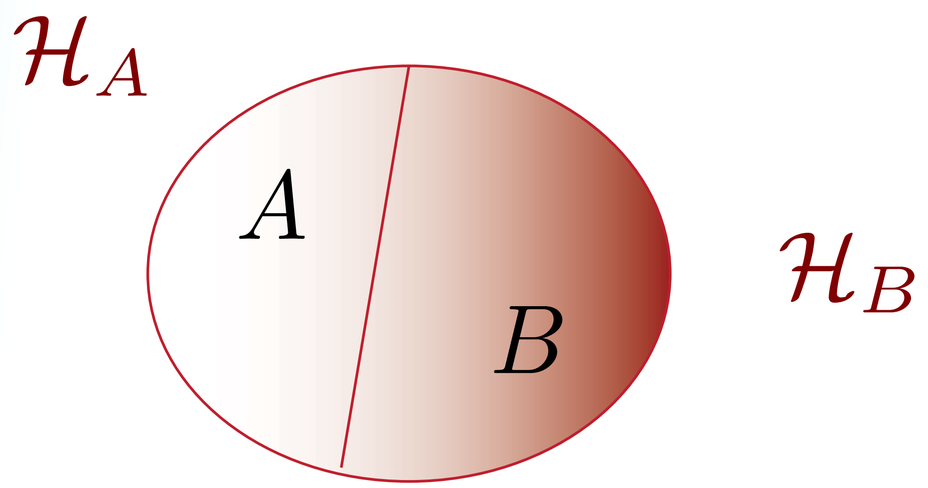
SVD ⇒ Schmidt decomposition



$$|\Psi\rangle = \sum_{ij} \Psi_{ij} |ij\rangle_{AB}$$

entanglement in TNS picture

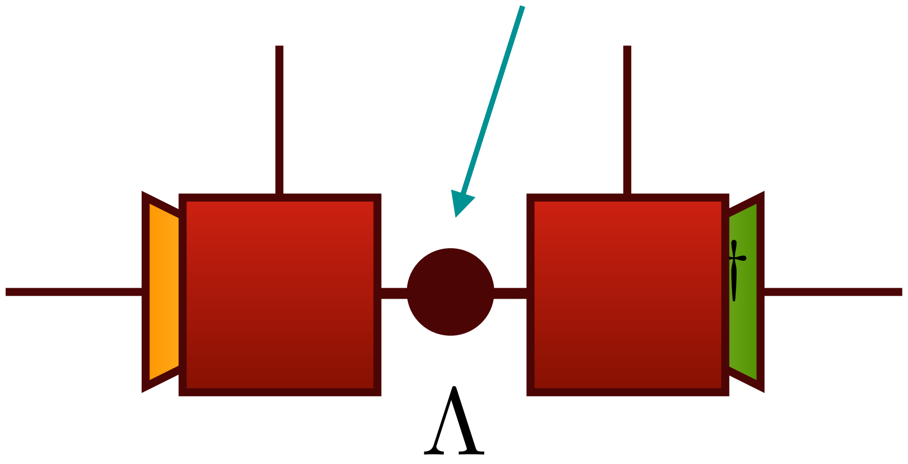
SVD $\Rightarrow$ Schmidt decomposition



$$|\Psi\rangle = \sum_{ij} \Psi_{ij} |i\rangle |j\rangle$$

$$|\Psi\rangle = \sum_k \lambda_k |u_k\rangle_A |v_k\rangle_B = \sum_k \lambda_k \left(\sum_i U_{ik} |i\rangle_A\right)\left(\sum_j V^\dagger_{kj} |j\rangle_B\right)$$

Schmidt coefficients



Schmidt rank: number of non-zero λ_k coefficients

$$\Psi_{ij} = \sum U_{ik} \lambda_k V^\dagger_{kj}$$

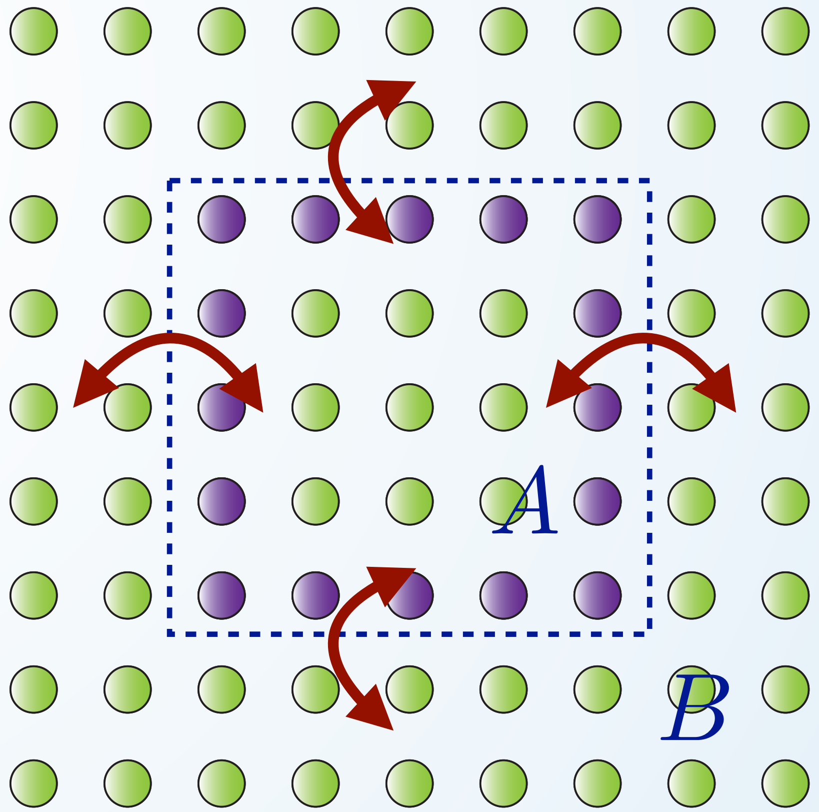
$$\mathrm{E}(|\Psi\rangle) = -\mathrm{tr}\,(\rho_A \log \rho_A) = -\sum_k \lambda_k^2 \log \lambda_k^2$$

finite range
gapped
Hamiltonians

$\Downarrow$

ground states with
little entanglement

Area law



$$S_{A\max} \propto |\delta A|$$

local gapped 1D Hamiltonians
have ground states
with area law of entanglement

$$S_{A\max} \propto |\delta A|$$

Hastings 2007

in 1D critical systems,
logarithmic corrections

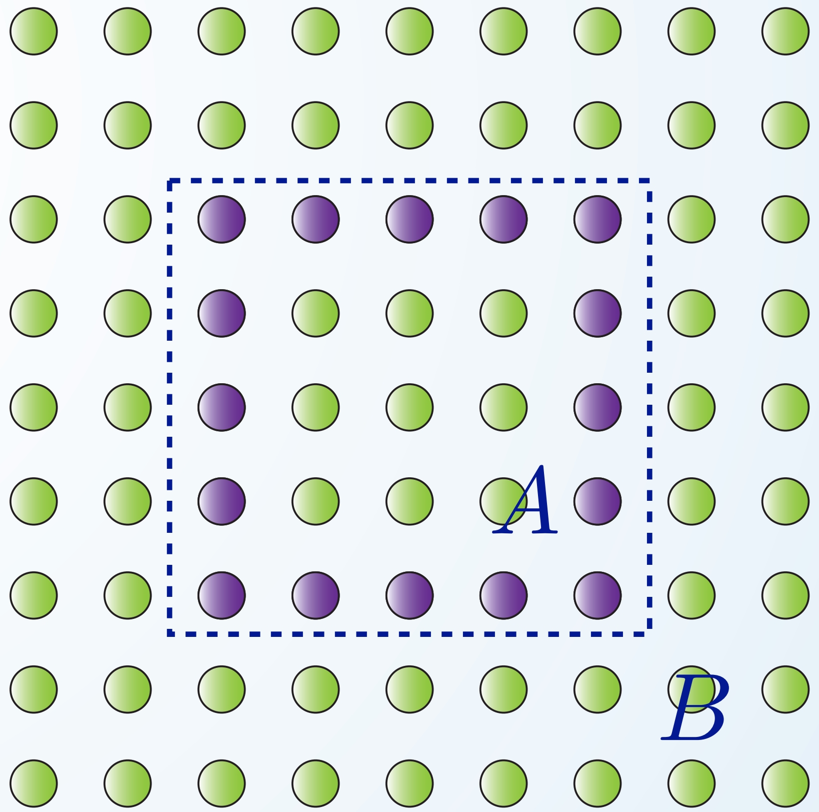
$$S_{A\max} \propto |\delta A| \log A$$

Calabrese, Cardy 2004

satisfied at finite temperature

Wolf, Verstraete, Hastings, Cirac, 2008

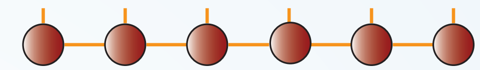
Area law



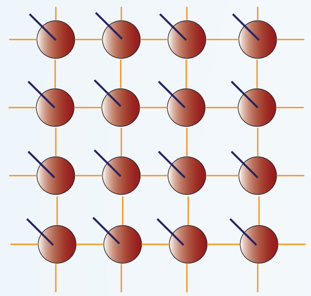
FINDING A GOOD ANSATZ

MPS & PEPS

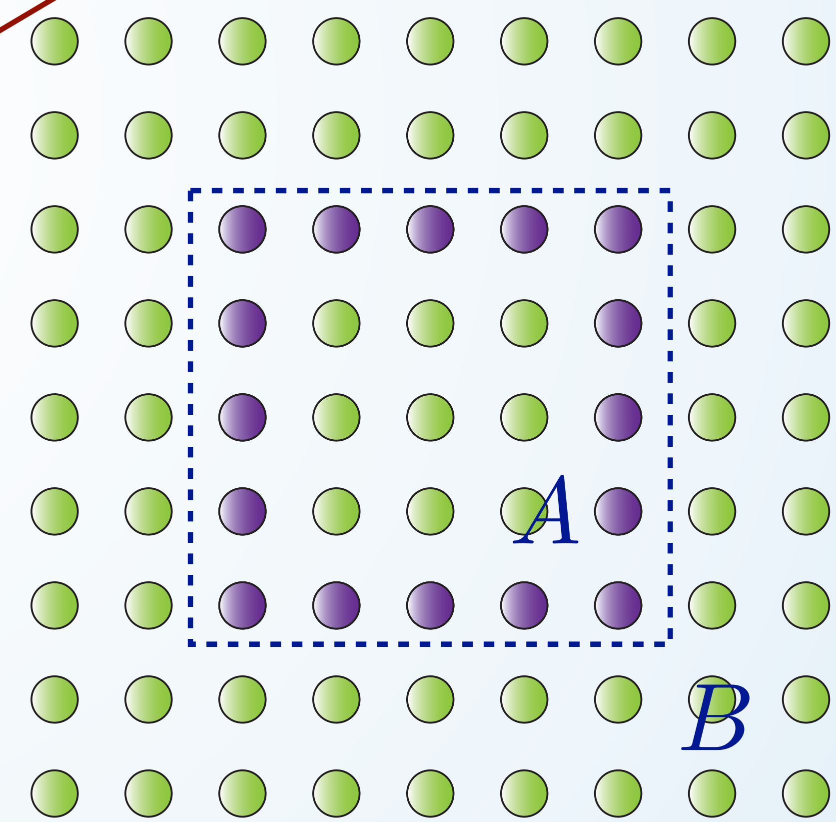
- MPS = Matrix Product States



- PEPS = Projected Entangled Pairs States



Area law

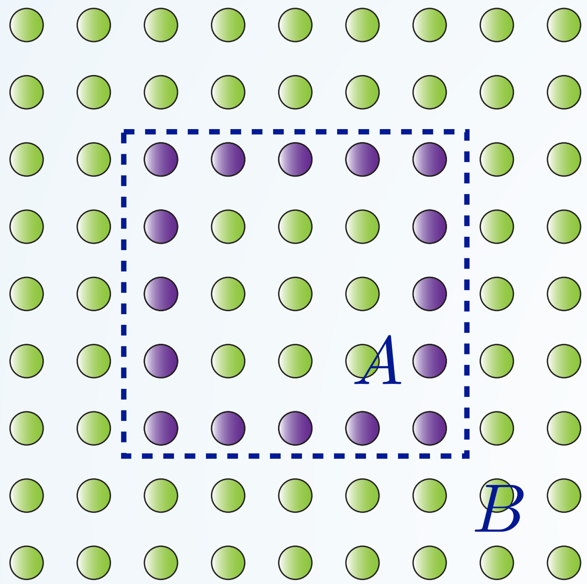


Ansätze satisfying
the area law
by construction

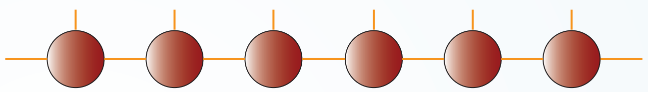
TNS = entanglement based ansatz

TNS = entanglement based ansatz

area law

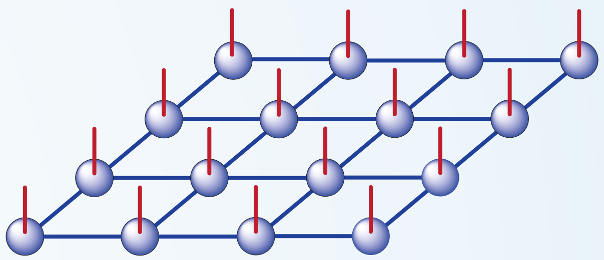


MPS



Schollwöck Ann.Phys.2011

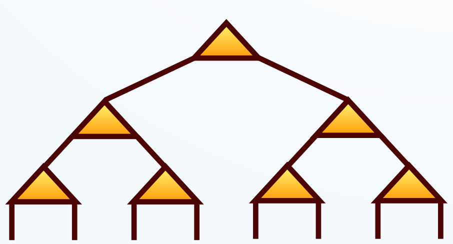
PEPS



Verstraete et al. Adv. Phys. 2008

other TNS

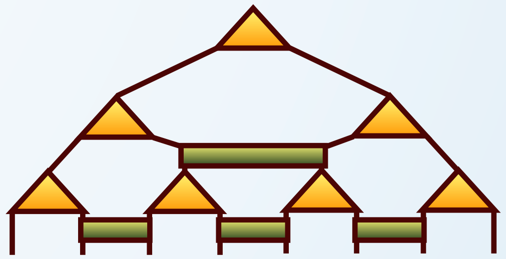
TTN

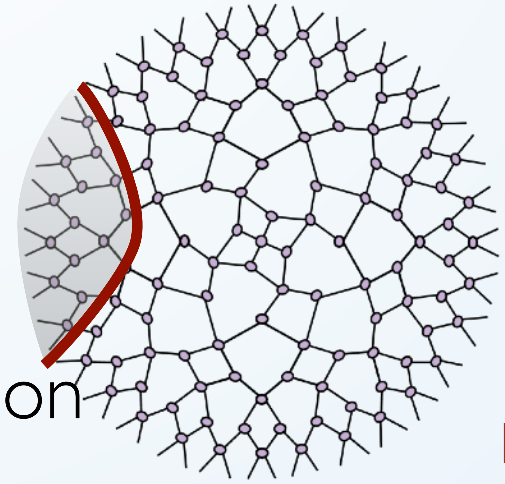


Shi et al PRA 2006

Vidal PRL 2007

MERA





suggested connection
to AdS/CFT

Swingle PRD 2012
Molina JHEP 2013
Nozaki et al JHEP 2012
Bao et al PRD 2015

MPS

Matrix Product States

MPS

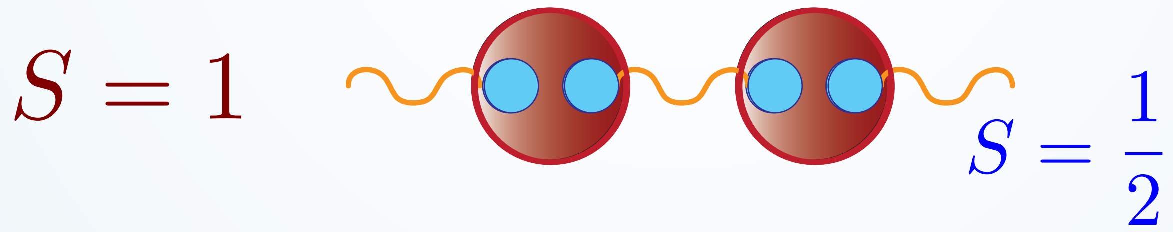
Matrix Product States

A bit of history...

AKLT exactly solvable spin model

Affleck, Kennedy, Lieb, Tasaki, PRL 1987

$$H_{ii+1} = \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}\left(\vec{S}_i \cdot \vec{S}_{i+1}\right)^2$$



The ground state is exactly a MPS (VBS)

MPS

Matrix Product States

A bit of history...

AKLT exactly solvable spin model

Affleck, Kennedy, Lieb, Tasaki, PRL 1987

↓

Finitely correlated states

Fannes, Nachtergaele, Werner, CMP 1992

Formal properties of generalized VBS on rings

MPS

Matrix Product States

A bit of history...

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Affleck, Kennedy, Lieb, Tasaki, PRL 1987

↓

Finitely correlated states

Fannes, Nachtergaele, Werner, CMP 1992

DMRG algorithm

White, PRL 1992

ground states of quantum spin chains

quasiexact

applied to other systems (Q.Chem., 2D)

MPS

Matrix Product States

A bit of history...

AKLT exactly solvable spin model

Affleck, Kennedy, Lieb, Tasaki, PRL 1987

↓

Finitely correlated states

Fannes, Nachtergaele, Werner, CMP 1992

DMRG algorithm

White, PRL 1992

DMRG variational over MPS

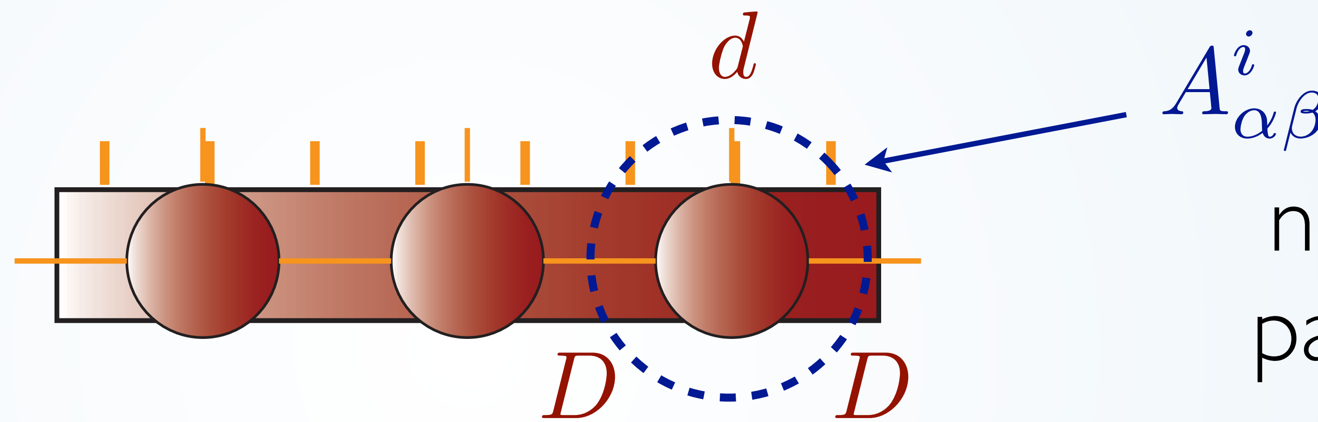
Ostlund, Rommer, PRL 1995
Dukelsky et al., Eur. Phys. Lett. 1998

Quantum Information perspective

Vidal, PRL 2003
Verstraete, Porras, Cirac, PRL 2004

MPS

Matrix Product States

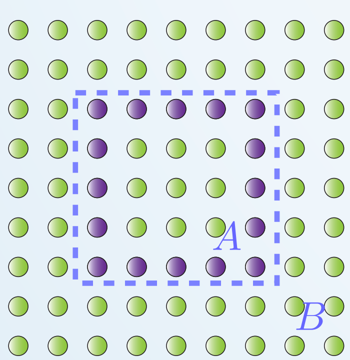


number of parameters

NdD^2

$$|\Psi\rangle = \sum_{i_1 \ldots i_N} c_{i_1 \ldots i_N} |i_1 \ldots i_N\rangle$$

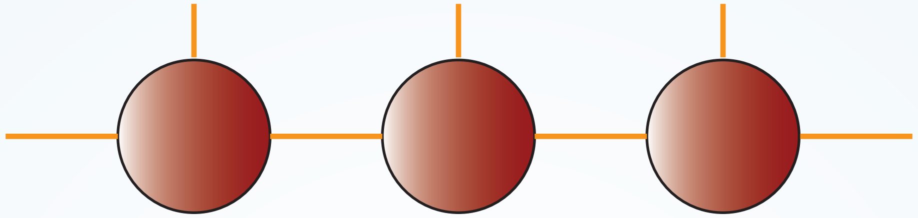
$$|\Psi\rangle = \sum_{i_1 \ldots i_N} \mathrm{tr}(A_1^{i_1} A_2^{i_2} \ldots A_N^{i_N}) |i_1 \ldots i_N\rangle$$



Area law by construction

Bounded entanglement $S(L/2) \leq \log D$

MPS EXAMPLE



$$|\Psi\rangle = \sum_{i_1 \dots i_N} \mathrm{tr}(A_1^{i_1} A_2^{i_2} \dots A_N^{i_N}) |i_1 \dots i_N\rangle$$

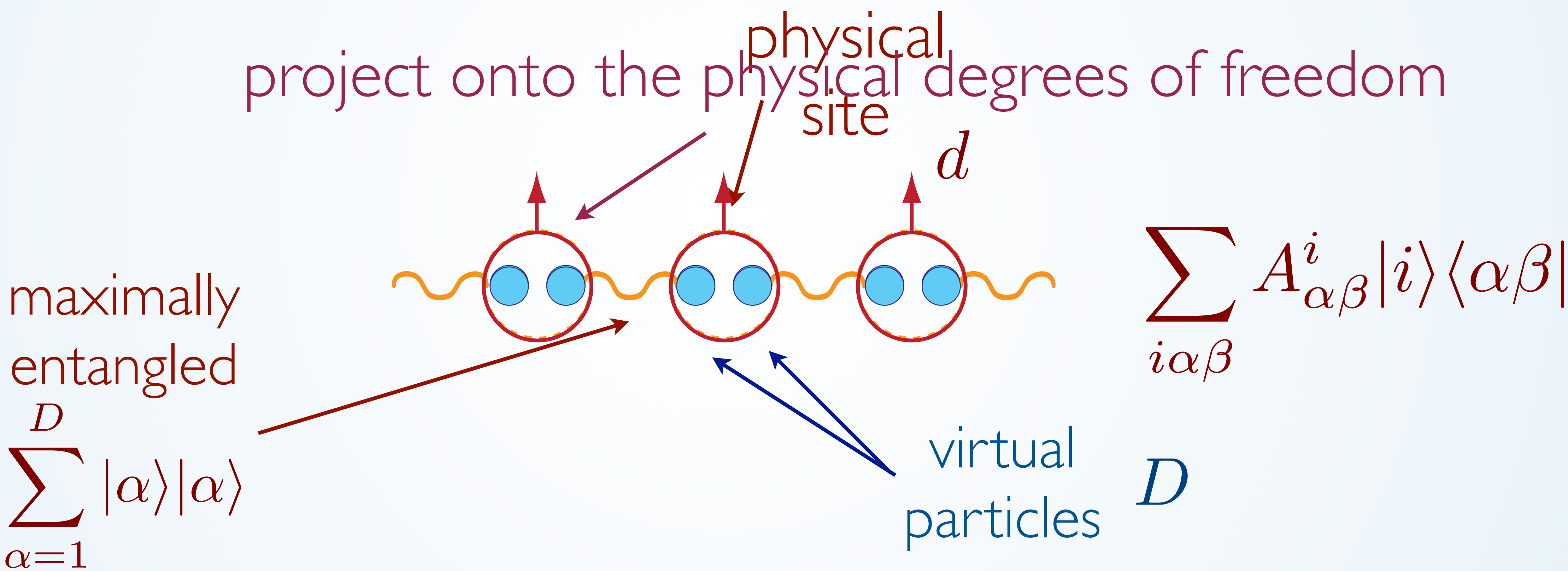
$$A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad A^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

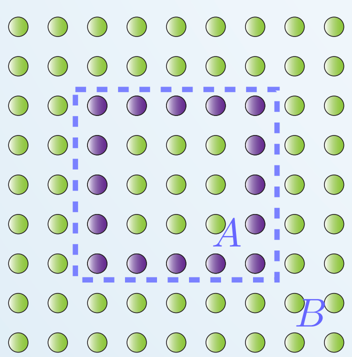
$$|100\dots\rangle + |010\dots\rangle + |001\dots\rangle + \dots$$

$$D = 2$$

MPS

Matrix Product States



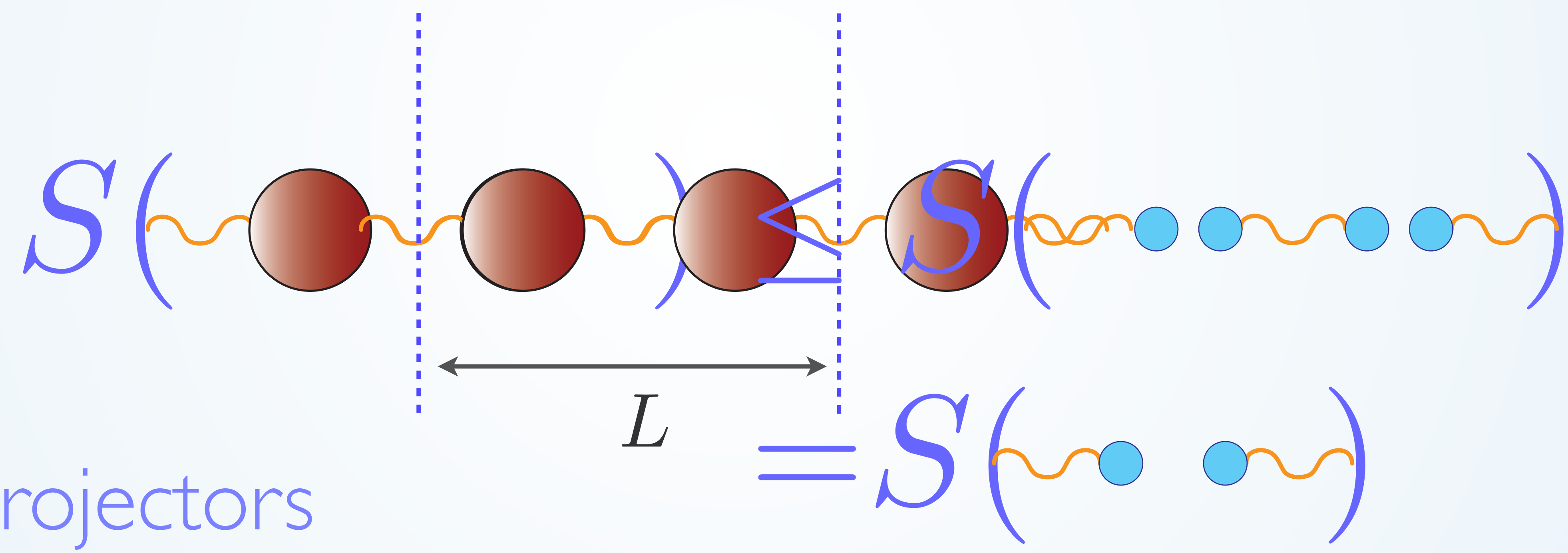


Area law by construction

Bounded entanglement $\quad S(L/2) \leq \log D$

MPS PROPERTIES

Area law by construction



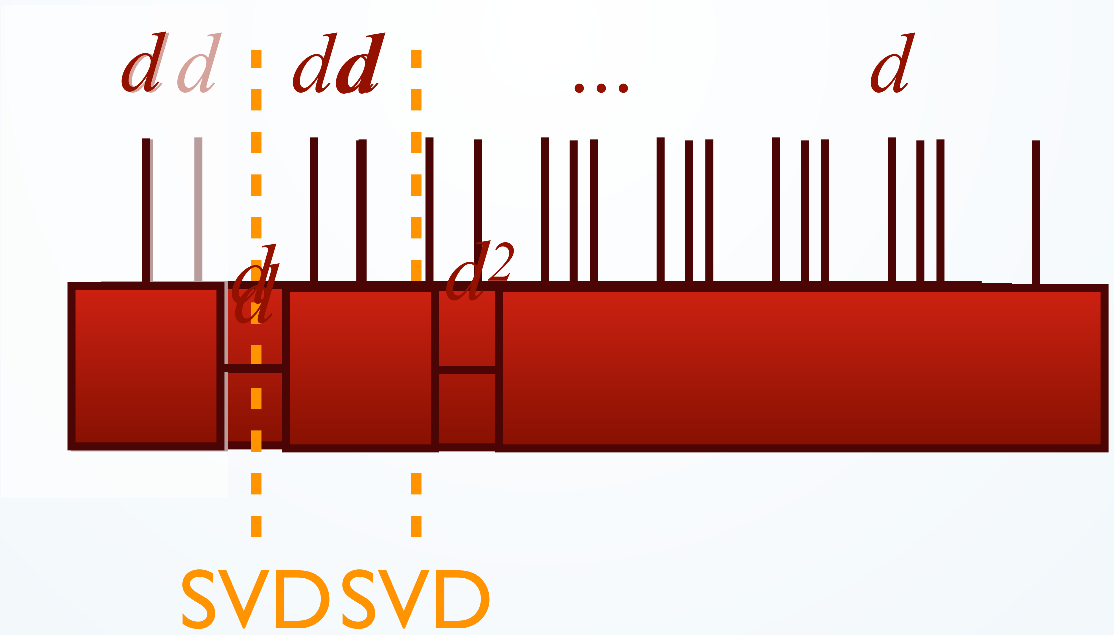
$$= 2 \log D$$

local projectors
cannot increase
the entropy

other properties of MPS

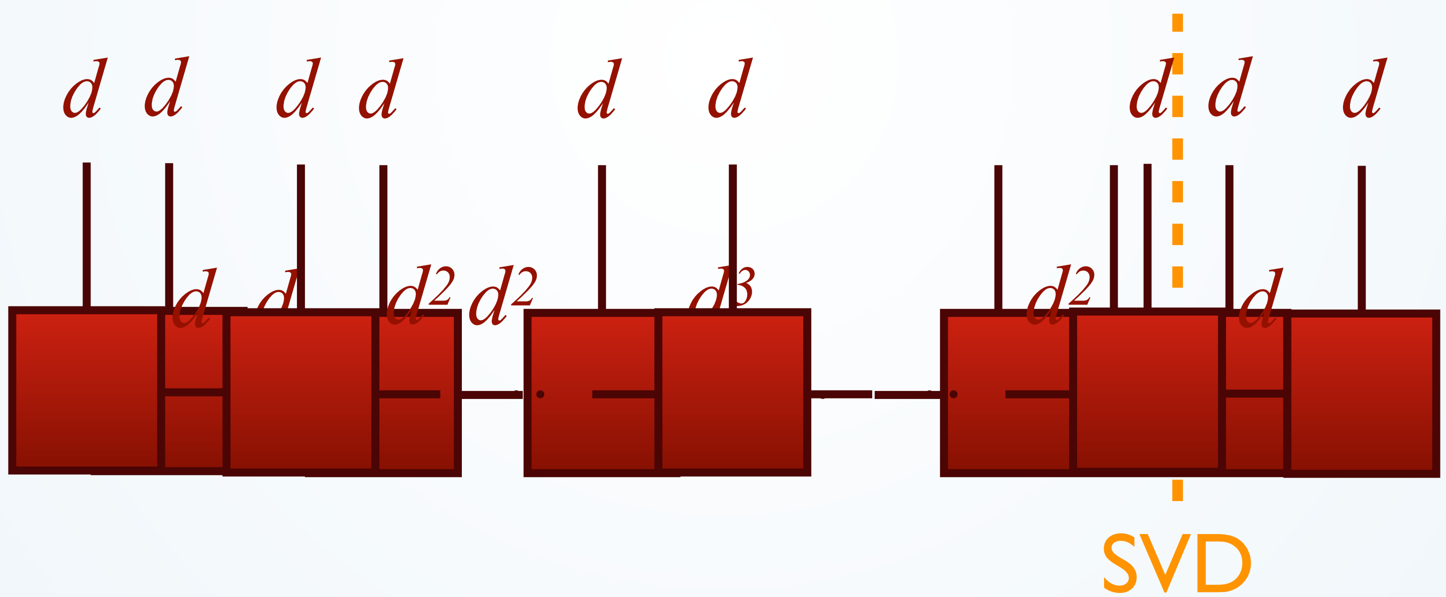
MPS PROPERTIES

any state can be written as MPS



MPS PROPERTIES

any state can be written as MPS



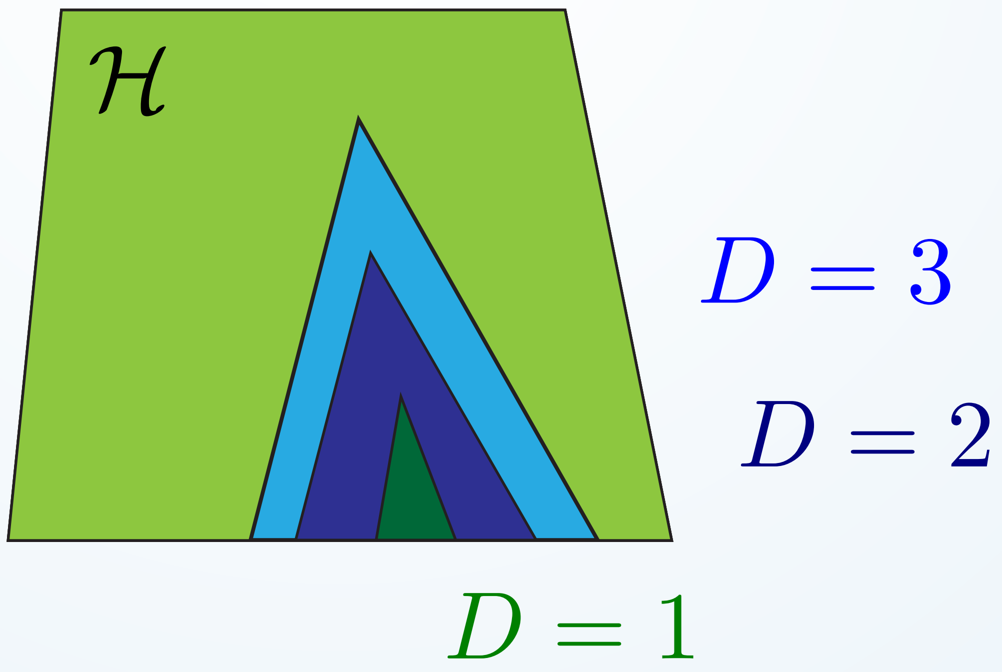
$$D \leq d^{N/2}$$

MPS PROPERTIES

MPS are a complete family

increasing the bond dimension, they can describe any state of the Hilbert space

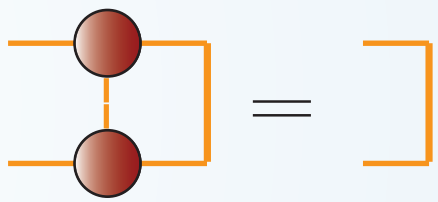
$$D \leq d^{N/2}$$



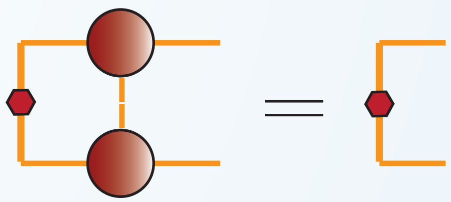
MPS PROPERTIES

canonical form

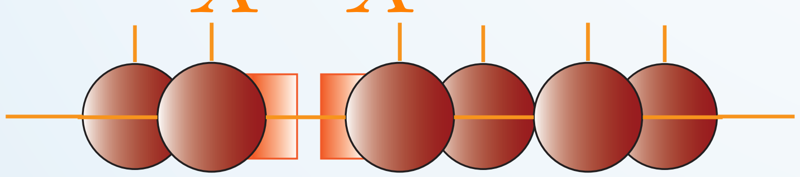
$$\sum_i A^{[m]i} A^{[m]i\dagger} = 1$$



$$\sum_i A^{[m]i\dagger} \Lambda^{[m-1]} A^{[m]i} = \Lambda^{[m]}$$



$X \cdot X^{-1}$



gauge freedom

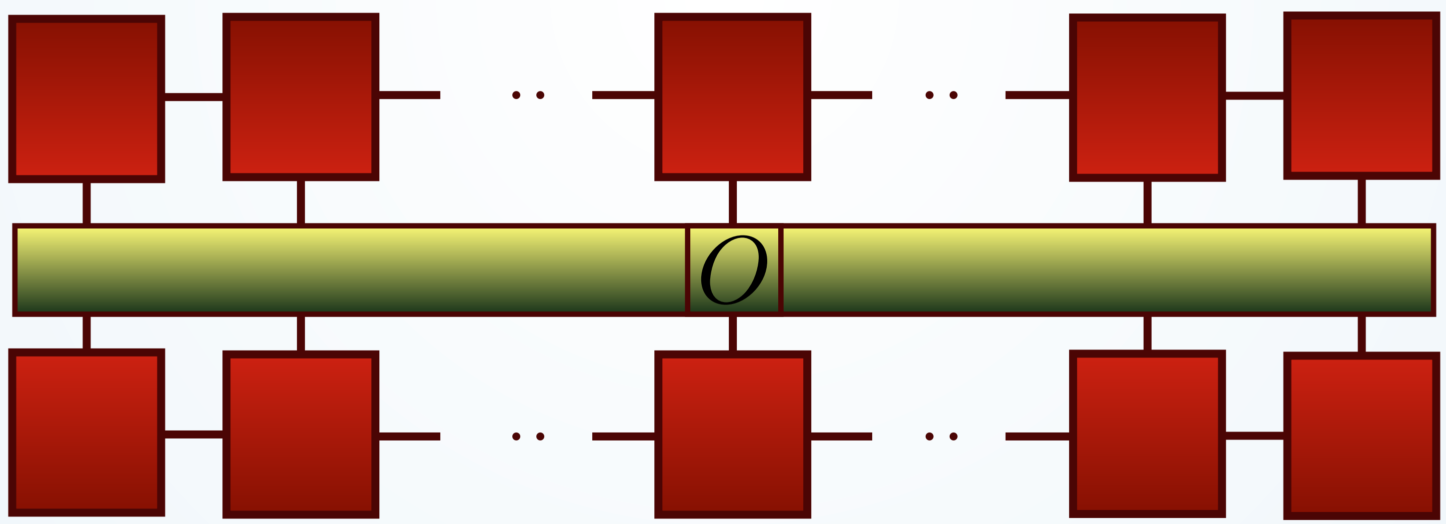
unique
imposed locally

Pérez-García, Verstraete, Wolf, Cirac, Q.Inf.Comp. 2007

MPS PROPERTIES

Efficient expectation values

$$|\Psi\rangle = \sum_{\{i_k\}} c_{i_1 i_2 \ldots i_N} |i_1 i_2 \ldots i_N\rangle$$

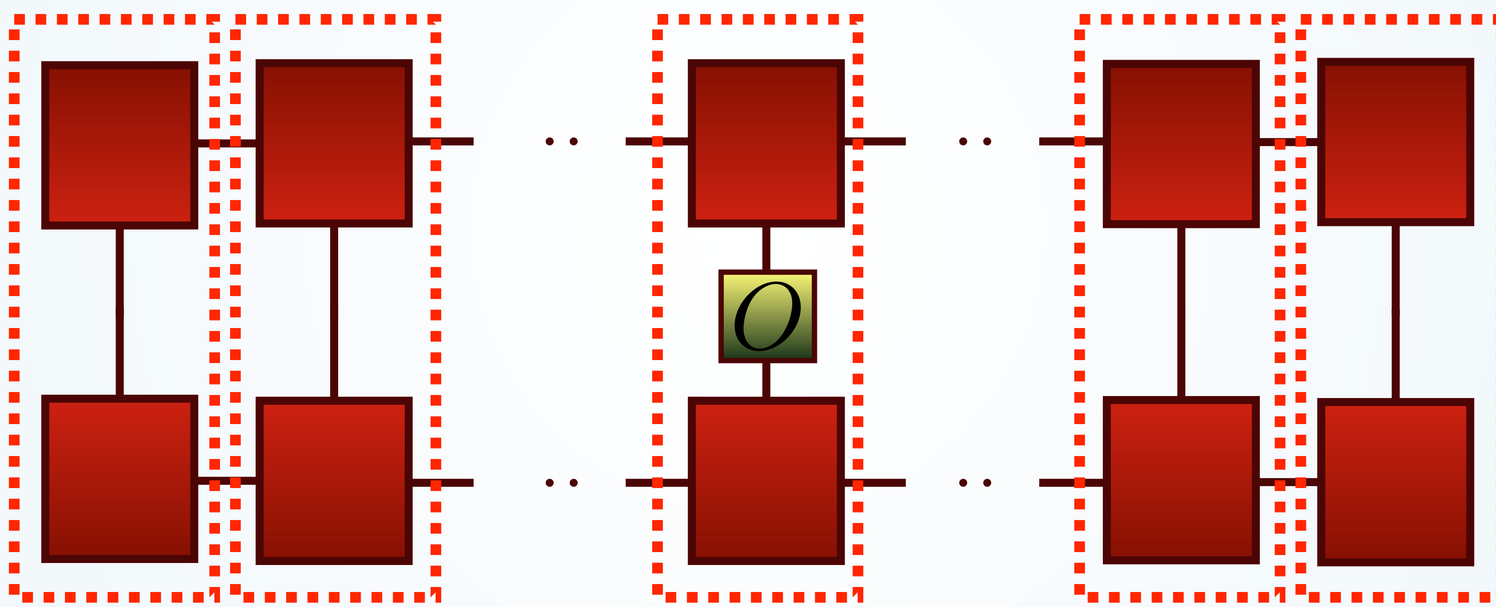


$$\langle\Psi|O|\Psi\rangle = \sum_{\{i_k\},\{j_k\}} c^*_{i_1 i_2 \ldots i_N} c_{j_1 j_2 \ldots j_N} \langle i_1 i_2 \ldots i_N|O|j_1 j_2 \ldots j_N\rangle$$

$$\langle\Psi|O^{[M]}|\Psi\rangle = \sum_{\{i_k\}_{k\neq M}} \sum_{i_M, j_M} c^*_{i_1 i_2 \ldots i_N} c_{i_1 \ldots j_M \ldots i_N} \langle i_M|O|j_M\rangle$$

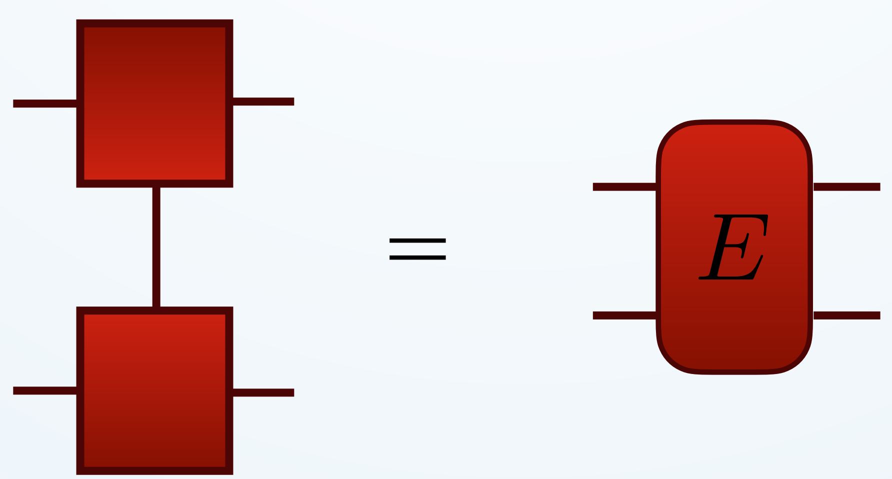
MPS PROPERTIES

Efficient expectation values



transfer operator

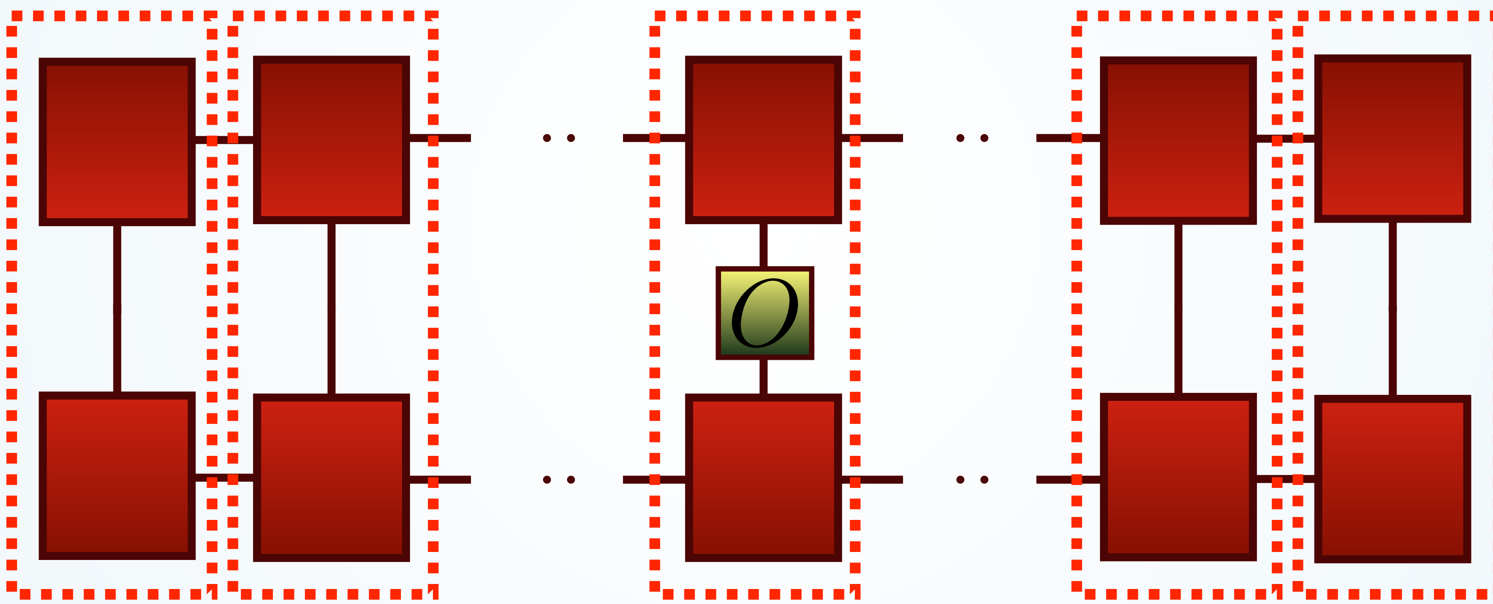
$D^2 \times D^2$ matrix



$$E = \sum_i A^{i*} \otimes A^i$$

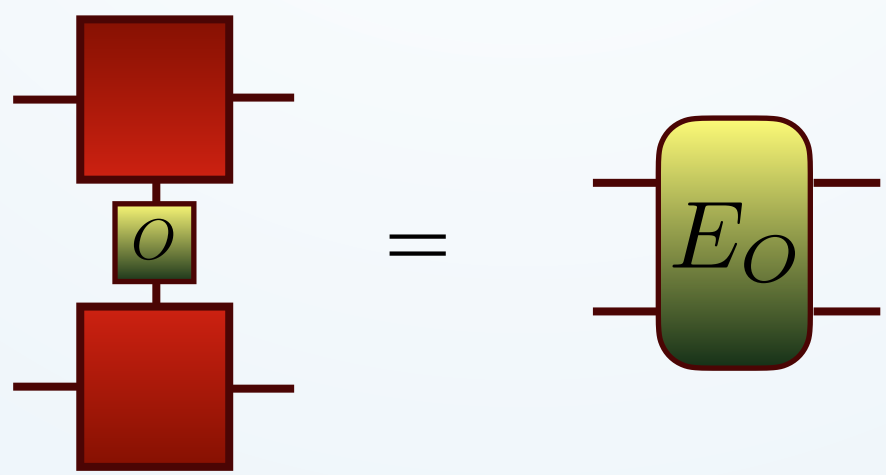
MPS PROPERTIES

Efficient expectation values



transfer operator

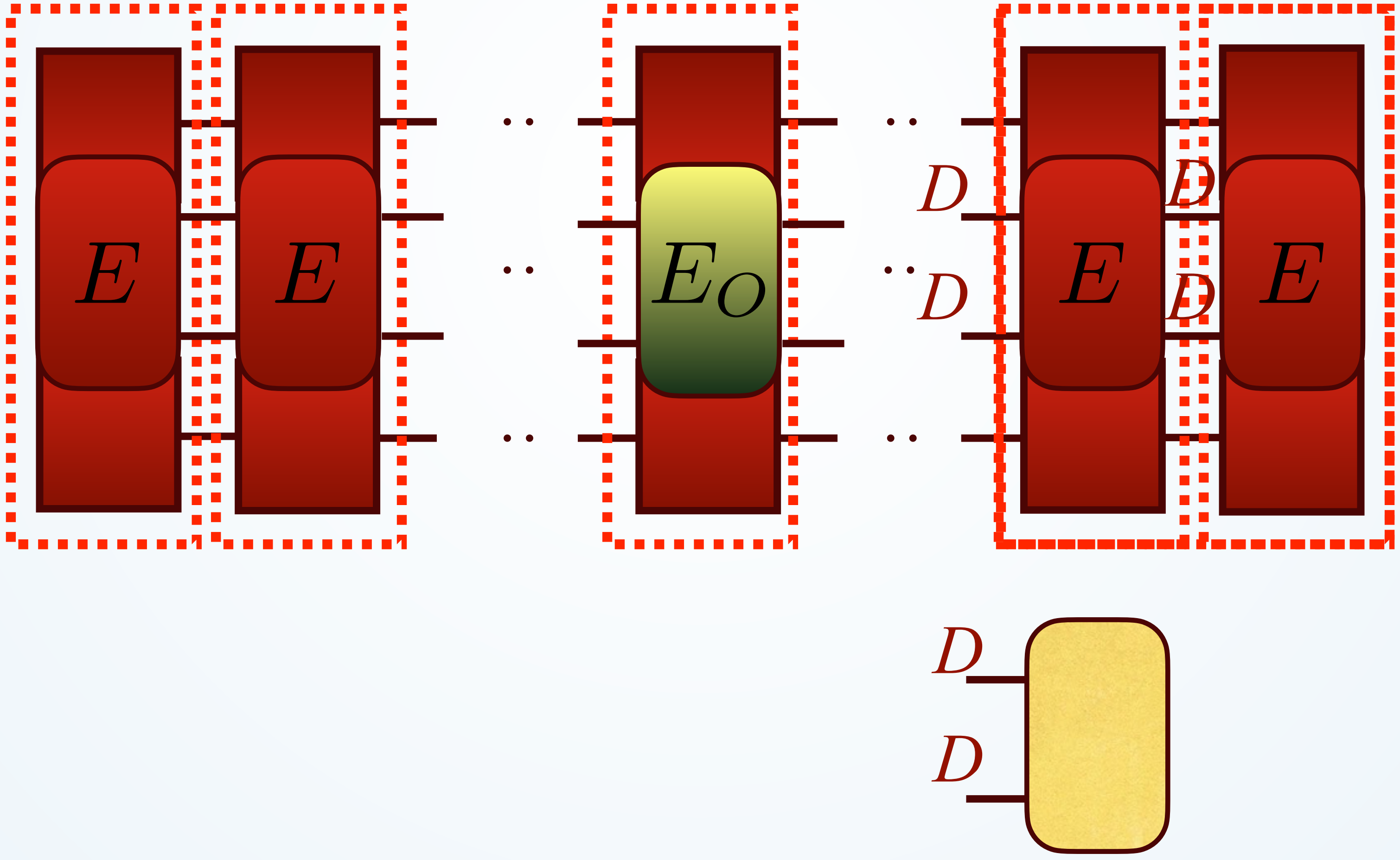
$D^2 \times D^2$ matrix



$$E_O = \sum_{ij} A^{i*} \otimes A^j \langle i|O|j\rangle$$

MPS PROPERTIES

Efficient expectation values

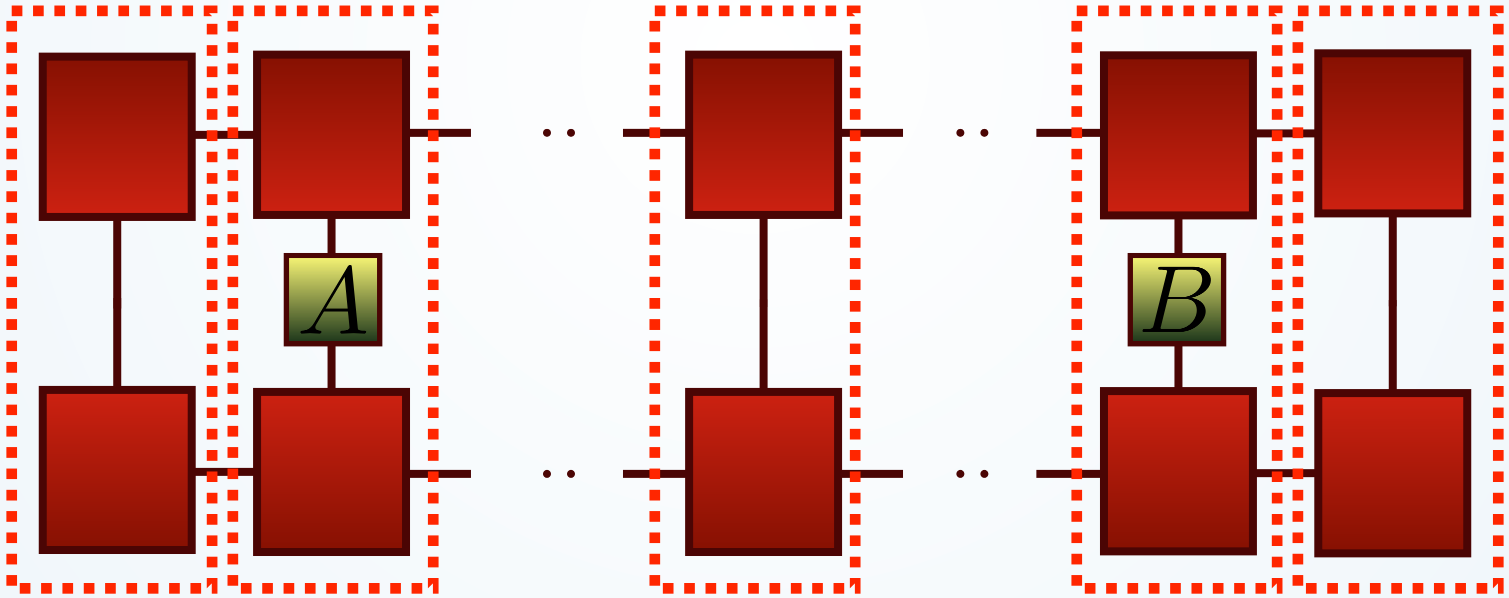


$O(D^4)$

MPS PROPERTIES

Exponentially decaying correlations

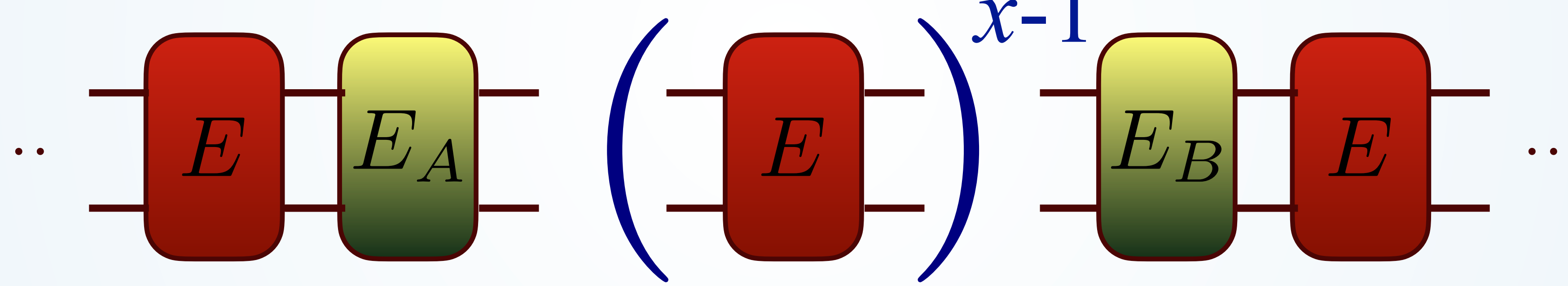
$$\langle A^{[p]} B^{[p+x]} \rangle - \langle A^{[p]} \rangle \langle B^{p+x} \rangle$$



MPS PROPERTIES

Exponentially decaying correlations

$$\langle A^{[p]} B^{[p+x]} \rangle$$

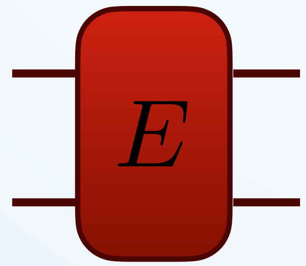


$$\lambda_1^{x-1} \left(|R_1\rangle\langle L_1| + \left(\frac{\lambda_2}{\lambda_1}\right)^{x-1} |R_2\rangle\langle L_2| + \dots \right)$$

normalize

disconnected component

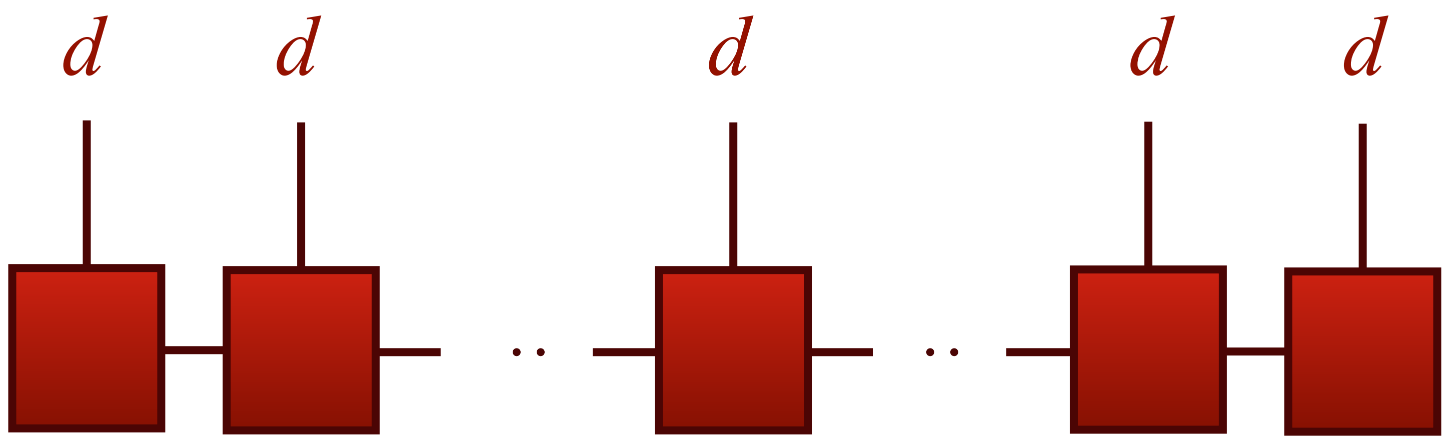
exponential decrease



$$E = \sum_i A^{i*} \otimes A^i = \sum_k \lambda_k |R_k\rangle\langle L_k|$$

summarizing…

MPS

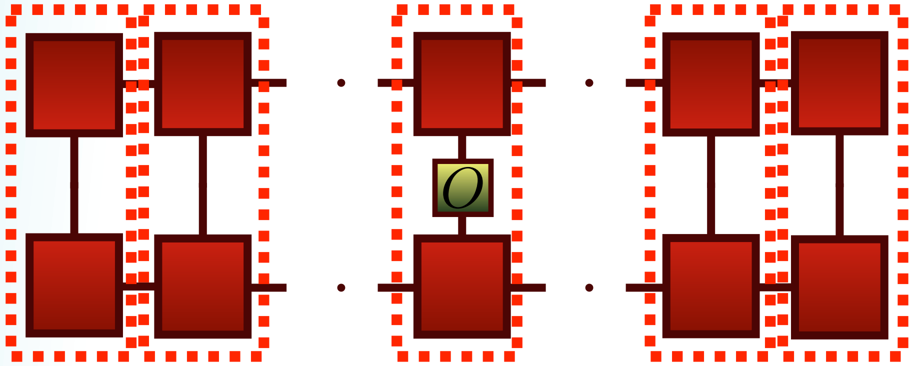


good approximation of ground states

gapped finite range Hamiltonian ⇒
area law (ground state)

efficient preparation

efficient calculation of expectation values



exponentially decaying correlations

complete family $D \leq d^{N/2}$

hierarchy of entanglement

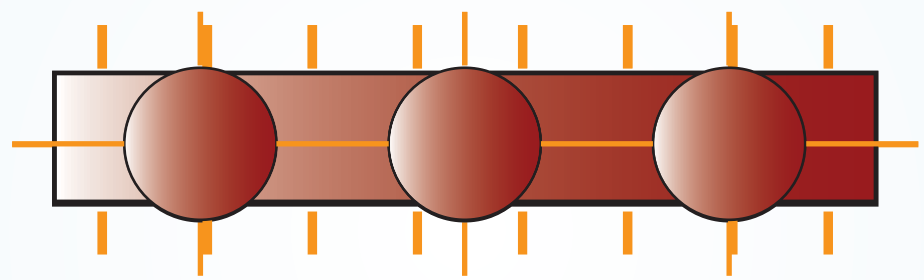
MPO

Matrix Product Operators

MPO

Matrix Product Operator

Same kind of ansatz for operators



$$\hat{M} = \sum_{i_1,j_1 \dots i_N,j_N} \mathrm{tr}(M_1^{i_1 j_1} M_2^{i_2 j_2} \dots M_N^{i_N j_N}) |i_1 \dots i_N\rangle\langle j_1 \dots j_N|$$

$$|\Psi\rangle = \sum_{i_1 \dots i_N} \mathrm{tr}(A_1^{i_1} A_2^{i_2} \dots A_N^{i_N}) |i_1 \dots i_N\rangle$$

MPO is an operator with MPS form in the chosen basis!

Verstraete et al., PRL 2004
Zwolak, Vidal, PRL 2004
Pirvu et al., NJP 2010

MPO

Matrix Product Operator

local Hamiltonians are simple MPOs

finite state automata ⟶ recognize regular expressions

$(0*)1(0*)$

accept	reject
1000	0000
0100	1100
0010	1010
0001	…

$$|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle$$

$$\boldsymbol{\sigma_x} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes \boldsymbol{\sigma_x} \otimes \mathbb{1} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes \boldsymbol{\sigma_x} \otimes \mathbb{1} + \mathbb{1} \otimes \mathbb{1} \otimes \mathbb{1} \otimes \boldsymbol{\sigma_x} = \sum_i \sigma_x^{[i]}$$

MPO

local Hamiltonians are simple MPOs

finite state automata ⟶ recognize regular expressions

FSA = computational model

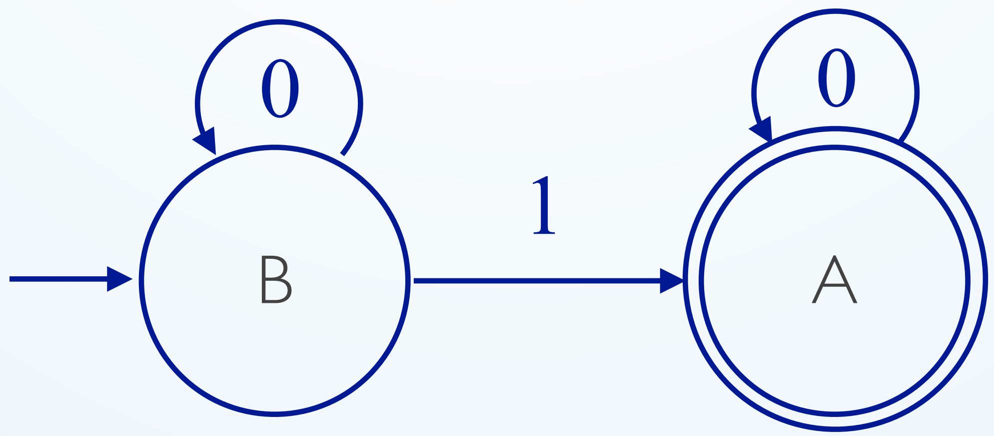
$(0*)1(0*)$

S states $S_0, S_f \in S$

B: before 1
A: after 1

Σ input alphabet 0, 1

$S \times \Sigma \to S$ transitions

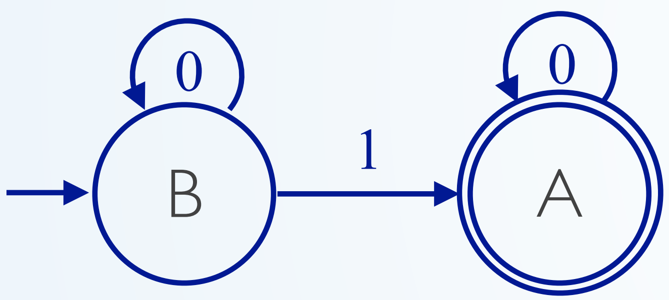


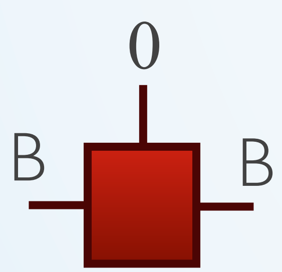
MPO

Matrix Product Operator

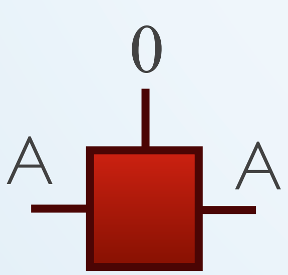
local Hamiltonians are simple MPOs

translate to MPS/MPO → input symbols = physical indices
nr of states = bond dimension
valid transitions = non-vanishing tensor elements





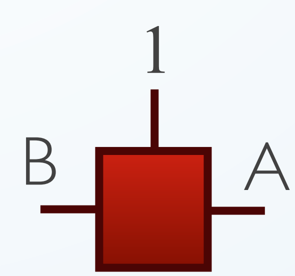
$= 1$



$= 1$

B A

$$M^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



$= 1$

$$M^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

boundaries M_L, M_R

MPO

Matrix Product Operator

local Hamiltonians are simple MPOs

$$M^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad M^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

$$\sum_{\{i_k\}} M_L^{i_1} M^{i_2} \ldots M^{i_{N-1}} M_R^{i_N} |i_1 \ldots i_N\rangle \qquad i_k = 0,\, 1$$

expressed as operator(vector) valued matrix

$$M = \begin{pmatrix} |0\rangle & |1\rangle \\ 0 & |0\rangle \end{pmatrix} \qquad M = \begin{pmatrix} \mathbb{1} & \sigma_x \\ 0 & \mathbb{1} \end{pmatrix}$$

$$|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle \qquad \sum_i \sigma_x^{[i]}$$

MPO for Ising Hamiltonian

$$H = J \sum \sigma_z^{[i]} \sigma_z^{[i+1]} + g \sum \sigma_x^{[i]}$$

$$\sum_{\{i_k\}} M_L^{i_1} M^{i_2} \dots M^{i_{N-1}} M_R^{i_N} |i_1 \dots i_N\rangle \qquad i_k = \mathbb{1}, \sigma_x, \sigma_z$$

M_L

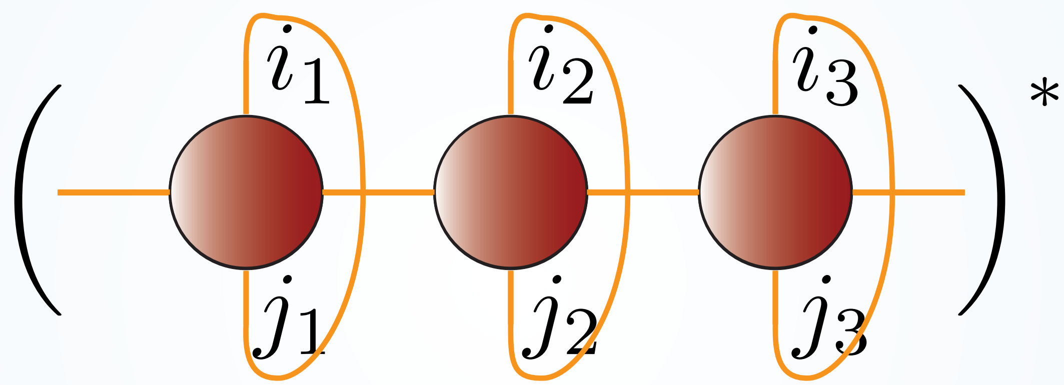
$$M = \begin{pmatrix} \mathbb{1} & J\sigma_z & g\sigma_x \\ 0 & 0 & \sigma_z \\ 0 & 0 & \mathbb{1} \end{pmatrix}$$

M_R

MPO

Matrix Product Operator

an ansatz for density matrices



need some properties

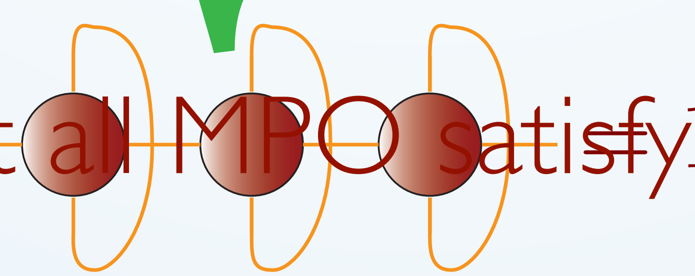
$$\rho = \sum_{i_1, j_1 \ldots i_N, j_N} \mathrm{tr}(M_1^{i_1 j_1} M_2^{i_2 j_2} \ldots M_N^{i_N j_N}) |i_1 \ldots i_N\rangle\langle j_1 \ldots j_N|$$

can we impose them *locally*?

$\rho = \rho^\dagger$ ✓

$\mathrm{tr}\rho = 1$ ✓

$\rho \geq 0$ ✗



not all MPO satisfy them!

there is a way

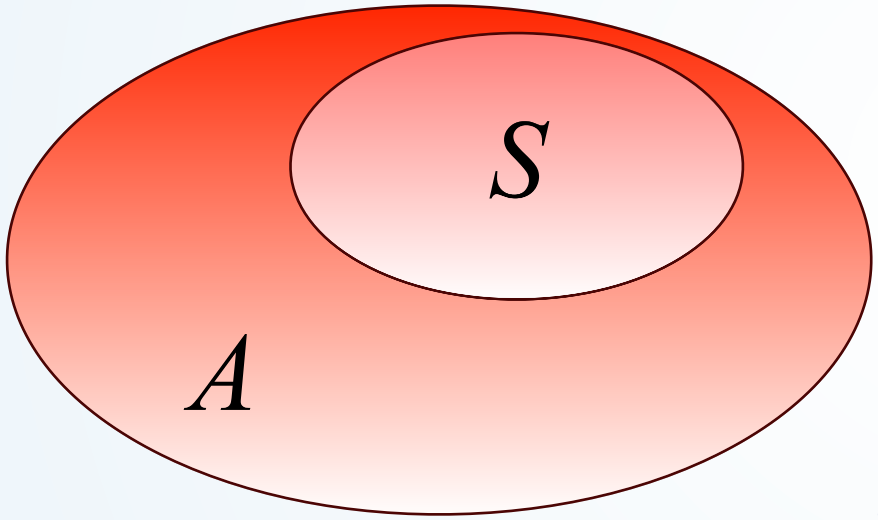
Kliesch et al., PRL 2014

de las Cuevas et al. J Math Phys 2016

MPO

Matrix Product Operator

purification



$$\rho_S = \sum_i \lambda_i |\varphi_i\rangle\langle\varphi_i|$$

$$0 \leq \lambda_i \leq 1$$

$$\sum_i \lambda_i = 1$$

ancillary system **A** $d_{\mathrm{A}} \leq d_{\mathrm{S}}$

$$|\Psi\rangle_{SA} = \sum_i \sqrt{\lambda_i} |\varphi_i\rangle_S \otimes |i\rangle_A$$

orthogonal

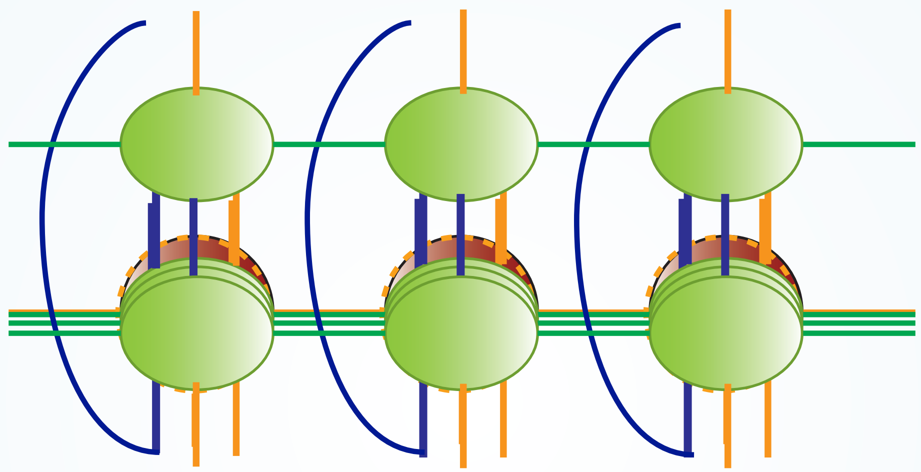
$$\rho_S = \mathrm{tr}_A\left(|\Psi_{SA}\rangle\langle\Psi_{SA}|\right)$$

unitary freedom on ancilla

MPO

Matrix Product Operator

purification



need some properties

$$\rho = \sum_{i_1, j_1 \dots i_N, j_N} \mathrm{tr}(M_1^{i_1 j_1} M_2^{i_2 j_2} \dots M_N^{i_N j_N}) |i_1 \dots i_N\rangle\langle j_1 \dots j_N|$$

can we impose them *locally*?

$\rho = \rho^\dagger$ ✓

$\mathrm{tr}\rho = 1$ ✓

$\rho \geq 0$ ✗

$$\rho_S = \mathrm{tr}_A |\Psi_{SA}\rangle\langle\Psi_{SA}|$$

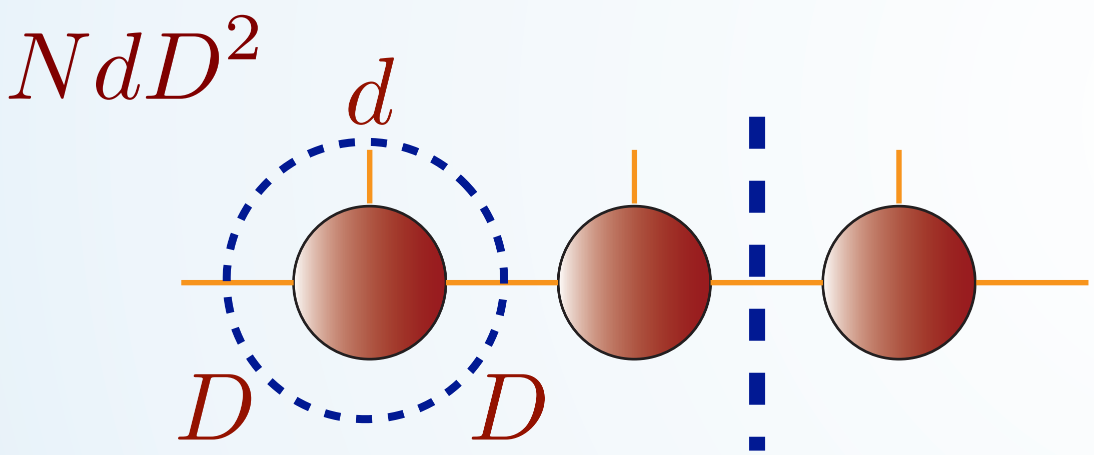
Verstraete et al., PRL 2004

Zwolak and Vidal, PRL 2004

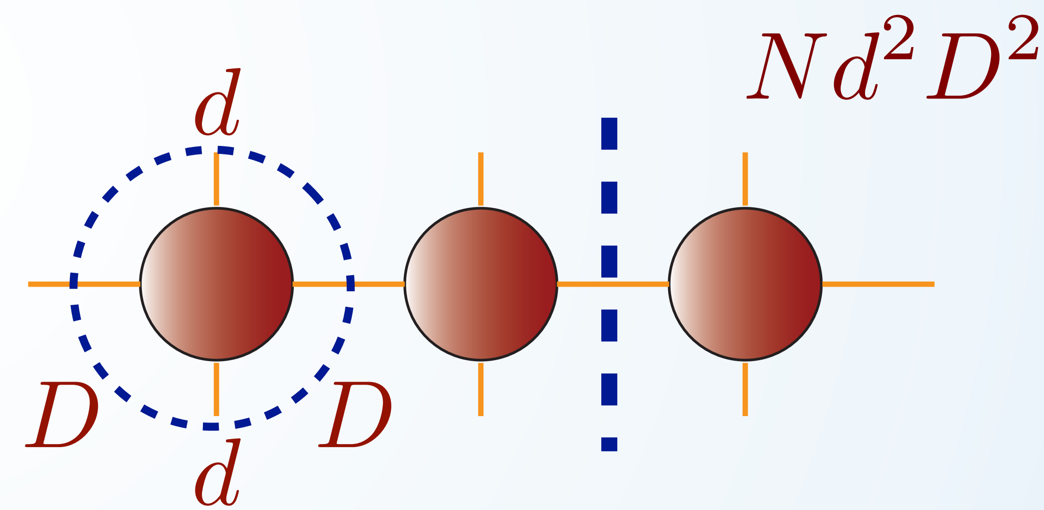
MPO

Matrix Product Operator

Bond dimension determines number of parameters



vs



Schmidt rank → entanglement

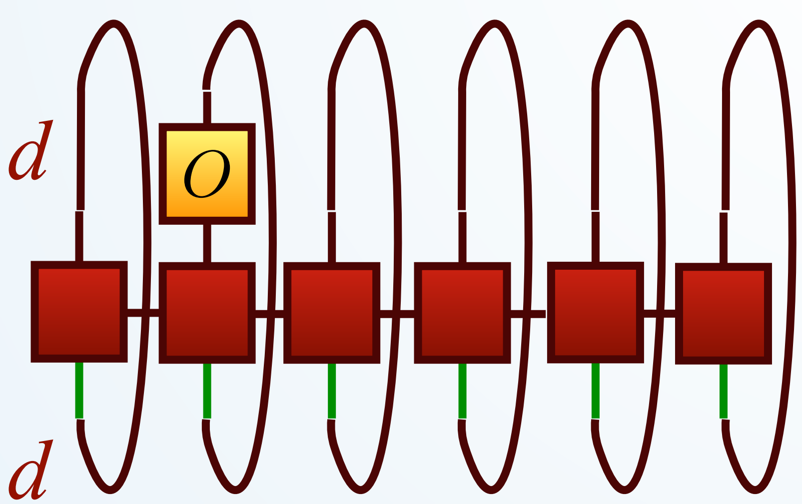
Schmidt rank in operator space → operator space entanglement entropy

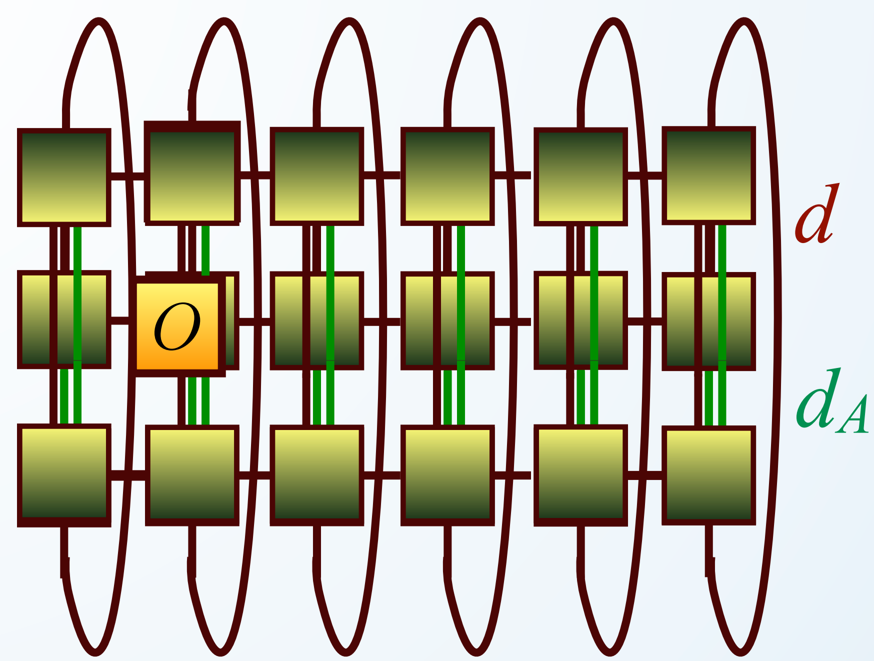
MPO

Matrix Product Operator

expectation values

$$\langle O \rangle_\rho = \mathrm{tr}(O\,\rho) = \mathrm{tr}_S[O\,\mathrm{tr}_A(|\Psi\rangle\langle\Psi|)] = \mathrm{tr}(O\,|\Psi\rangle\langle\Psi|)$$
$$= \langle\Psi|O|\Psi\rangle$$





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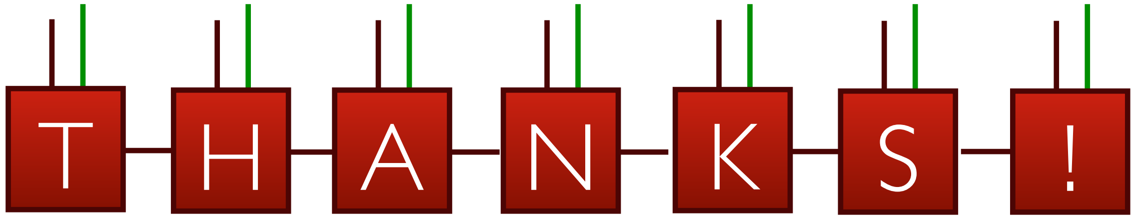

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TUTORIAL:

NOTES