TENSOR NETWORKS FOR QUANTUM MANY-BODY SYSTEMS

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In this tutorial…

introducing Tensor Network States

basic numerical techniques (for QMB systems)

In this session…

Tensor networks? What? Why?

MPS, MPO

PEPS

others

What are tensor networks?

WHAT ARE TNS?

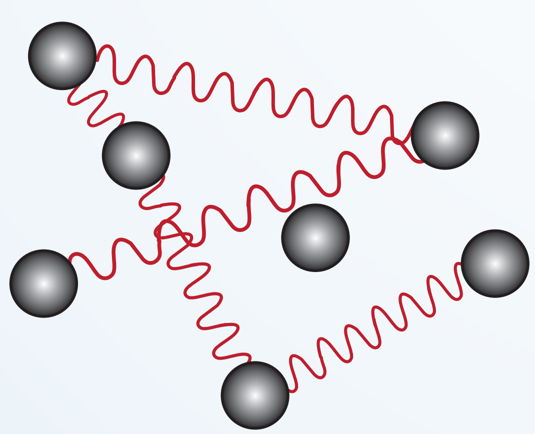
- TNS = Tensor Network States

Context: quantum many body systems

interacting with each other

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

N



Goal: describe equilibrium states

ground, thermal states

WHAT ARE TNS?

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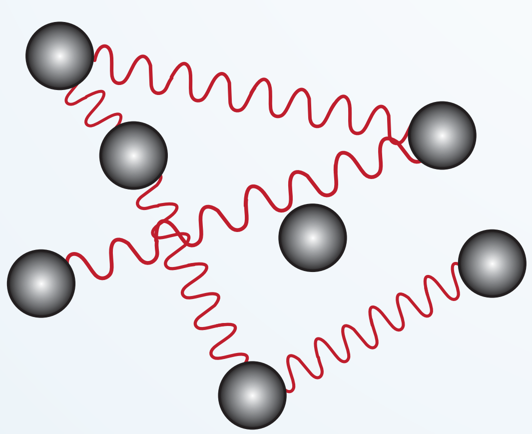


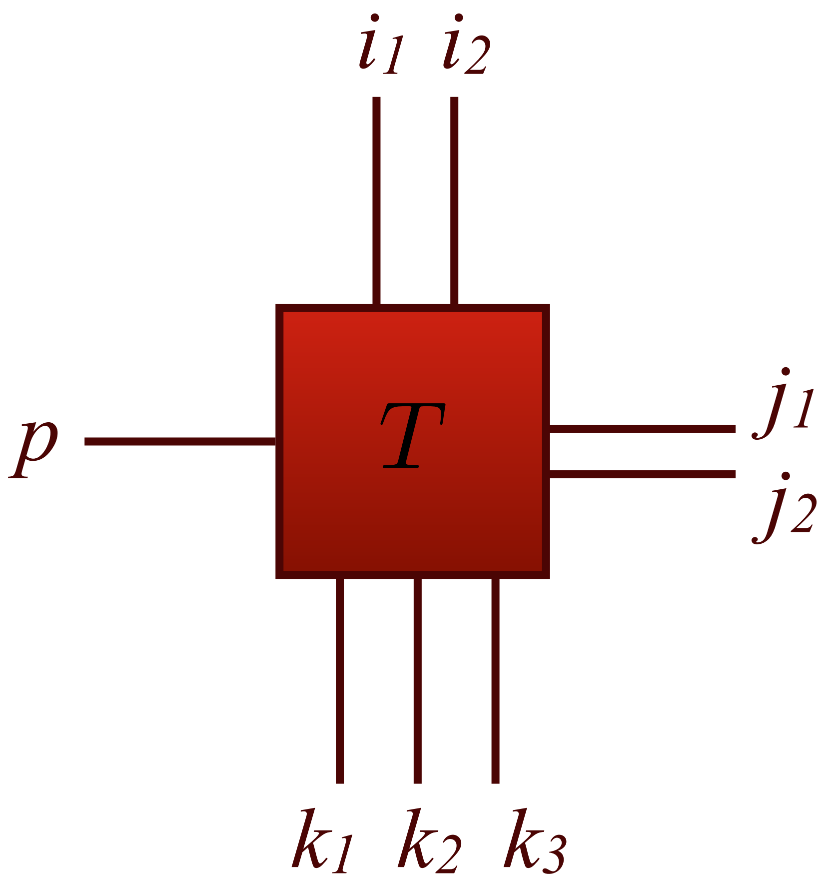
Goal: describe interesting states

ground, thermal states

pictorial representation

pictorial representation

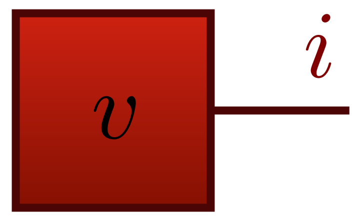
tensor = multidimensional array



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

pictorial representation

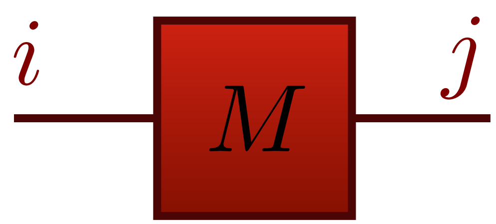
vector



v_i

$i = 1, \dots D$

matrix

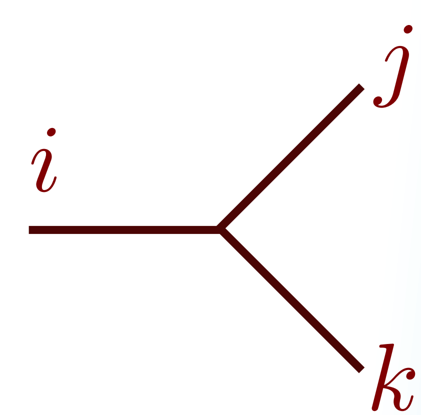


M_{ij}

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

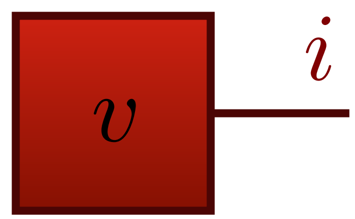
a special case

δ_{ij}



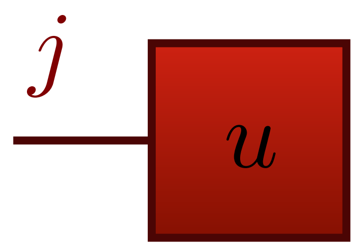
contractions

vector



v_i

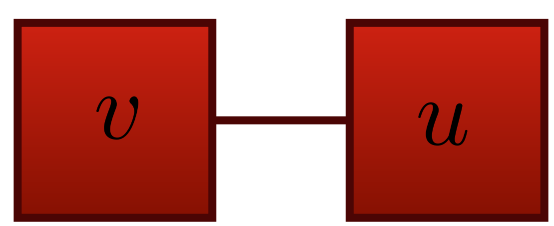
$i = 1, \ldots D$



u_j

$j = 1, \ldots D$

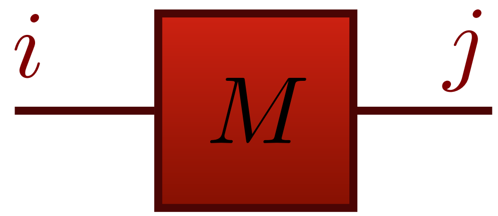
vector-vector



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

contractions

matrix

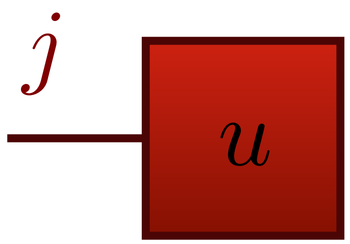


M_{ij}

$i = 1, \ldots D_1$

$j = 1, \ldots D_2$

vector



u_j

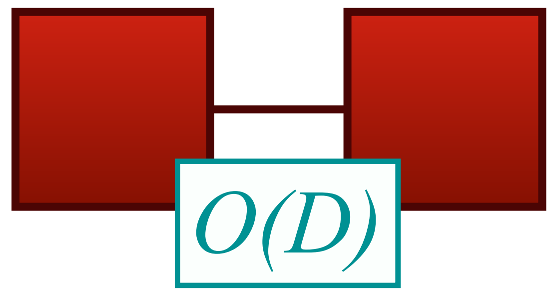
$j = 1, \ldots D_2$

matrix-vector

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

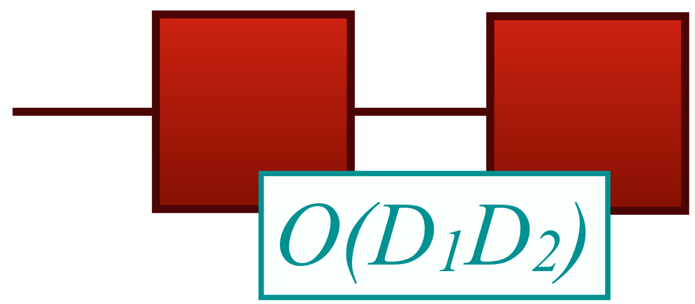
computational costs

vector-vector



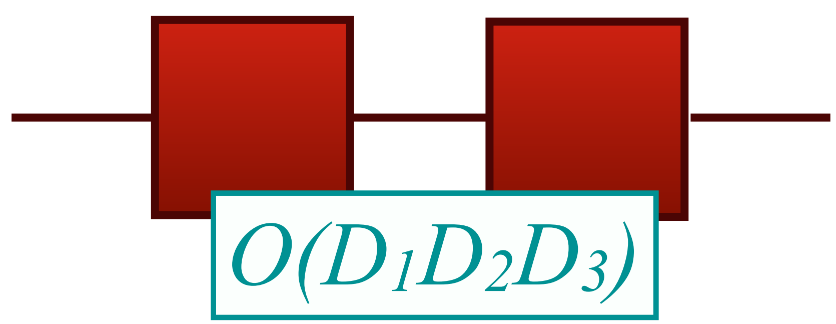
$$v \cdot u = \sum_i v_i u_i$$

matrix-vector



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

matrix-matrix

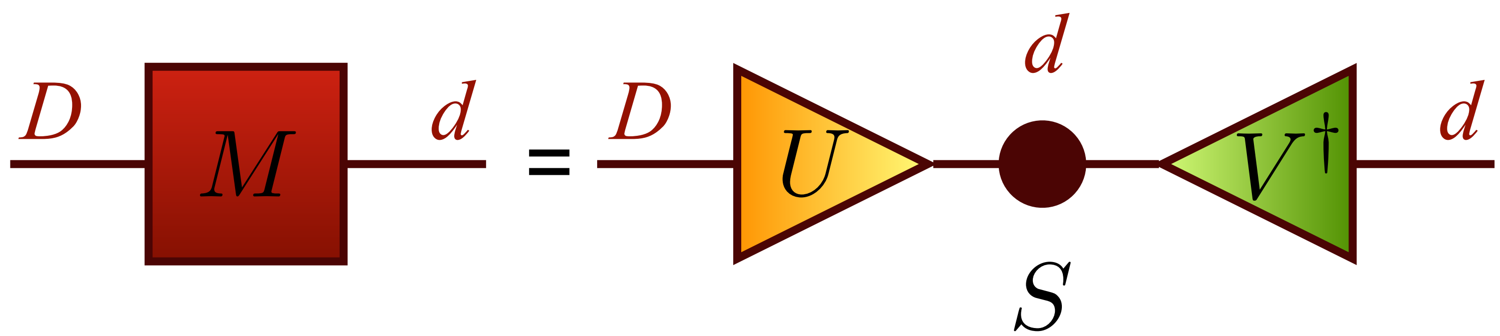


$$M \cdot N = \sum_j M_{ij} N_{jk}$$

in general: product of open and contracted dimensions

basic routines

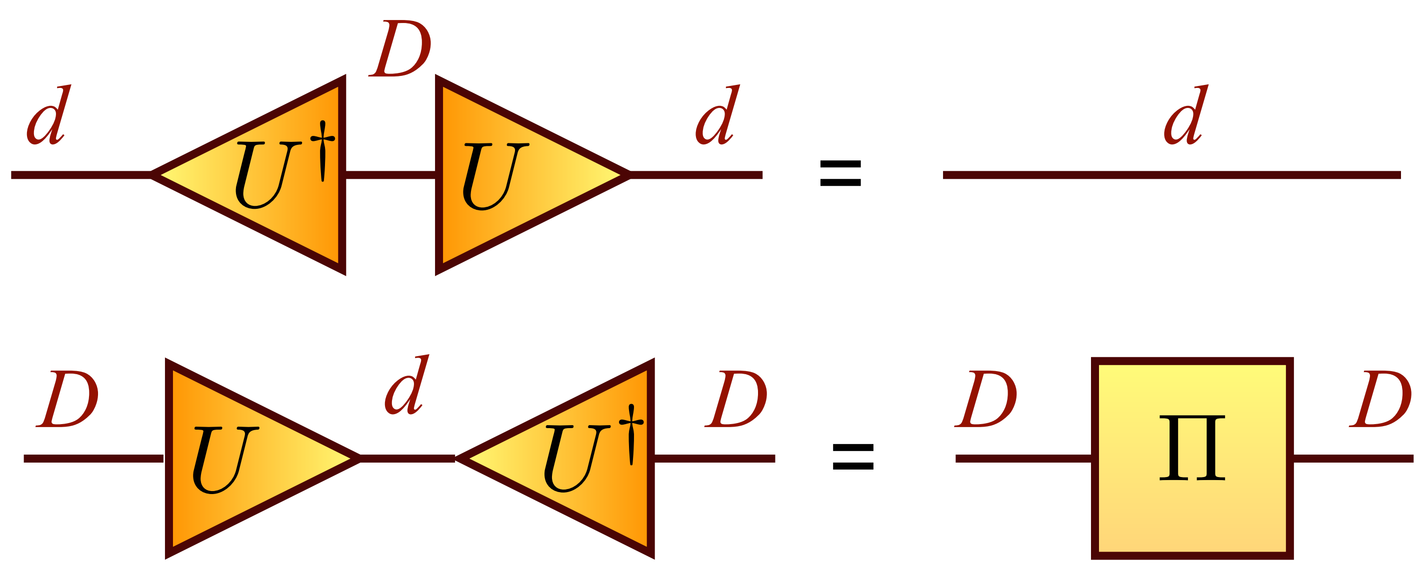
SVD



$M = USV^\dagger$

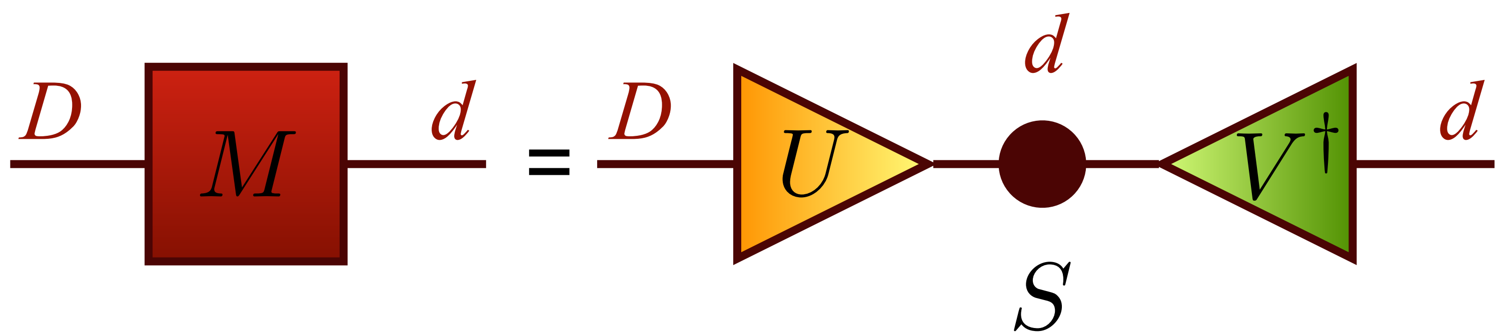
$O(Dd^2)$

isometry



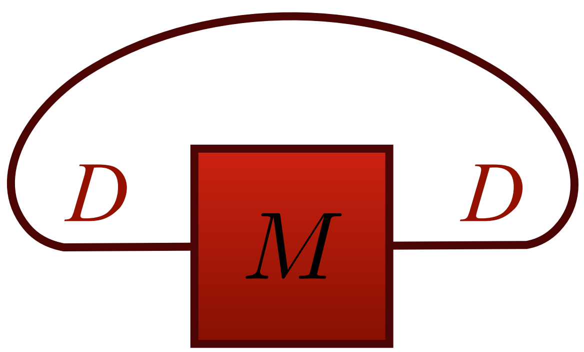
basic routines

SVD



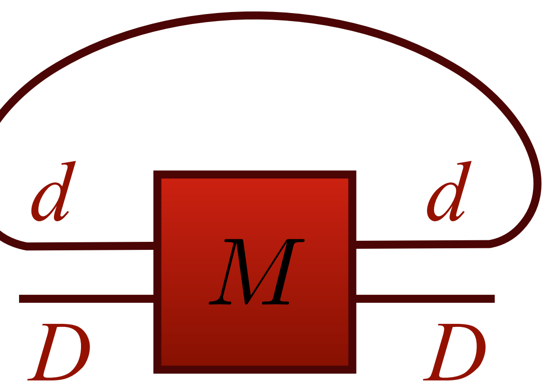
$$M = USV^\dagger$$

trace



$$\sum_{ij} M_{ij}\delta_{ij} = \sum_i M_{ii} = \mathrm{tr} M$$

partial trace



$$\sum_{ij} M_{ia,jb}\delta_{ij} = \sum_i M_{ia,ib} = \mathrm{tr}_d M$$

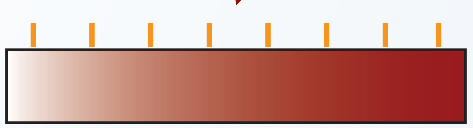
pictorial representation

WHAT ARE TNS?

- TNS = Tensor Network States

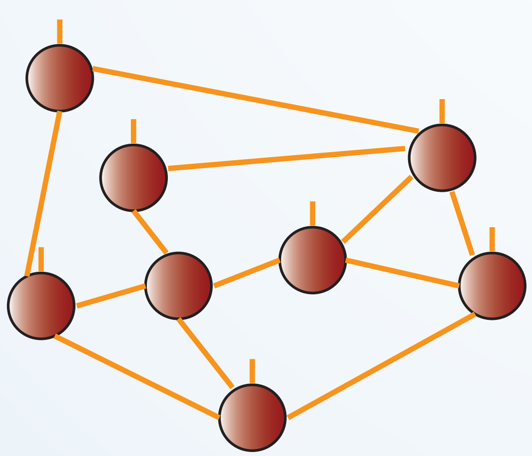
A general state of the N-body Hilbert space has exponentially many coefficients

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



N-legged tensor

d^N



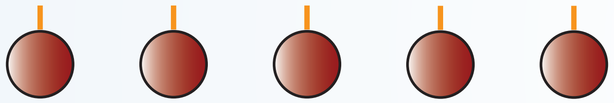
$\mathrm{poly}(N)$

A TNS has only a polynomial number of parameters

WHAT ARE TNS?

- TNS = Tensor Network States

A particular example



Mean field approximation

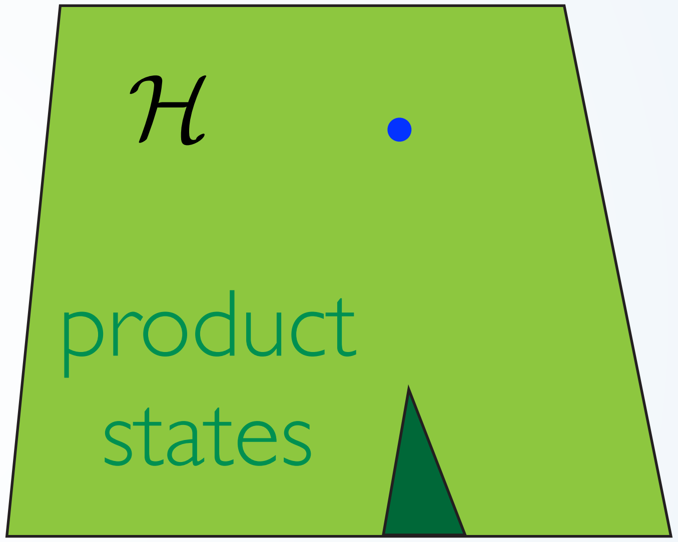
product state

Can still produce good results in some cases

WHY SHOULD TNS BE USEFUL?

States appearing in Nature are peculiar

State at random from Hilbert space is not close to product



- TNS = Tensor Network States

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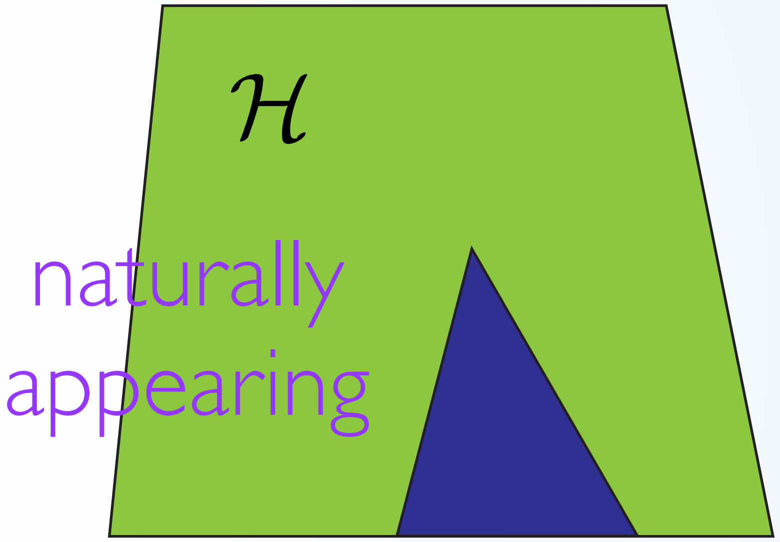


We look for the particular "*corner*" of the Hilbert space

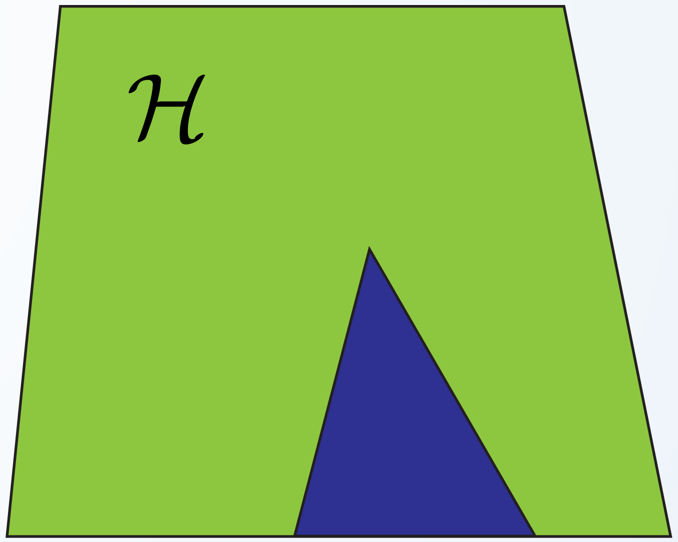
- TNS = Tensor Network States

WHY SHOULD TNS BE USEFUL?

The goal is to find good descriptions of physical states

WANTED

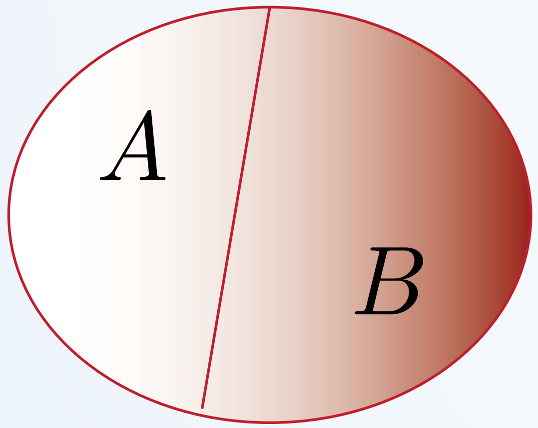
- ➡ efficient representation
- ➡ computable observables
- ➡ (variational) algorithms



FINDING A GOOD ANSATZ

Which properties characterize physically interesting states?

ENTANGLEMENT STRUCTURE



$$|a\rangle \otimes |b\rangle$$

$$|a\rangle \otimes |b\rangle + |b\rangle \otimes |a\rangle$$

$$S(A) = -\mathrm{tr}(\rho_A \log(\rho_A))$$

entanglement entropy

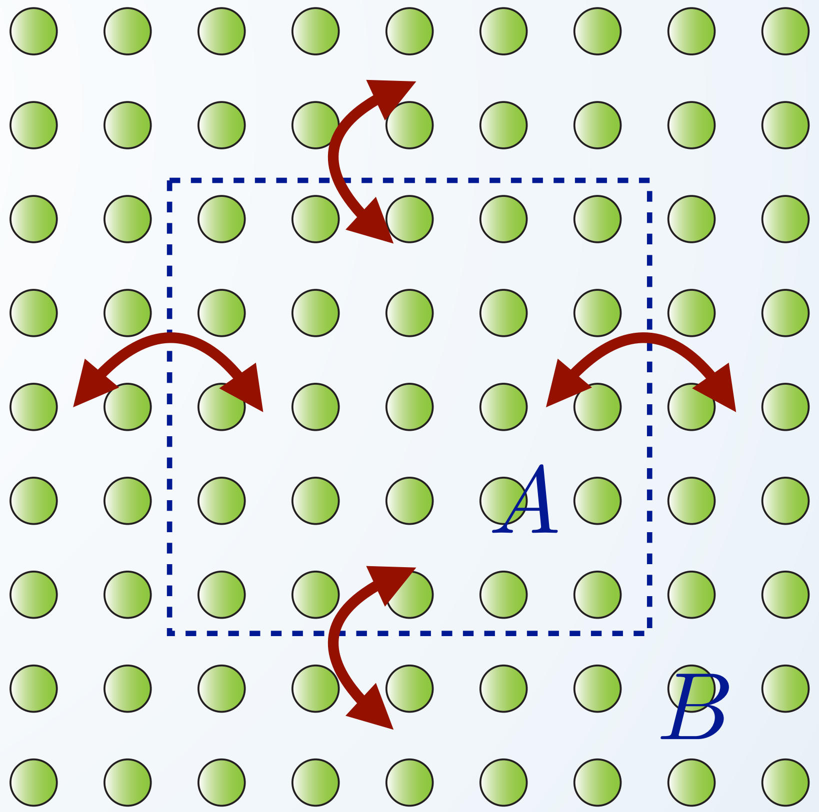
FINDING A GOOD ANSATZ

Which properties characterize ground states of relevant Hamiltonians?

finite range
gapped
Hamiltonians

states with
little entanglement

Area law



FINDING A GOOD ANSATZ

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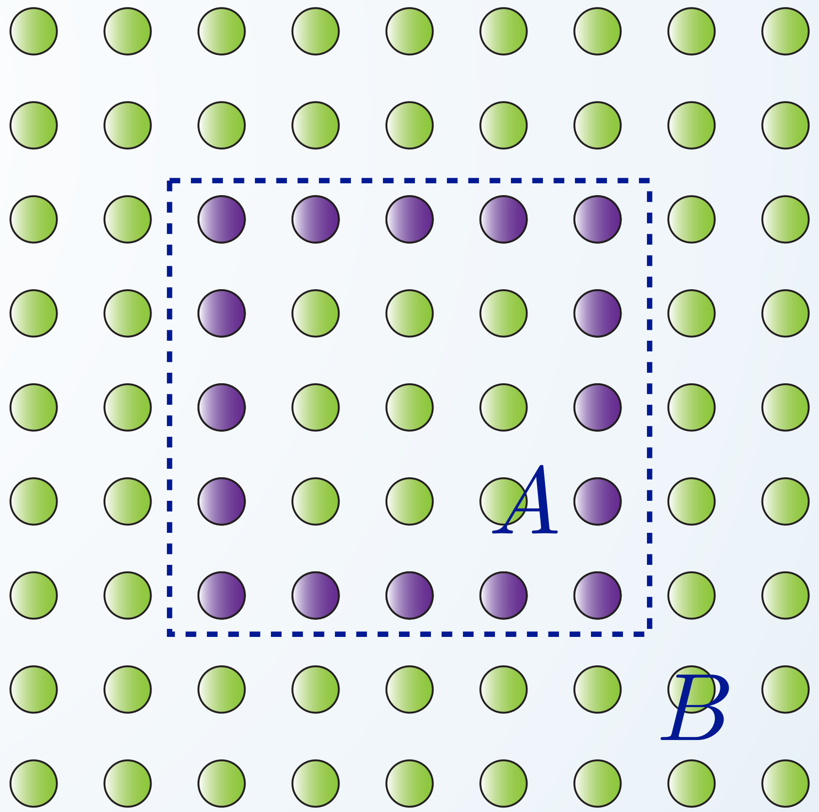


local gapped 1D Hamiltonians

have ground states

with area law of entanglement

$$S_{A\max} \propto |\delta A|$$ Hastings 2007

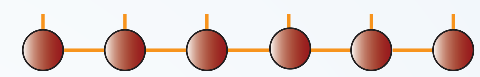
in 1D critical systems, logarithmic corrections

$$S_{A\max} \propto |\delta A| \log A$$ Calabrese, Cardy 2004

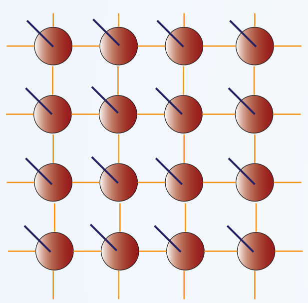
satisfied at finite temperature Wolf, Verstraete, Hastings, Cirac, PRL 2008

MPS & PEPS

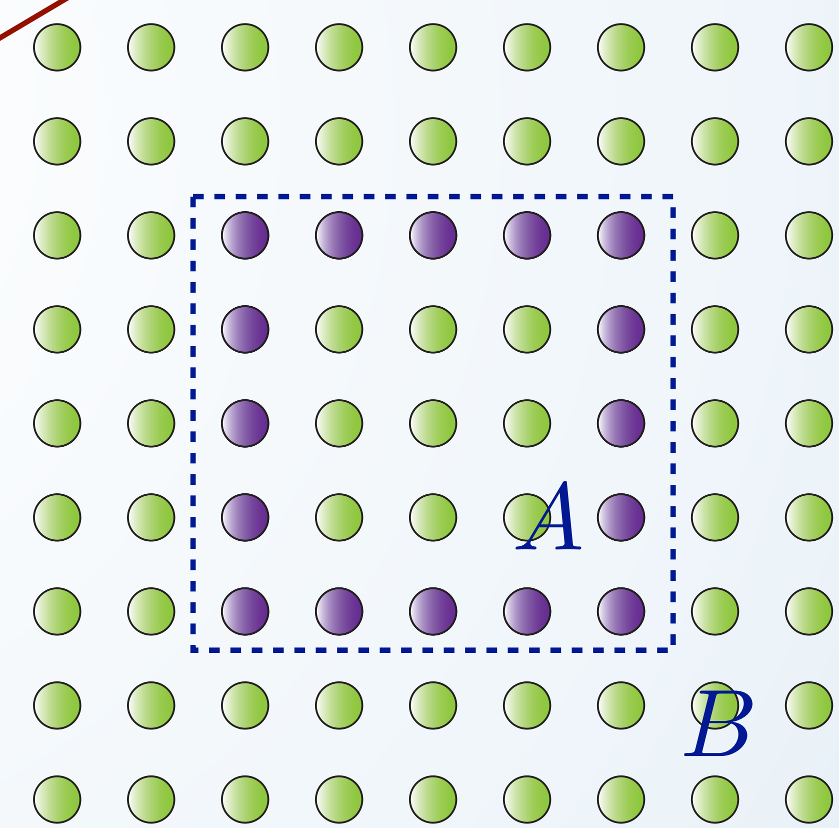
- MPS = Matrix Product States



- PEPS = Projected Entangled Pairs States



Area law

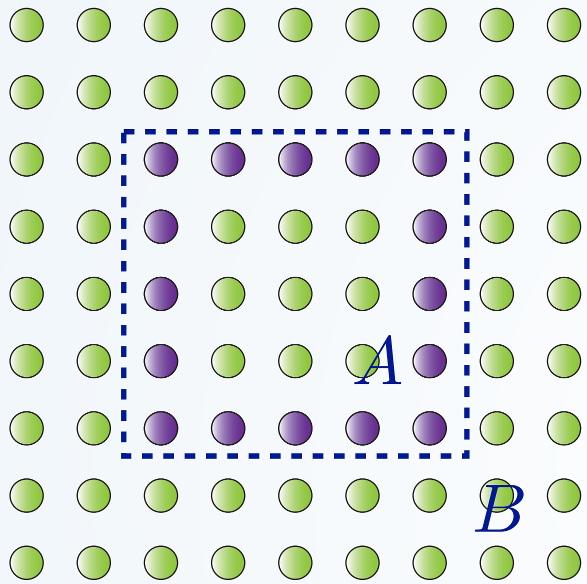


Ansätze satisfying
the area law
by construction

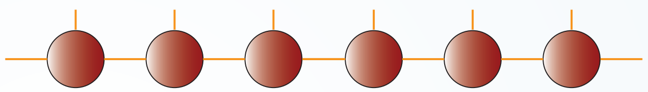
TNS = entanglement based ansatz

TNS = entanglement based ansatz

area law

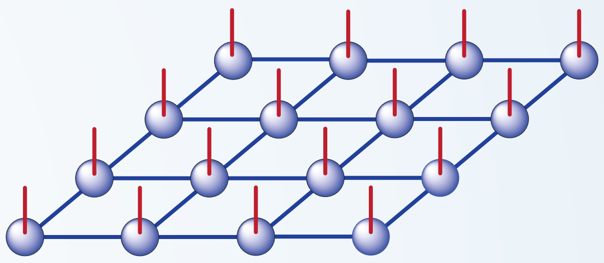


MPS



Schollwöck Ann.Phys.2011

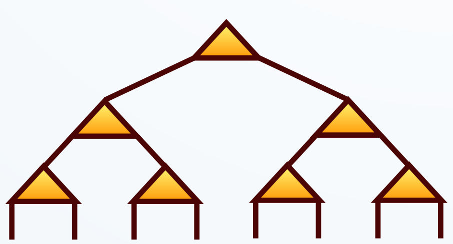
PEPS



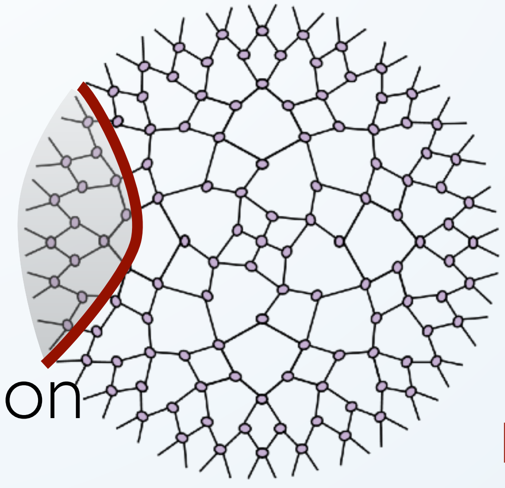
Verstraete et al. Adv. Phys. 2008

other TNS

TTN



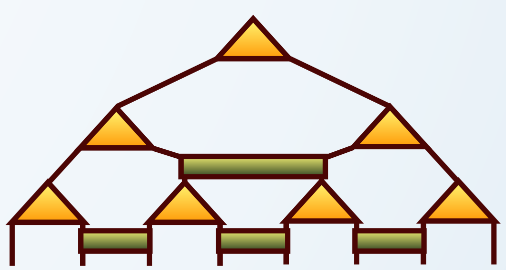
Shi et al PRA 2006



suggested connection
to AdS/CFT

Vidal PRL 2007

MERA



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

MPS

Matrix Product States

MPS

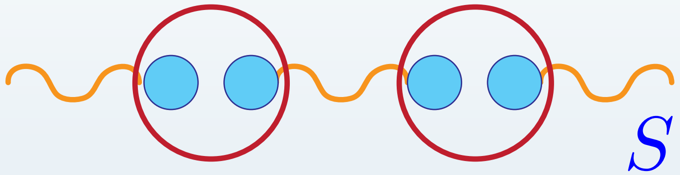
Matrix Product States

A bit of history...

AKLT exactly solvable spin model

Affleck, Kennedy, Lieb, Tasaki, PRL 1987

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



$S = \frac{1}{2}$

The ground state is exactly a MPS (VBS)

MPS

Matrix Product States

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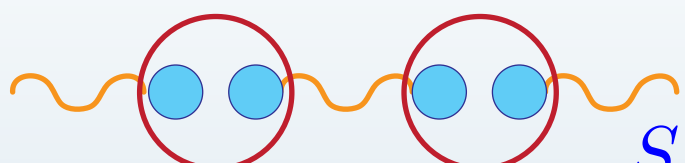

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The ground state is exactly a MPS (VBS)

MPS

Matrix Product States

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↓

Finitely correlated states

Fannes, Nachtergaele, Werner, CMP 1992

DMRG algorithm

White, PRL 1992

DMRG variational over MPS

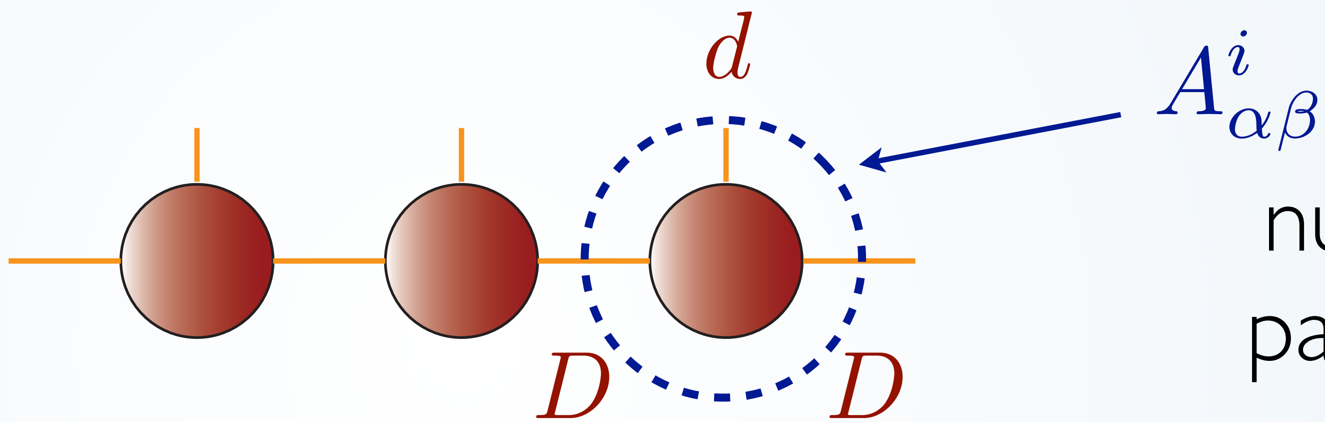
Ostlund, Rommer, PRL 1995
Dukelsky et al., Eur. Phys. Lett. 1998

Quantum Information perspective

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

MPS

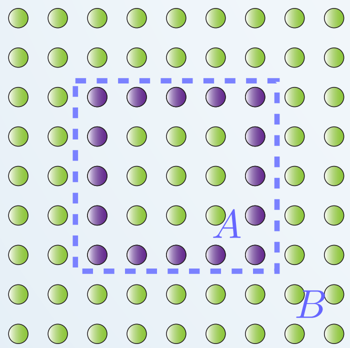
Matrix Product States



number of parameters

$$NdD^2$$

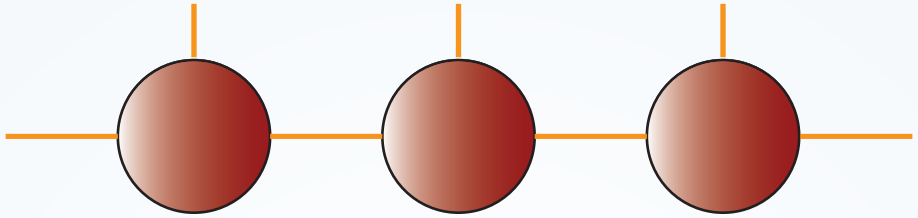
$$|\Psi\rangle = \sum_{i_1 \dots i_N} \mathrm{tr}(A_1^{i_1} A_2^{i_2} \dots A_N^{i_N}) |i_1 \dots i_N\rangle$$



Area law by construction

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

MPS EXAMPLE



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

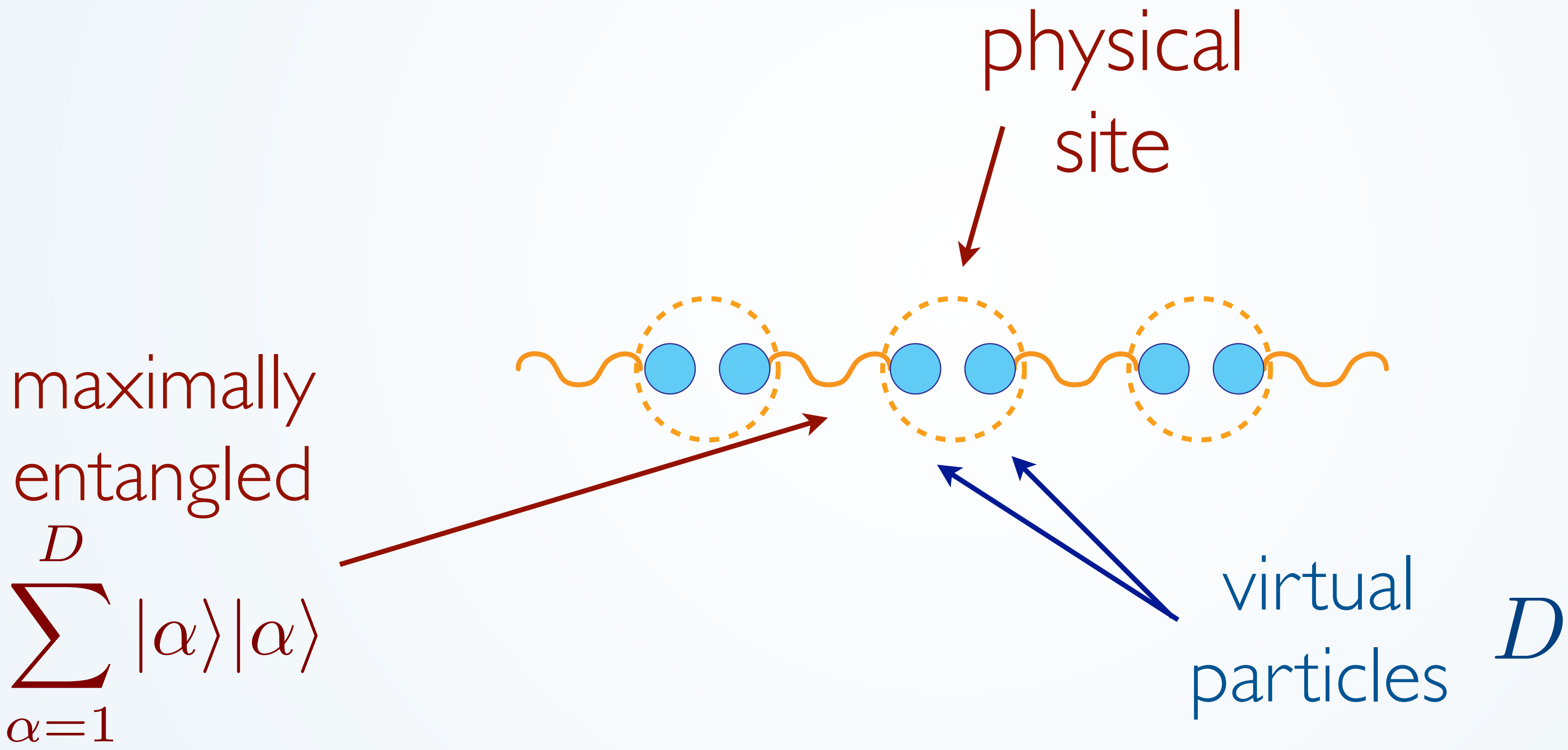
$$A^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad A^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

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

$$D = 2$$

MPS

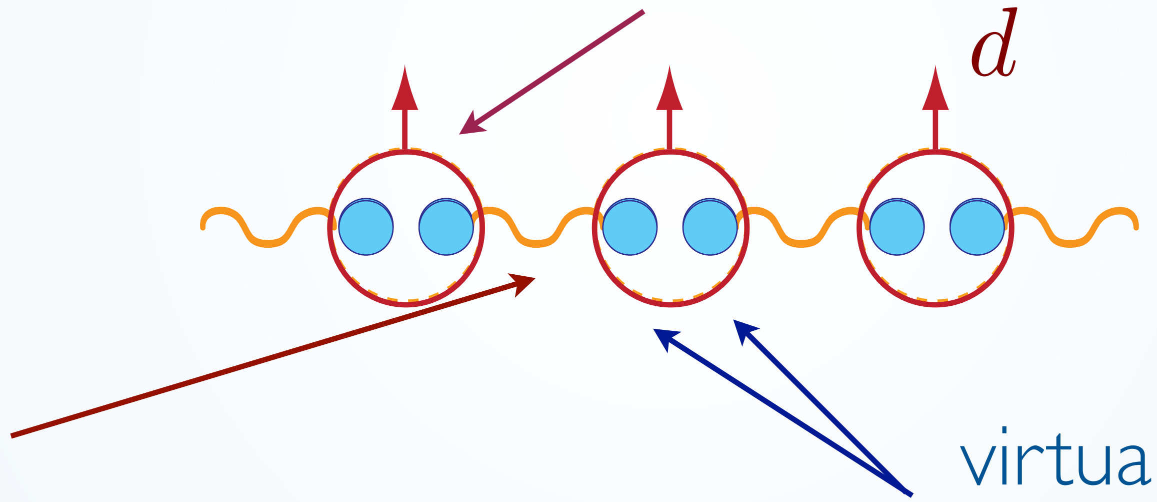
Matrix Product States



MPS

Matrix Product States

project onto the physical degrees of freedom



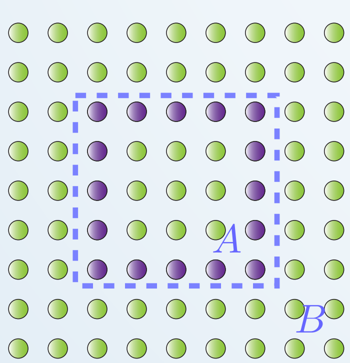
d

maximally entangled

$$\sum_{\alpha=1}^{D} |\alpha\rangle|\alpha\rangle$$

$$\sum_{i\alpha\beta} A^{i}_{\alpha\beta}|i\rangle\langle\alpha\beta|$$

virtual particles D

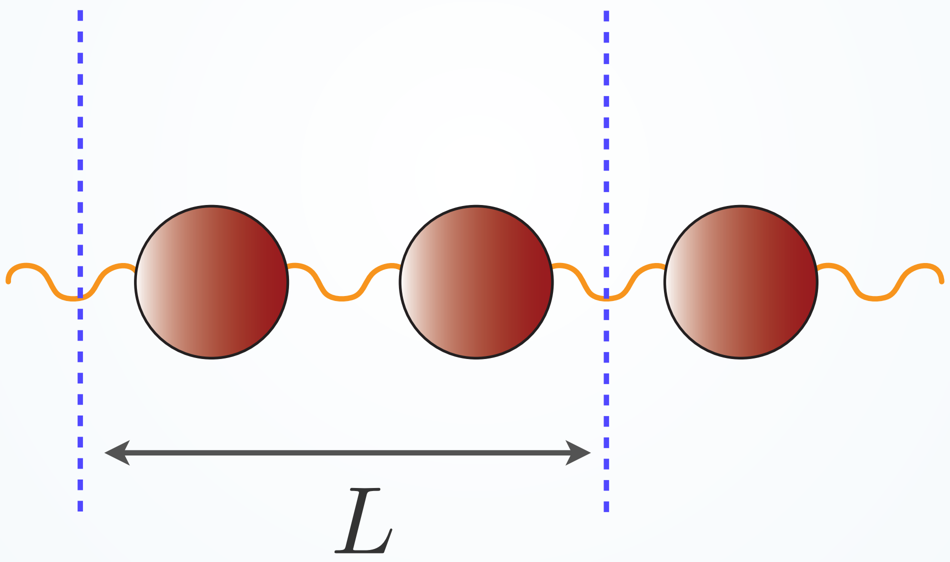


Area law by construction

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

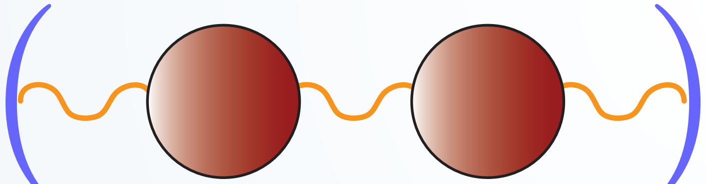
MPS PROPERTIES

Area law by construction



MPS PROPERTIES

Area law by construction

$S\Big($  $\Big) \leq S\Big($  $\Big)$

$= S\Big($  $\Big)$

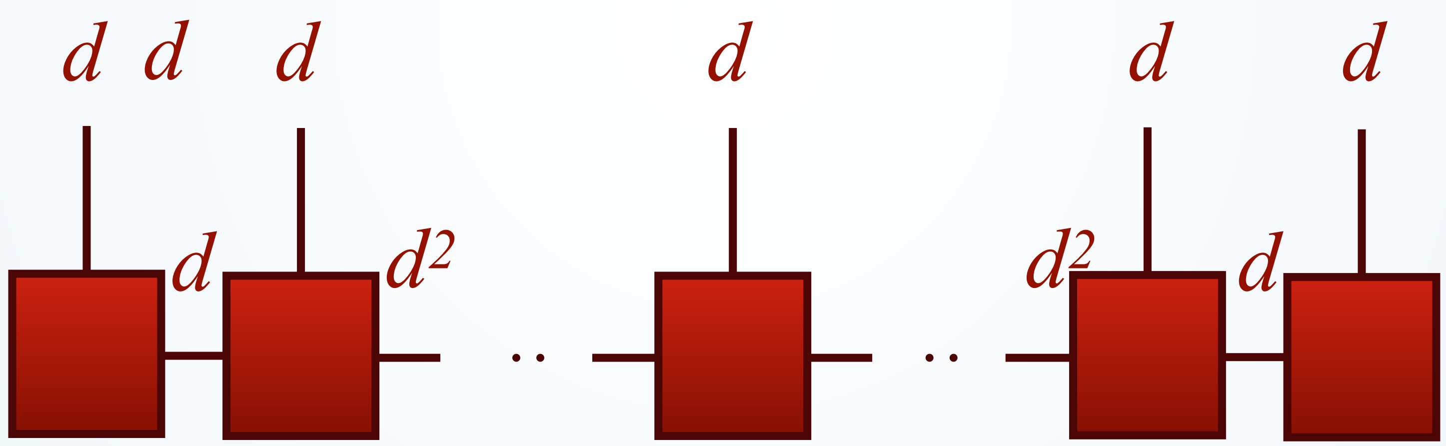
$= 2 \log D$

local projectors
cannot increase
the entropy

SOME OTHER PROPERTIES

MPS PROPERTIES

any state can be written as MPS



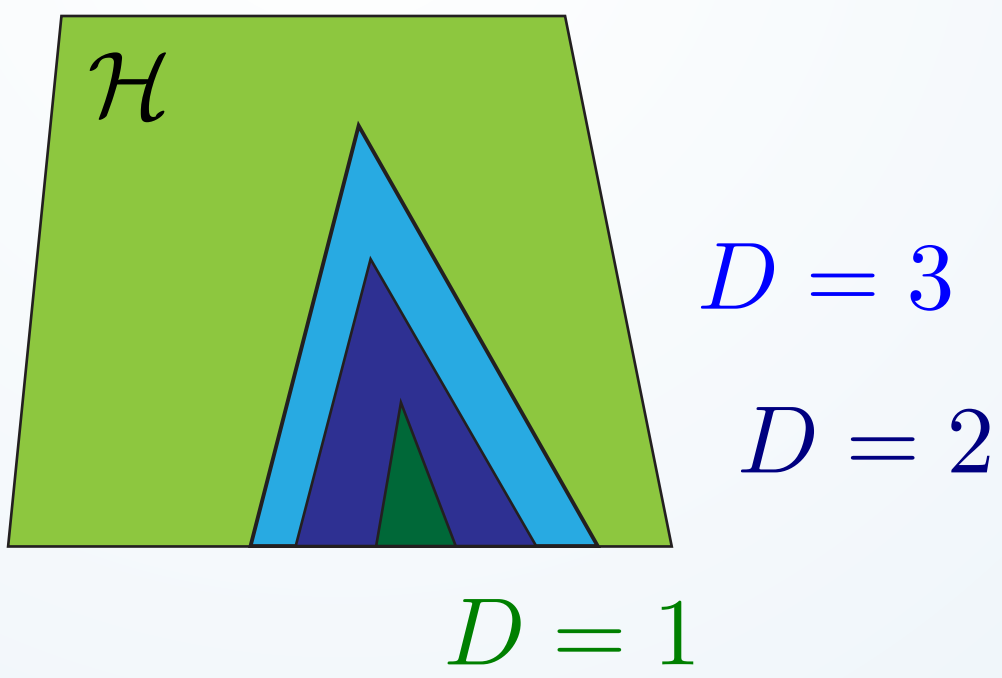
$$D \leq d^{N/2}$$

MPS PROPERTIES

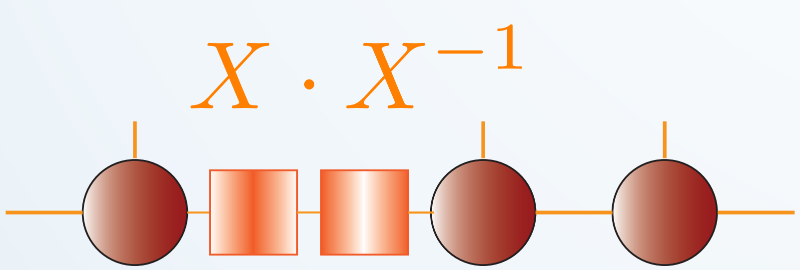
MPS are a complete family

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

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



MPS PROPERTIES



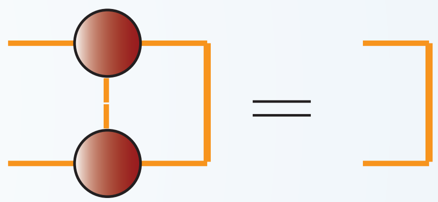
gauge freedom

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

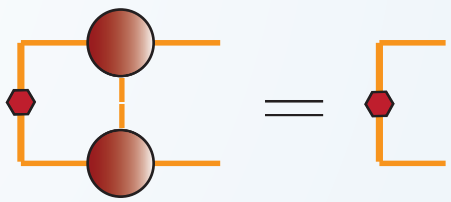
MPS PROPERTIES

canonical form

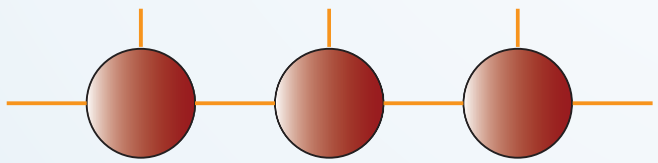
$$\sum_i A^{[m]i} A^{[m]i\dagger} = 1$$



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



unique
imposed locally

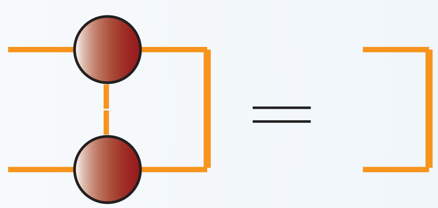


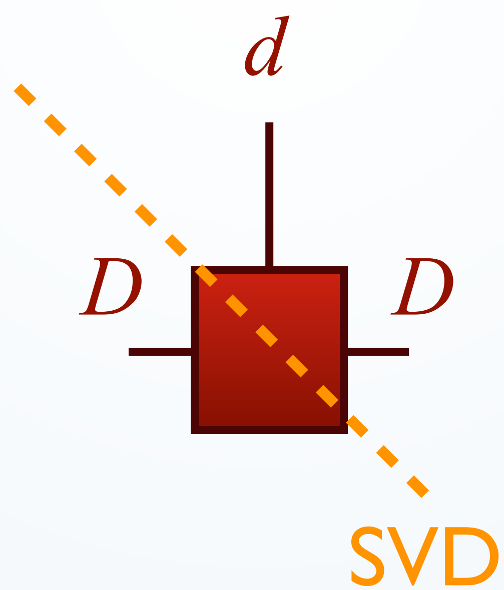
gauge freedom

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

MPS PROPERTIES

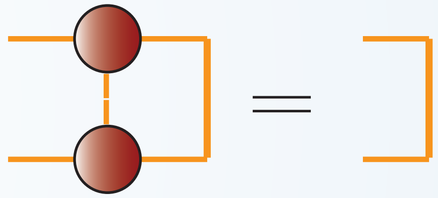
finding the canonical form

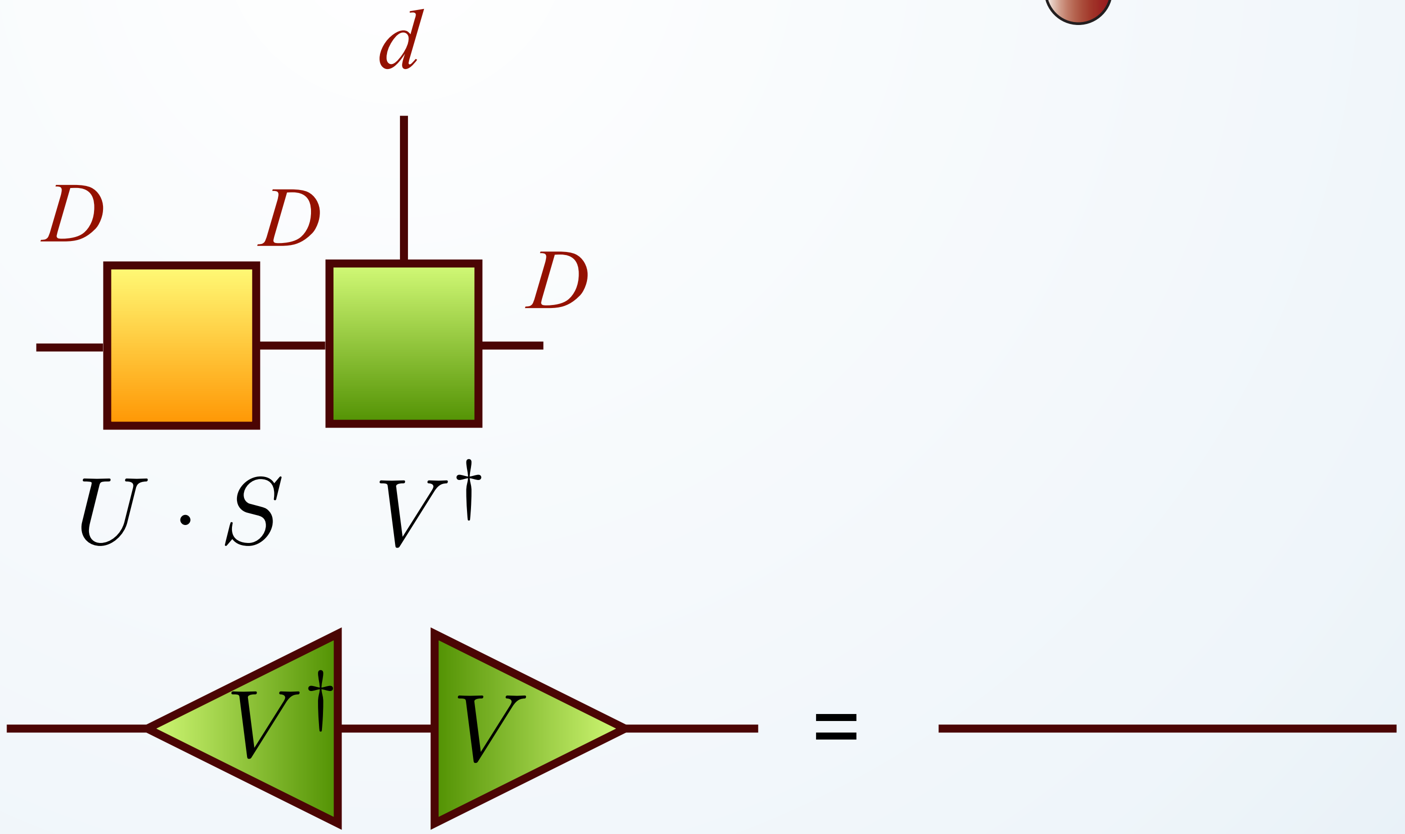




MPS PROPERTIES

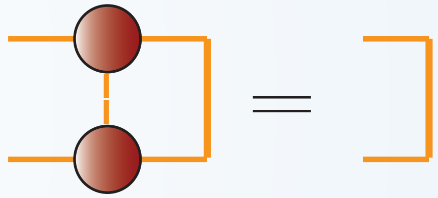
finding the canonical form

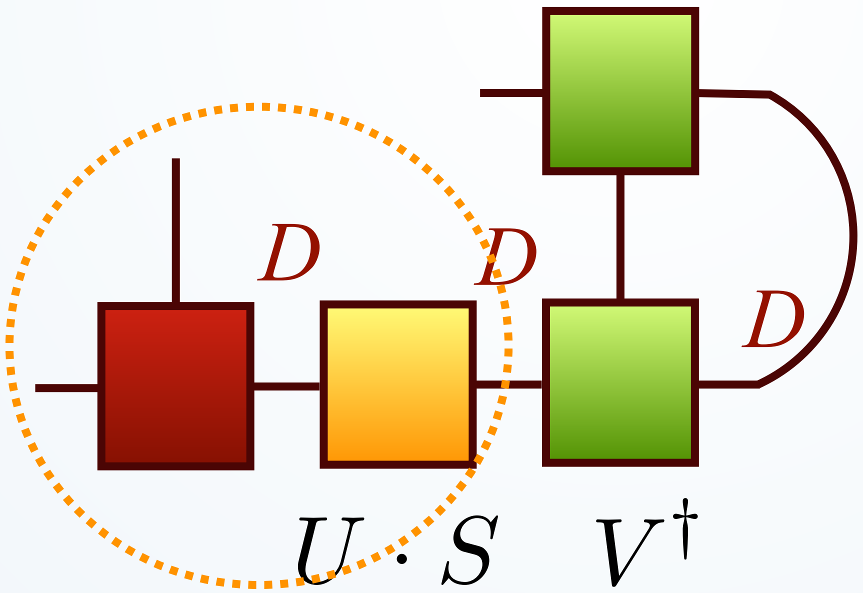


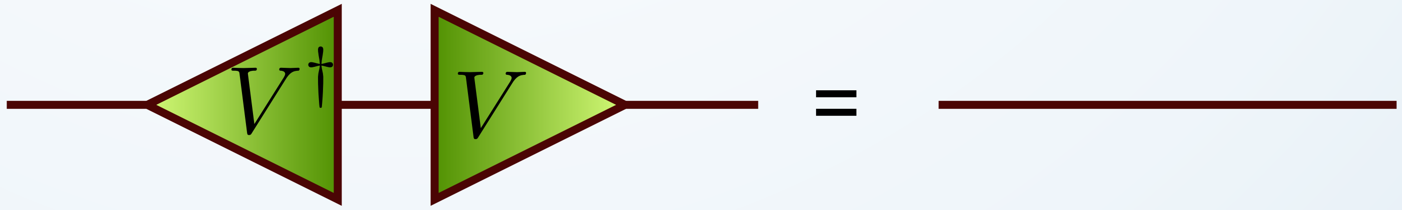


MPS PROPERTIES

finding the canonical form



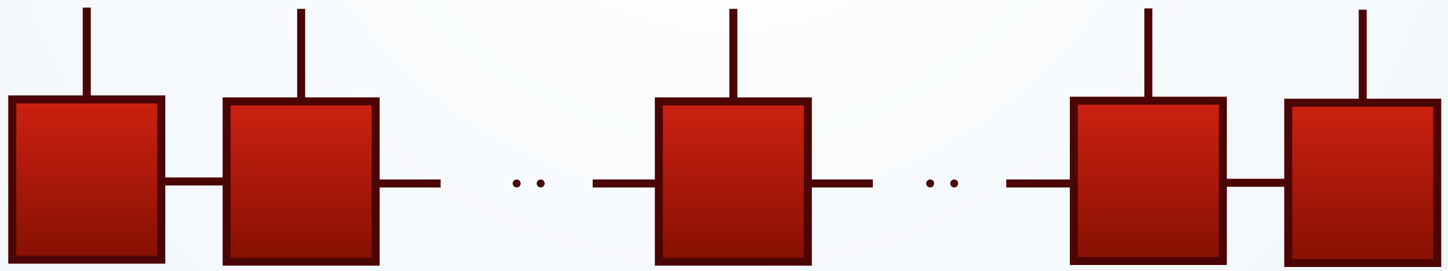




MPS PROPERTIES

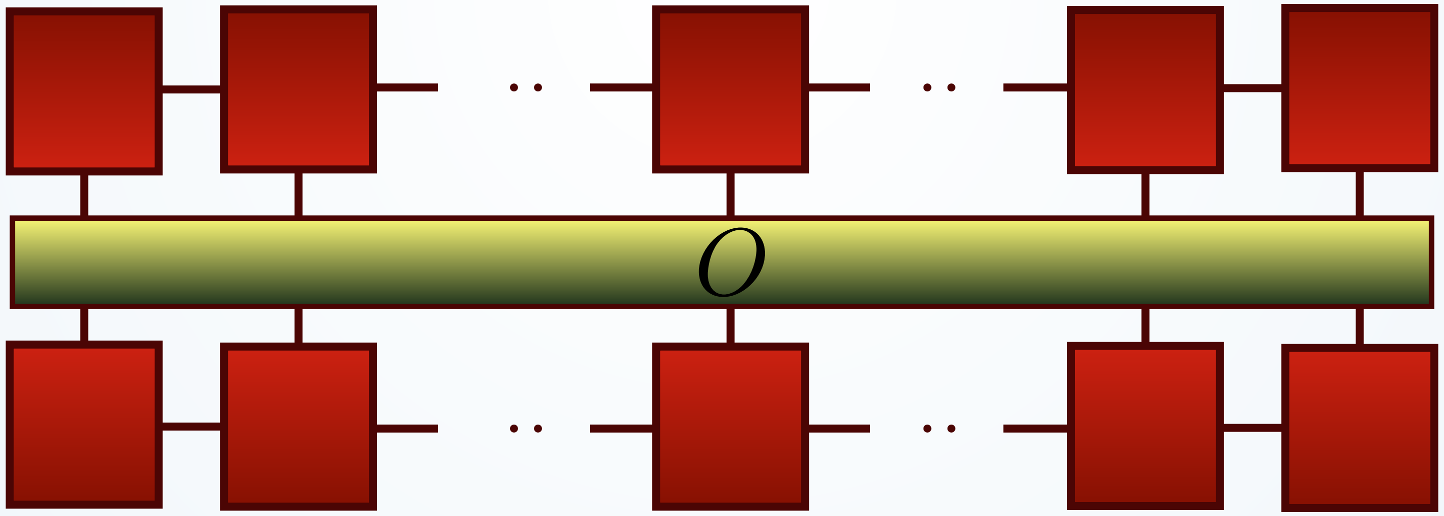
Efficient expectation values

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



MPS PROPERTIES

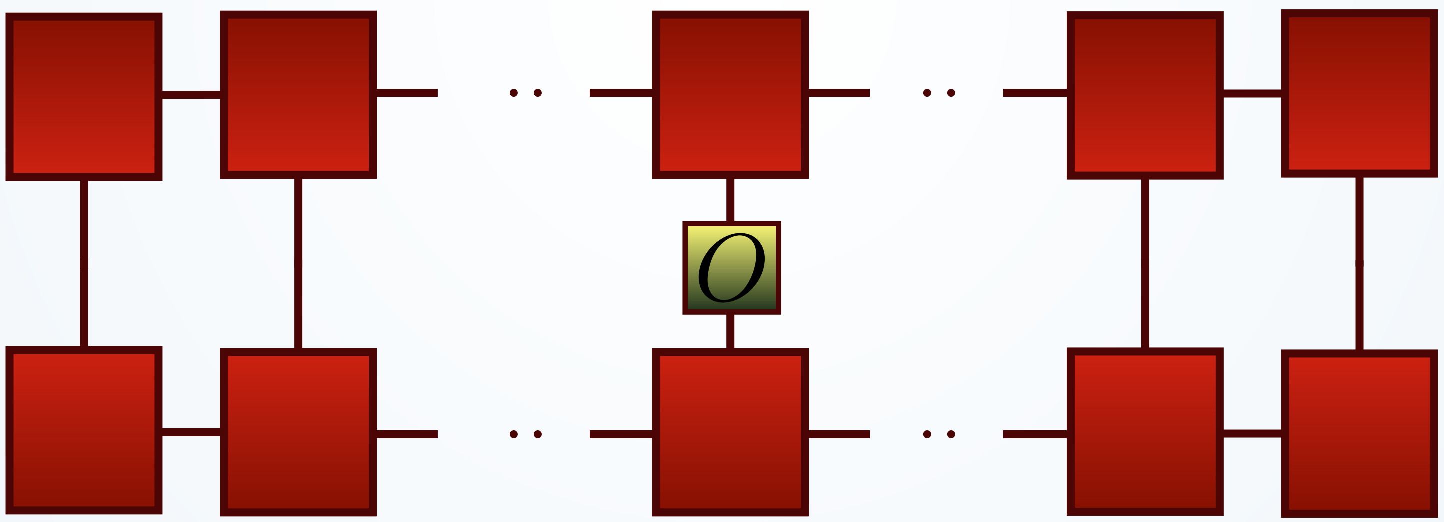
Efficient expectation values



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

MPS PROPERTIES

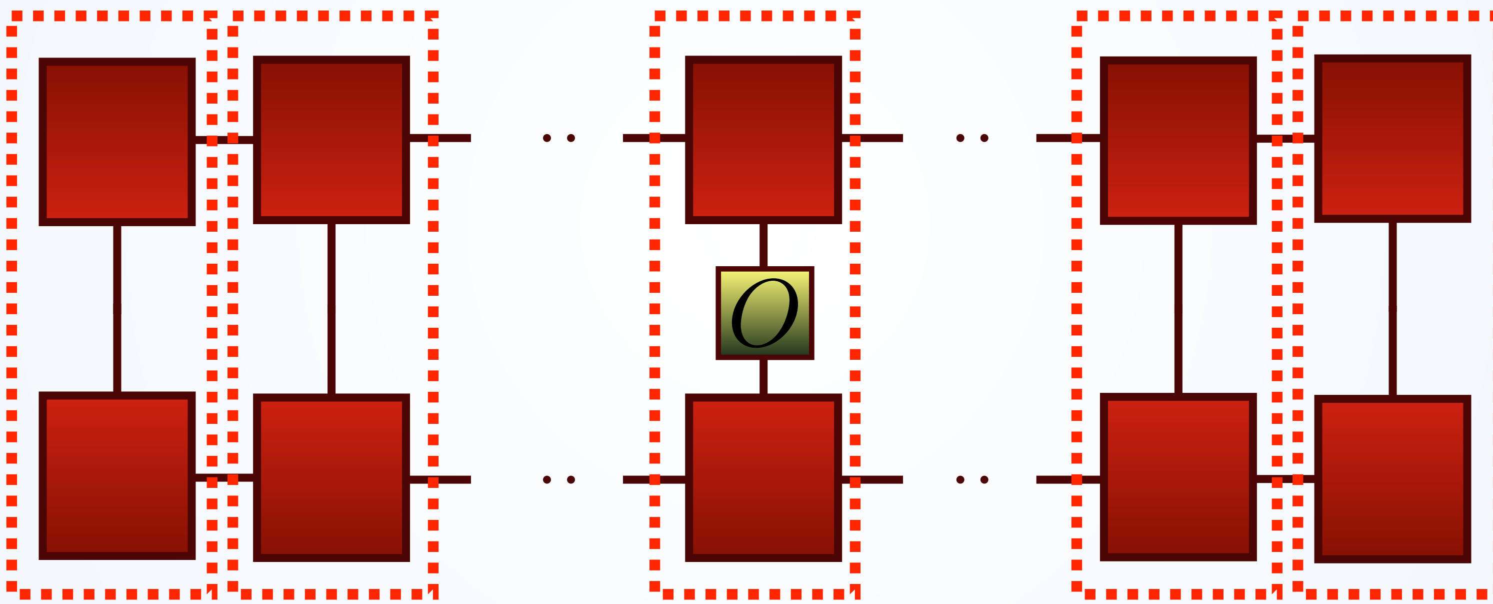
Efficient expectation values



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

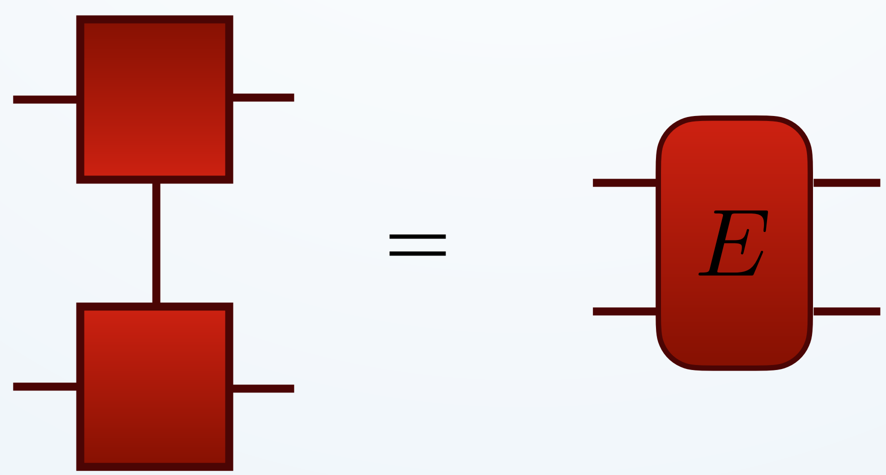
MPS PROPERTIES

Efficient expectation values



transfer operator

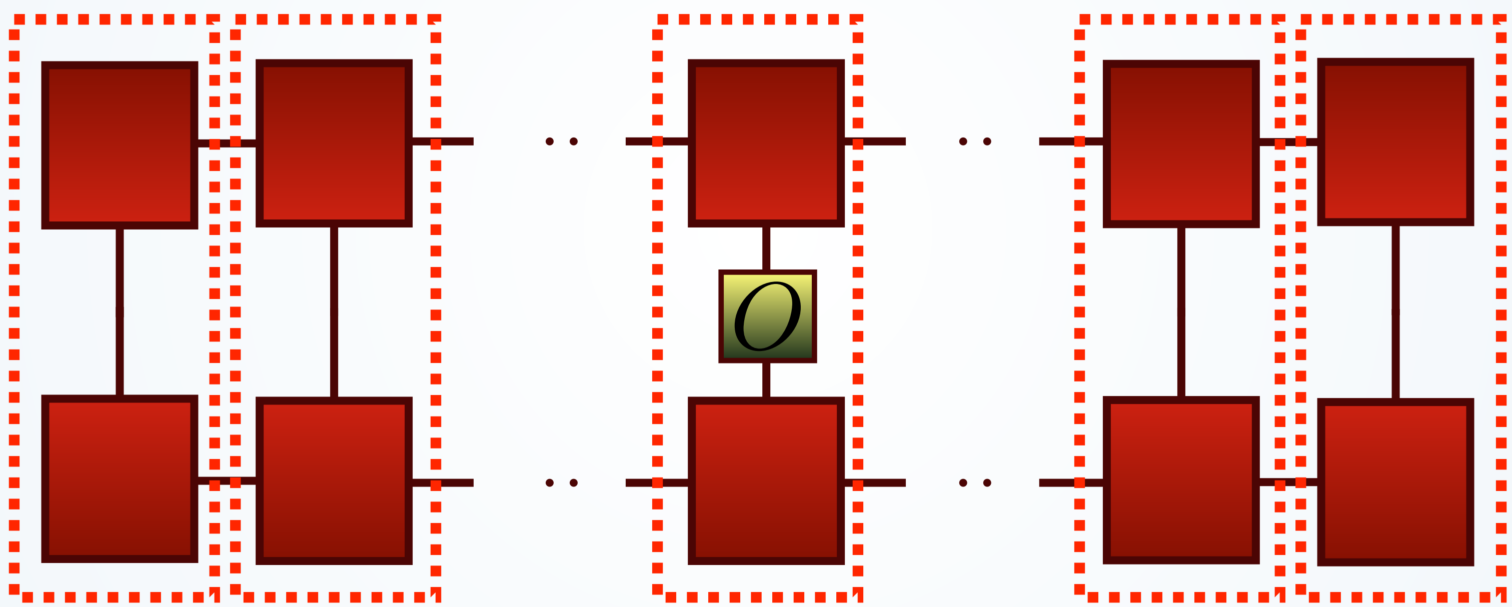
$D^2 \times D^2$ matrix



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

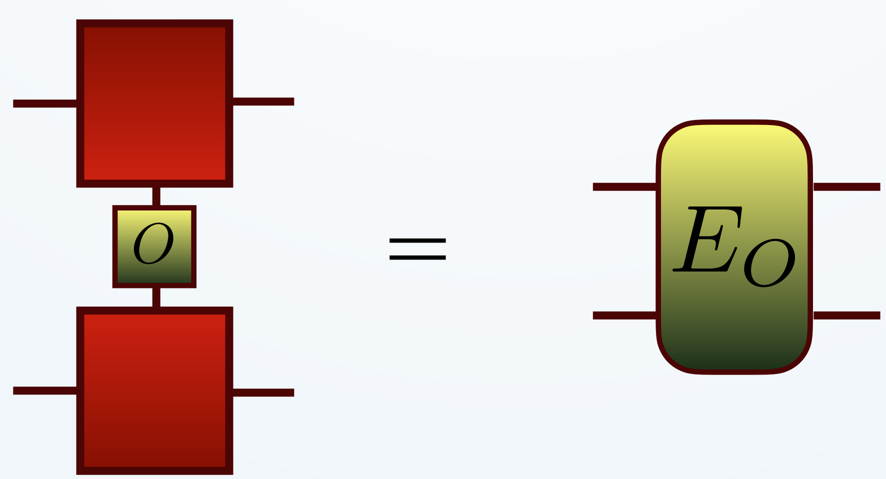
MPS PROPERTIES

Efficient expectation values



transfer operator

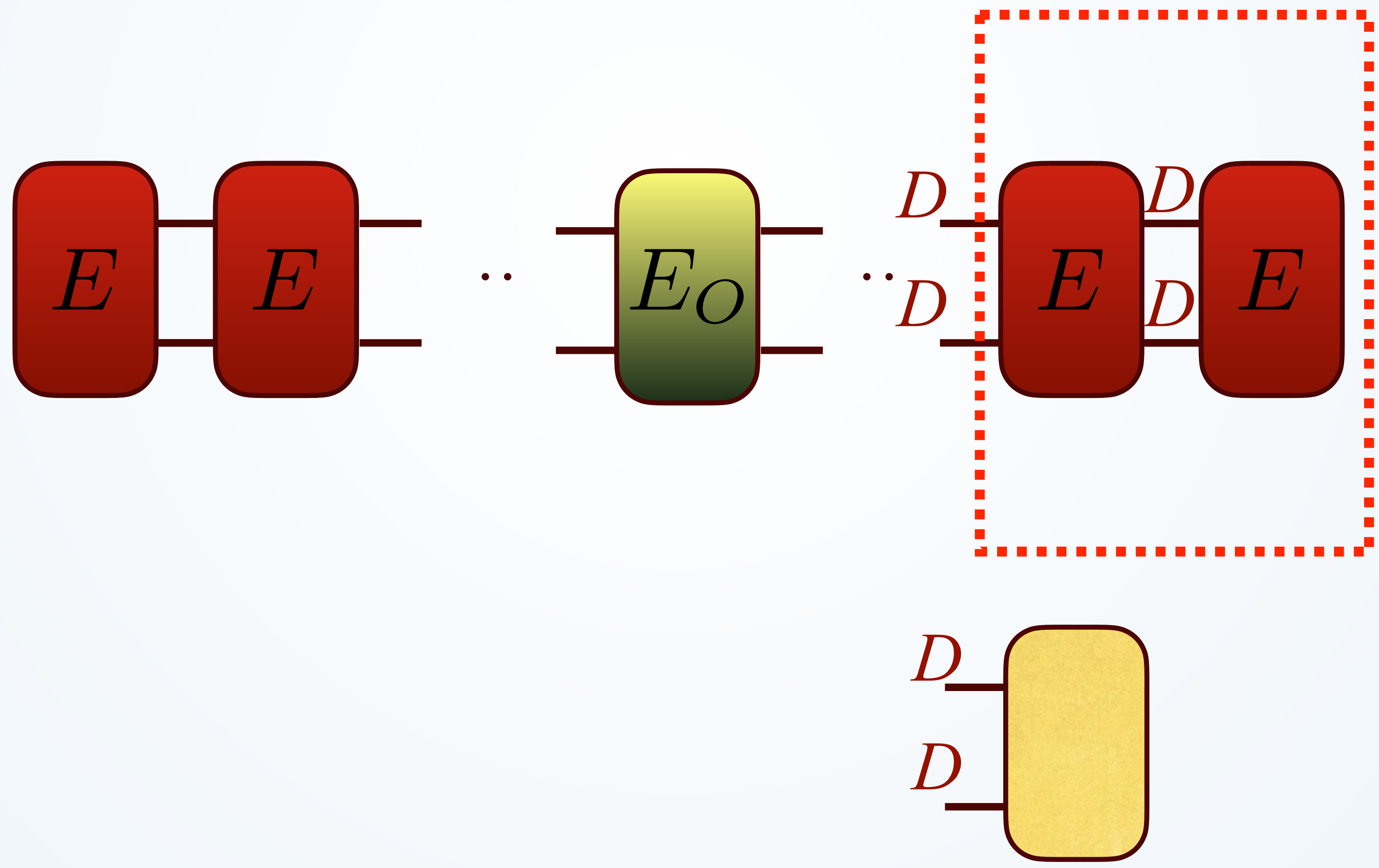
$D^2 \times D^2$ matrix



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

MPS PROPERTIES

Efficient expectation values

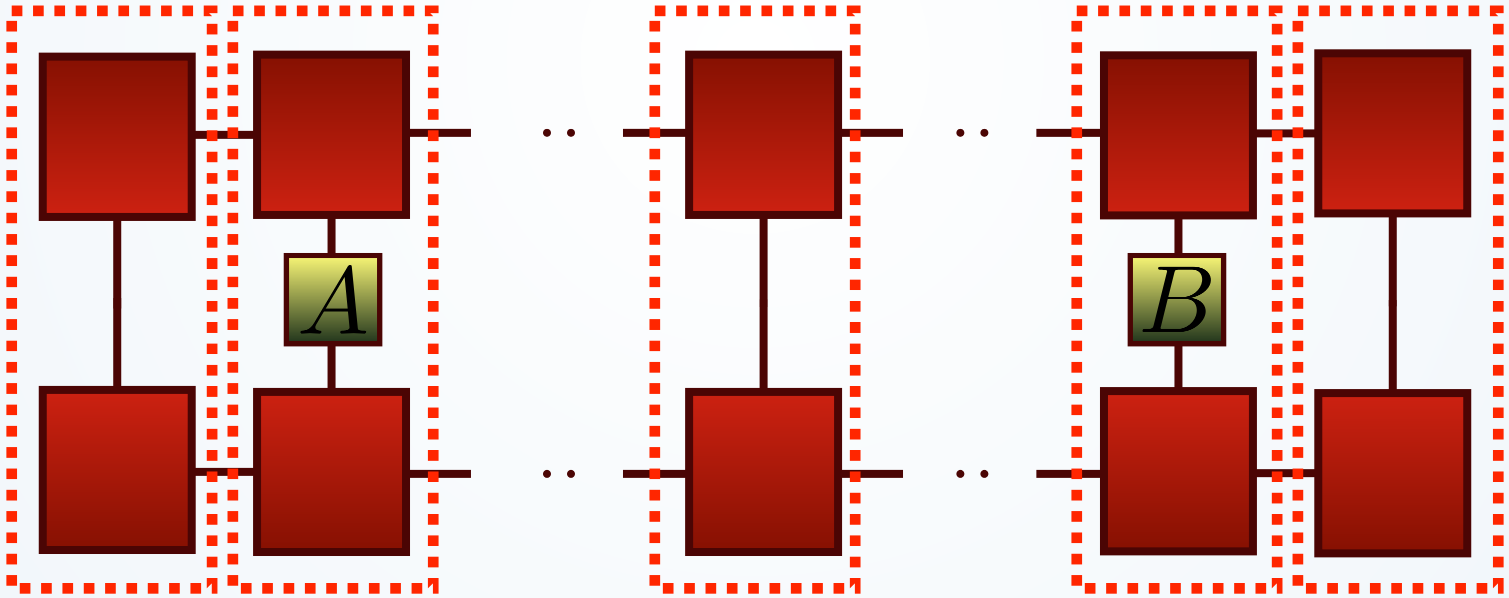


$O(D^4)$

MPS PROPERTIES

Exponentially decaying correlations

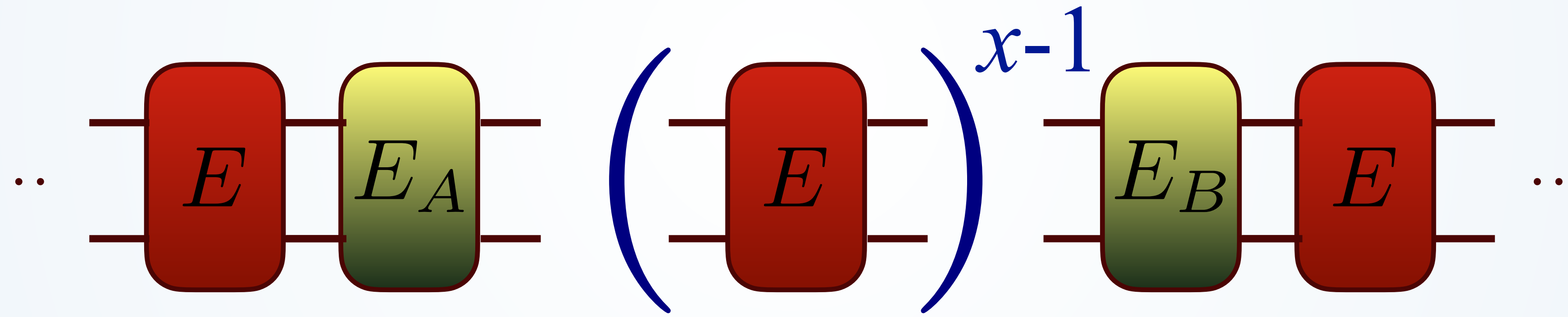
$$\langle A^{[p]} B^{[p+x]} \rangle - \langle A^{[p]} \rangle \langle B^{p+x} \rangle$$



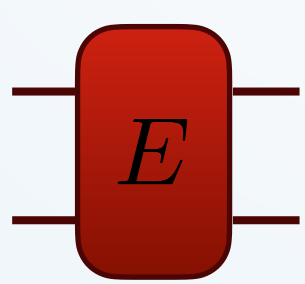
MPS PROPERTIES

Exponentially decaying correlations

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



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

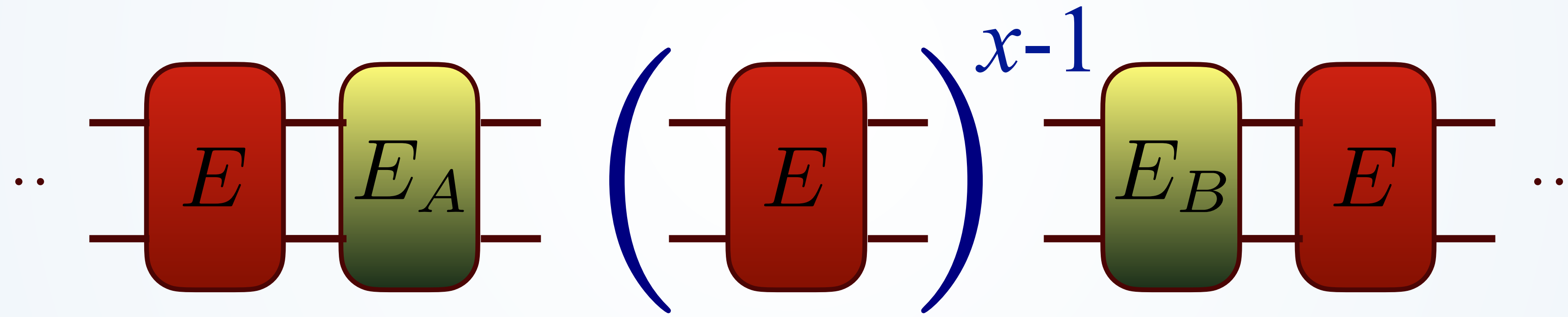


$$E = \sum_i A^{i*} \otimes A^i = \sum_k \lambda_k |R_k\rangle\langle L_k|$$

MPS PROPERTIES

Exponentially decaying correlations

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



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

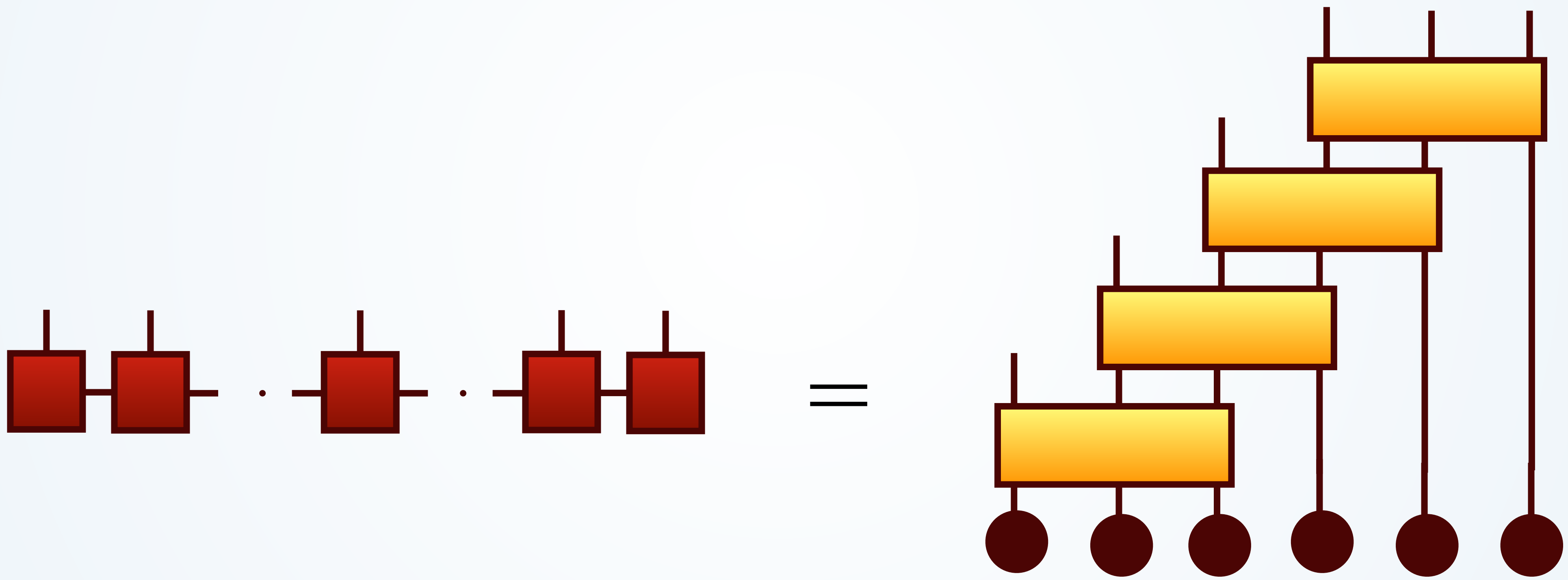
normalize

disconnected component

exponential decrease

MPS PROPERTIES

Efficient preparation



equivalent to an ancilla with dimension D

MPS PROPERTIES

Approximate ground states efficiently

$$\| |\Psi\rangle - |\Psi_D\rangle \|^2 \leq 2 \sum_{\alpha=1}^{N-1} \epsilon_\alpha(D)$$

truncation per link

$$\epsilon_\alpha(D) = \sum_{k=D+1}^{M_\alpha} \mu_k^{(\alpha)}$$

squared Schmidt values

quality of approximation depends on how fast Schmidt values decay

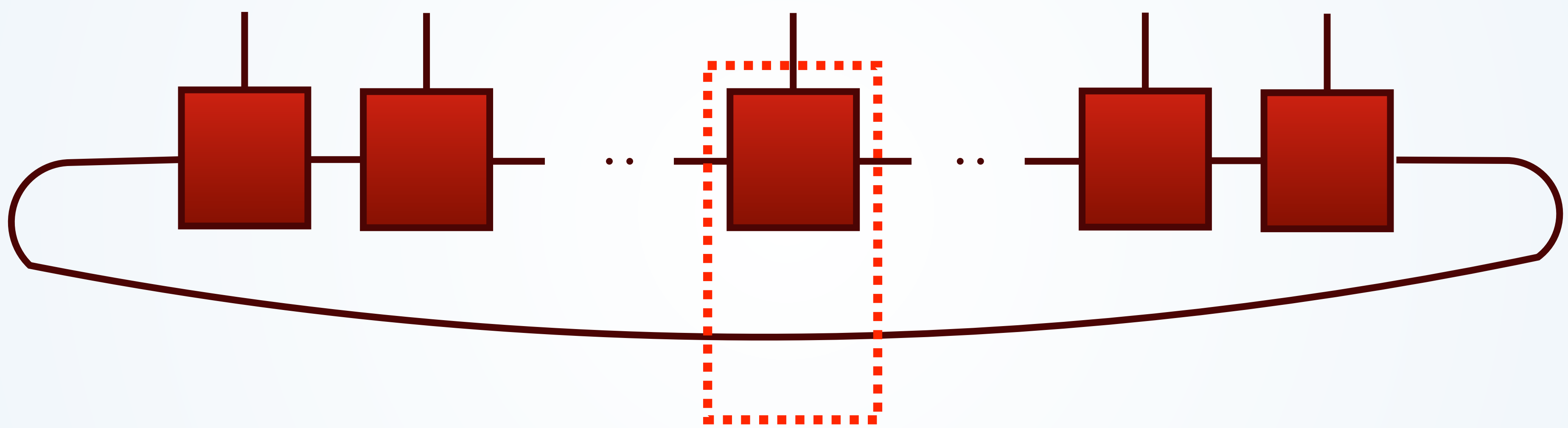
for ground states of local gapped 1D Hamiltonians

$$\epsilon_\alpha(D) \leq C D^{-\frac{1}{\xi' \log d}}$$

Hastings JStatMech 2007

MPS PROPERTIES

Also periodic boundary conditions



more expensive (still efficient) contractions $\mathbf{O}(D^5)$

could be written as OBC with D^2

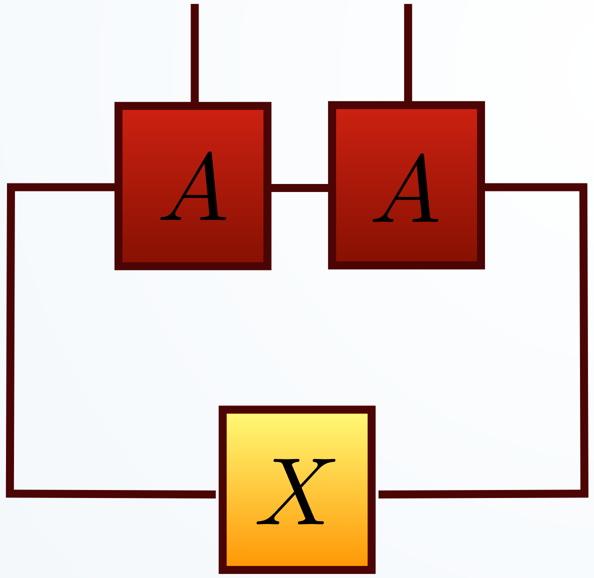
(twice the entropy at half chain)

MPS PROPERTIES

local parent Hamiltonian

Generalization of AKLT construction

S_2



$X \in \mathbb{C}^{D\times D}$

$$H = \sum_{i=1}^{N-1} (1 - \Pi_{S_2})$$

local, frustration-free

MPS injectivity ⇔ unique ground state

MPS PROPERTIES

Symmetries

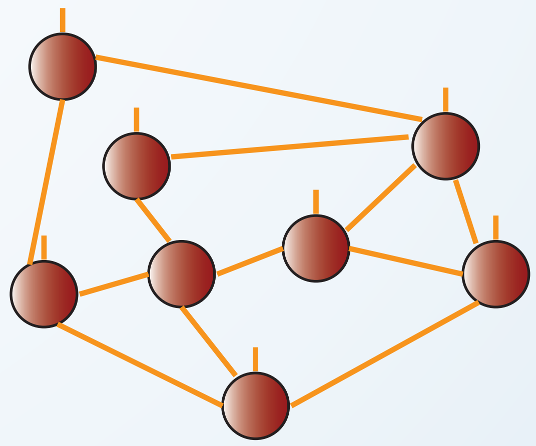
fundamental physical concept

invariant Hamiltonian ➞ symmetric (covariant) eigenstate

$$UHU^\dagger = H \qquad\qquad U|E_n\rangle = e^{i\phi}|E_n\rangle$$

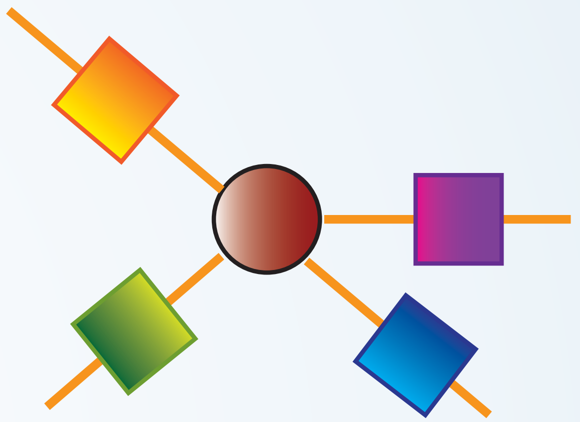
restrict effective Hilbert space to given quantum numbers

role of tensors symmetry?



MPS PROPERTIES

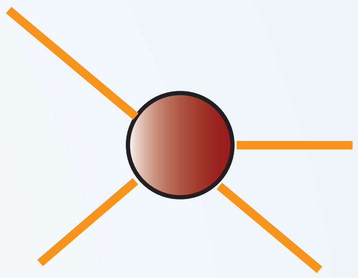
Tensors can be symmetric ⇒ state invariant



Pérez-García et al., PRL 2008
Sanz et al., PRA 2009
Schuch et al., Ann. Phys. 2010
Singh et al., NJP 2007, PRA 2010

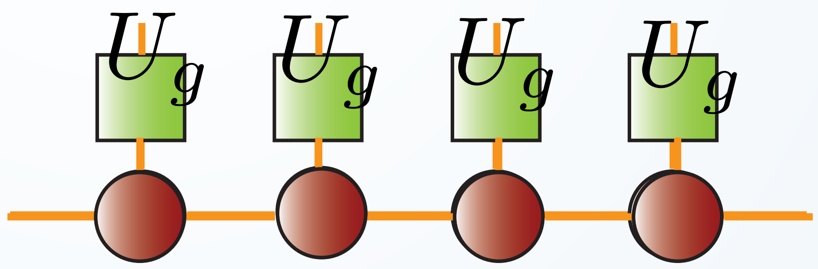
MPS PROPERTIES

Tensors can be symmetric ⇒ state invariant



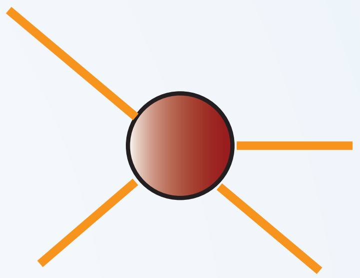
Pérez-García et al., PRL 2008
Sanz et al., PRA 2009
Schuch et al., Ann. Phys. 2010
Singh et al., NJP 2007, PRA 2010

state invariant ⇔



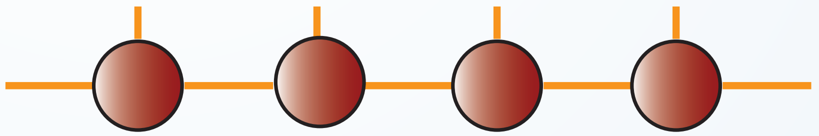
MPS PROPERTIES

Tensors can be symmetric ⇒ state invariant



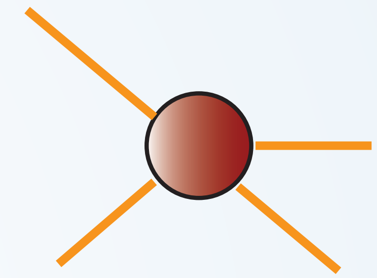
Pérez-García et al., PRL 2008
Sanz et al., PRA 2009
Schuch et al., Ann. Phys. 2010
Singh et al., NJP 2007, PRA 2010

state invariant ⇔



MPS PROPERTIES

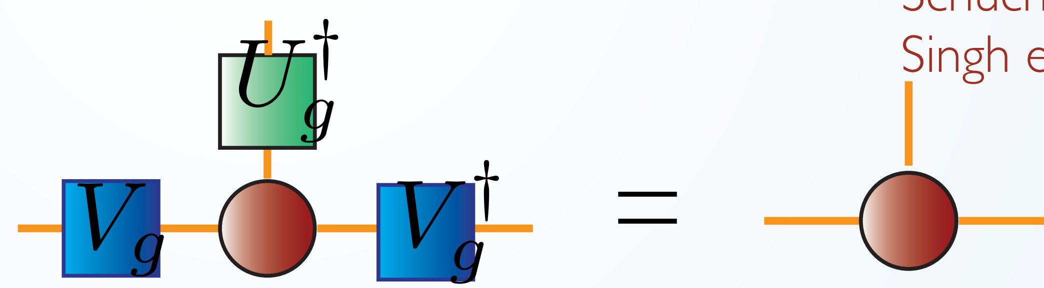
Tensors can be symmetric ⇒ state invariant



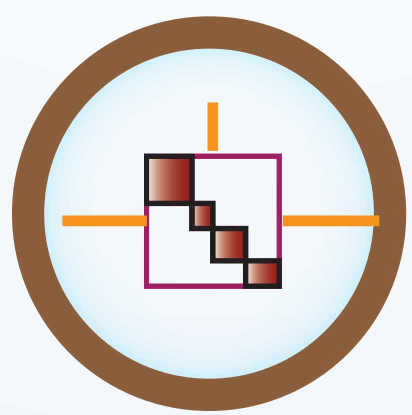
For MPS and PEPS, there is a canonical form

Pérez-García et al., PRL 2008
Sanz et al., PRA 2009
Schuch et al., Ann. Phys. 2010
Singh et al., NJP 2007, PRA 2010

state invariant ⇔



In general: structure of tensor → symmetry properties



gauge symmetries
- Tagliacozzo et al. PRX 2014
- Haegeman et al. PRX 2015

topological order
- Wahl et al., PRL 2013
- Buerschaper, Ann. Phys. 2014
- Sahinoglu et al. arXiv:1409.2150

MPS PROPERTIES

RECAP

good approximation of ground states

gapped finite range Hamiltonian ⇒ area law (ground state)

efficient calculation of expectation values

exponentially decaying correlations

can be prepared efficiently

PEPS

Projected Entangled Pairs

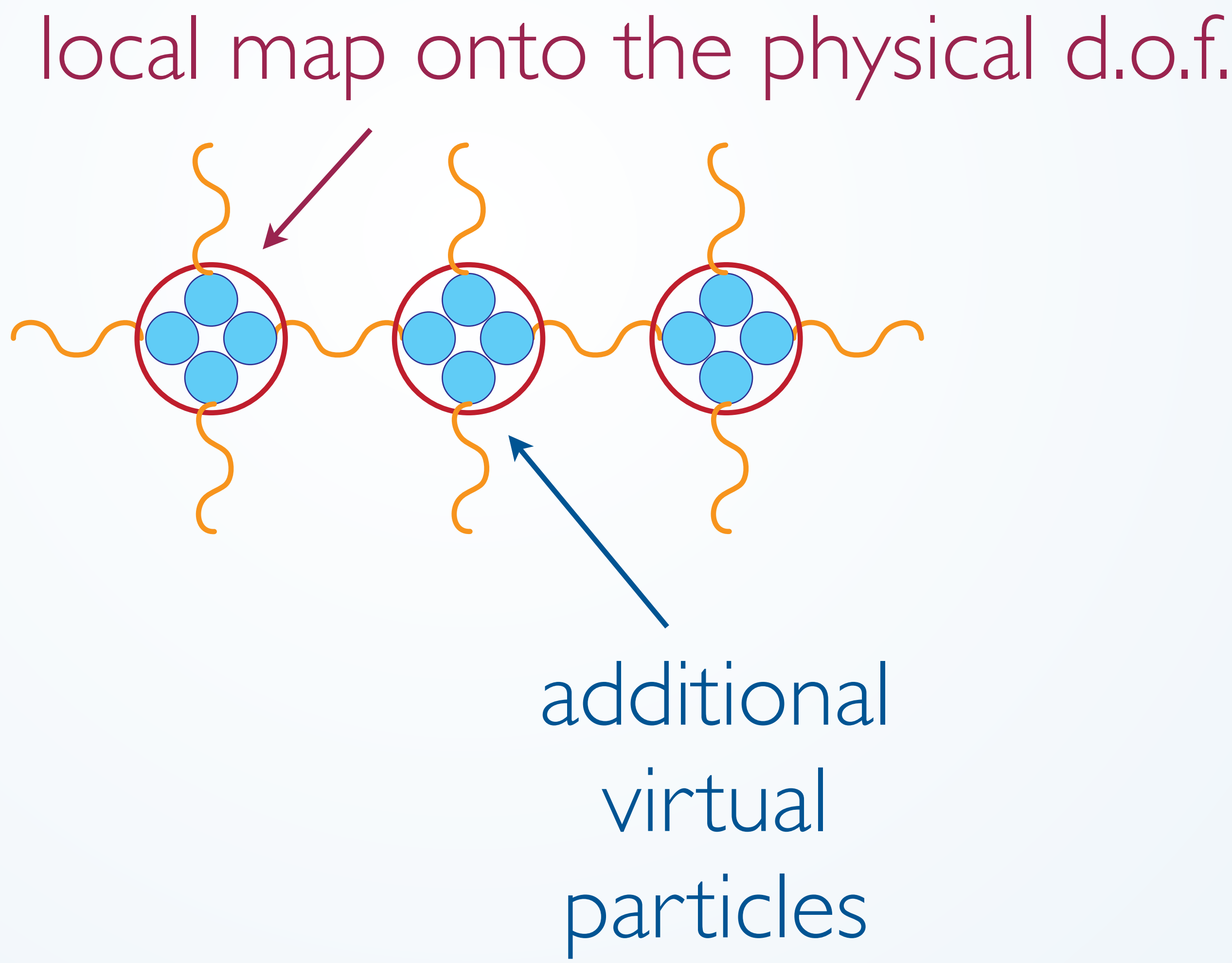
natural generalization of MPS

PEPS

Projected Entangled Pairs States

area law by construction

any lattice

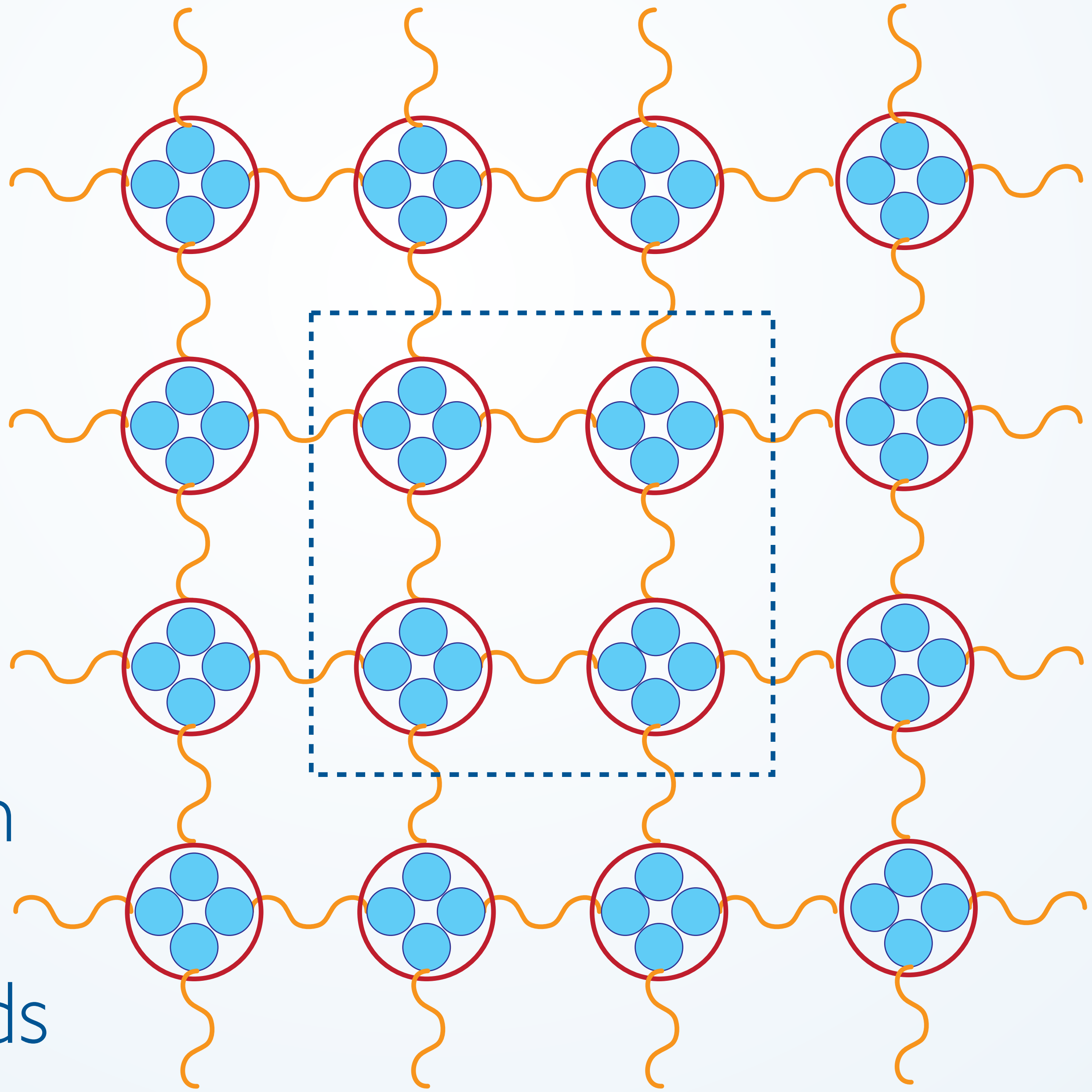


PEPS

Projected Entangled Pairs States

area law by construction

any lattice



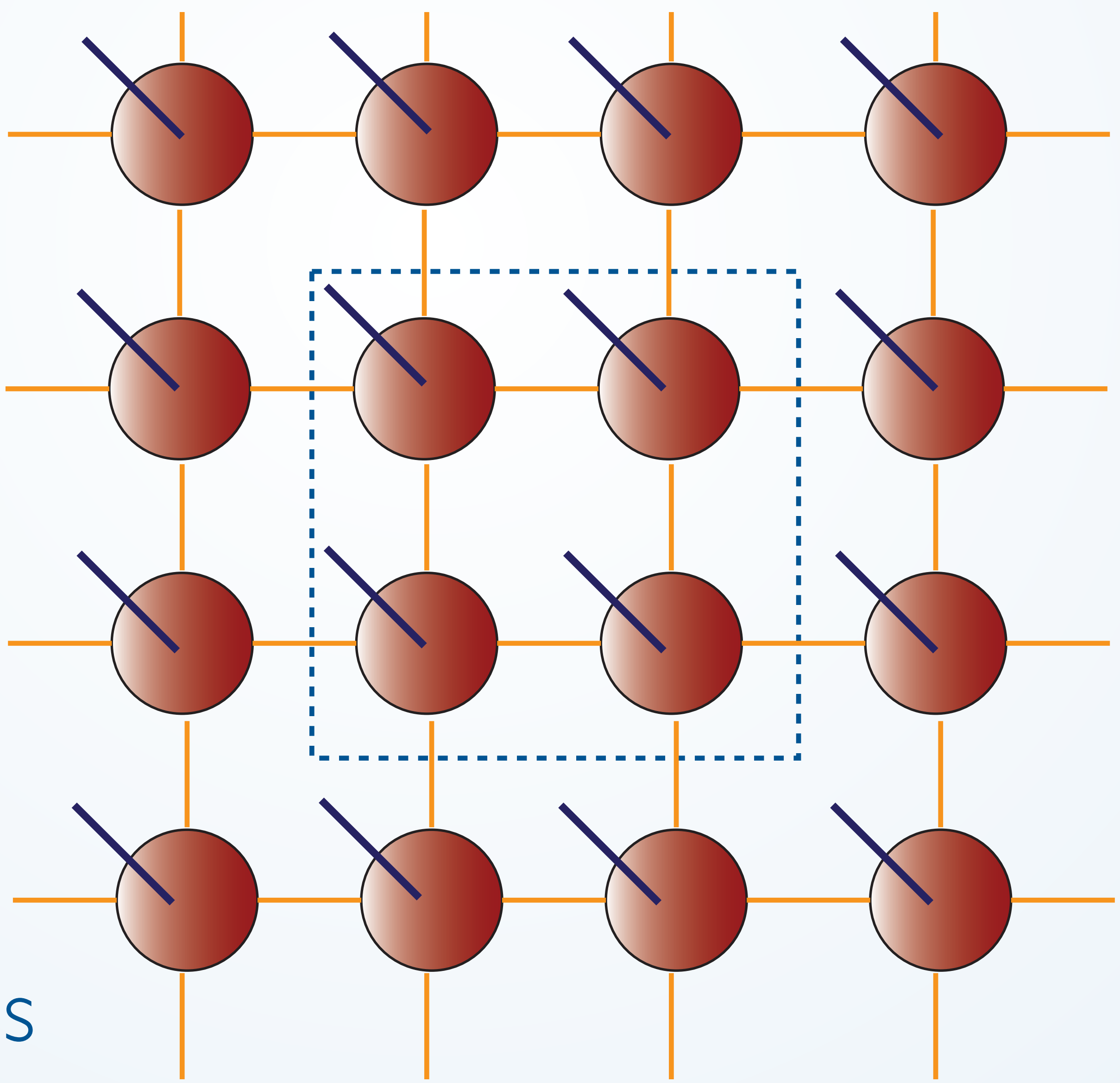
Entropy of a region bounded by the number of cut bonds

PEPS

Projected Entangled Pairs States

area law by construction

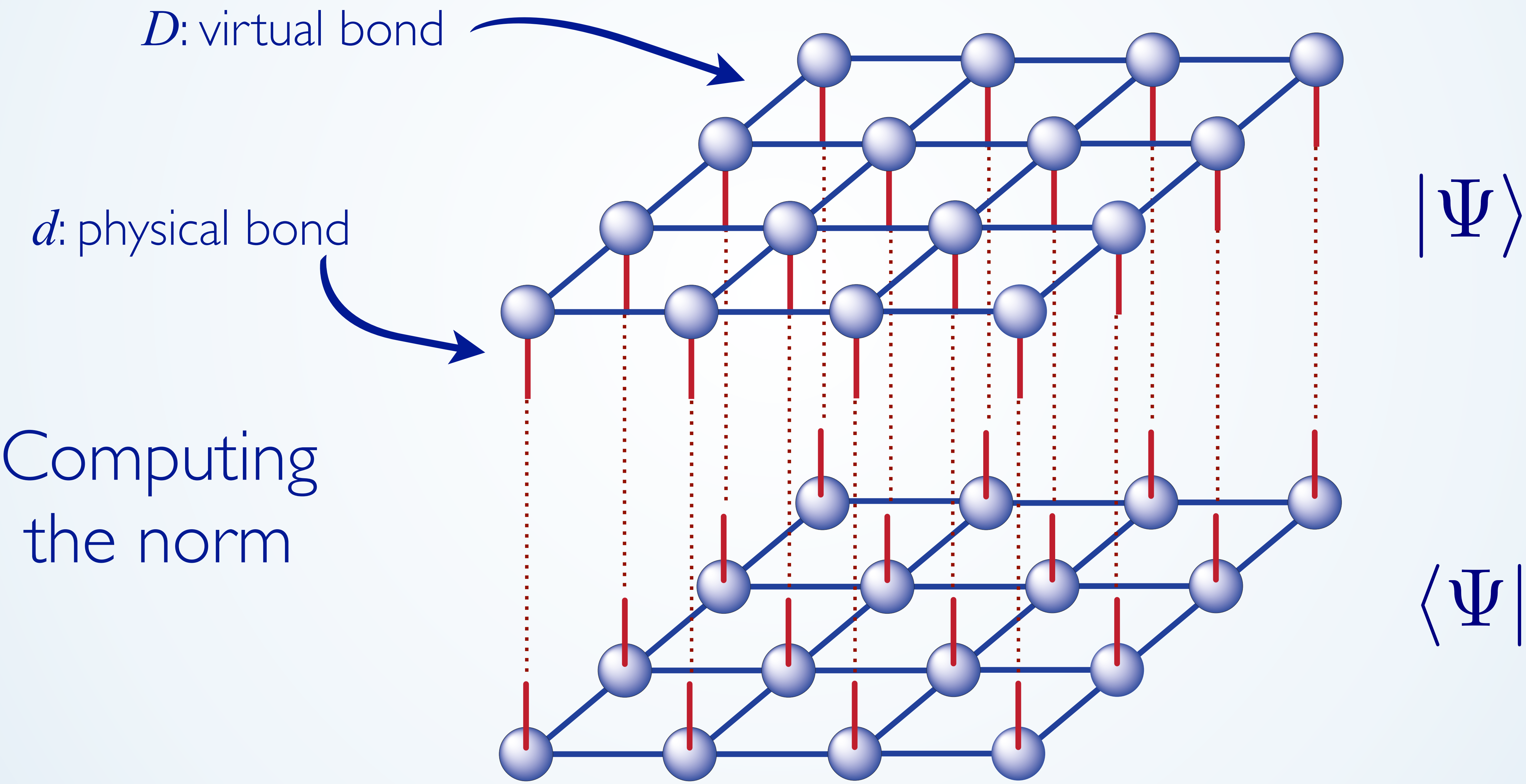
any lattice



Entropy of a region bounded by the number of cut bonds

PEPS

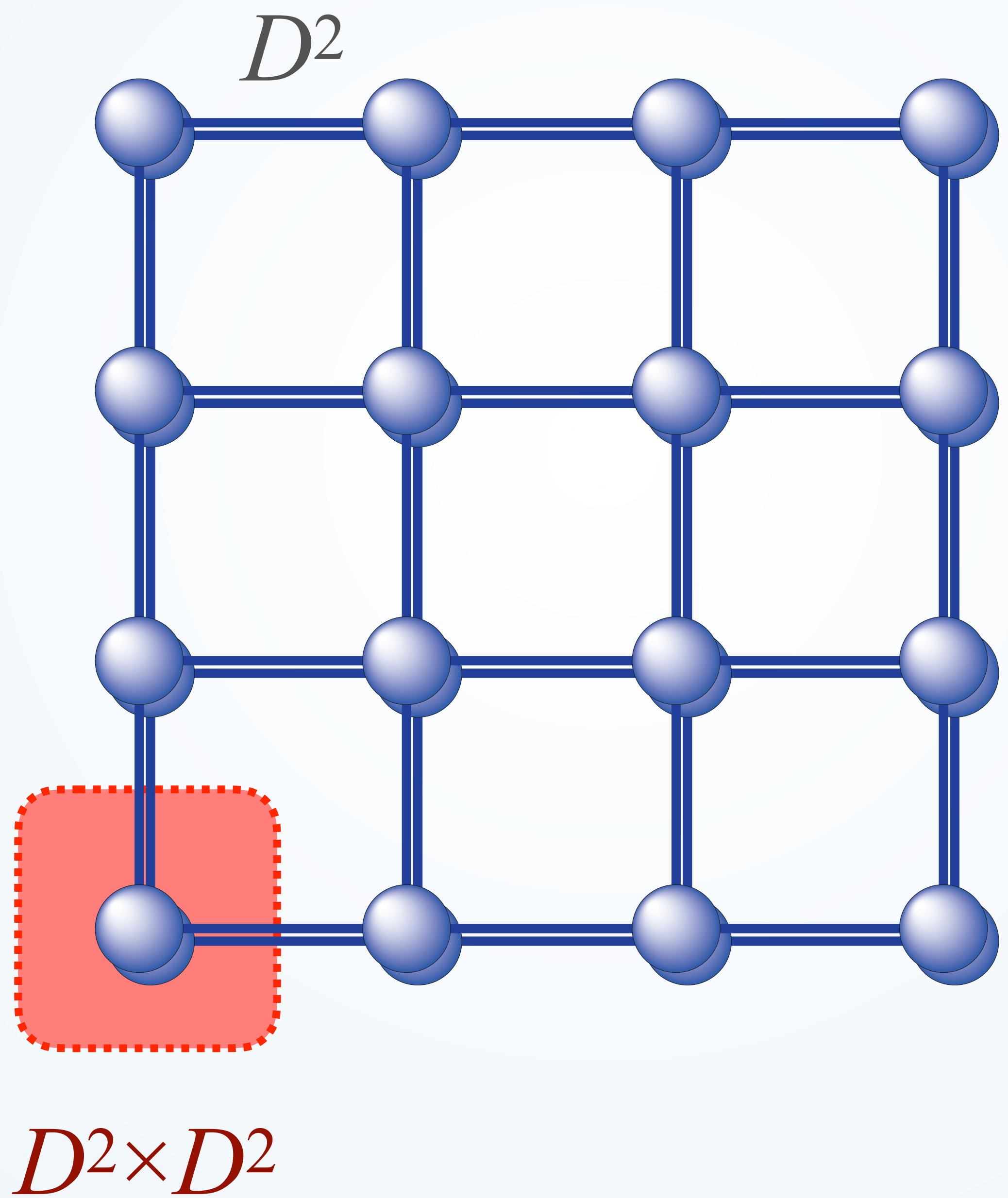
Projected Entangled Pairs States



Computing the norm

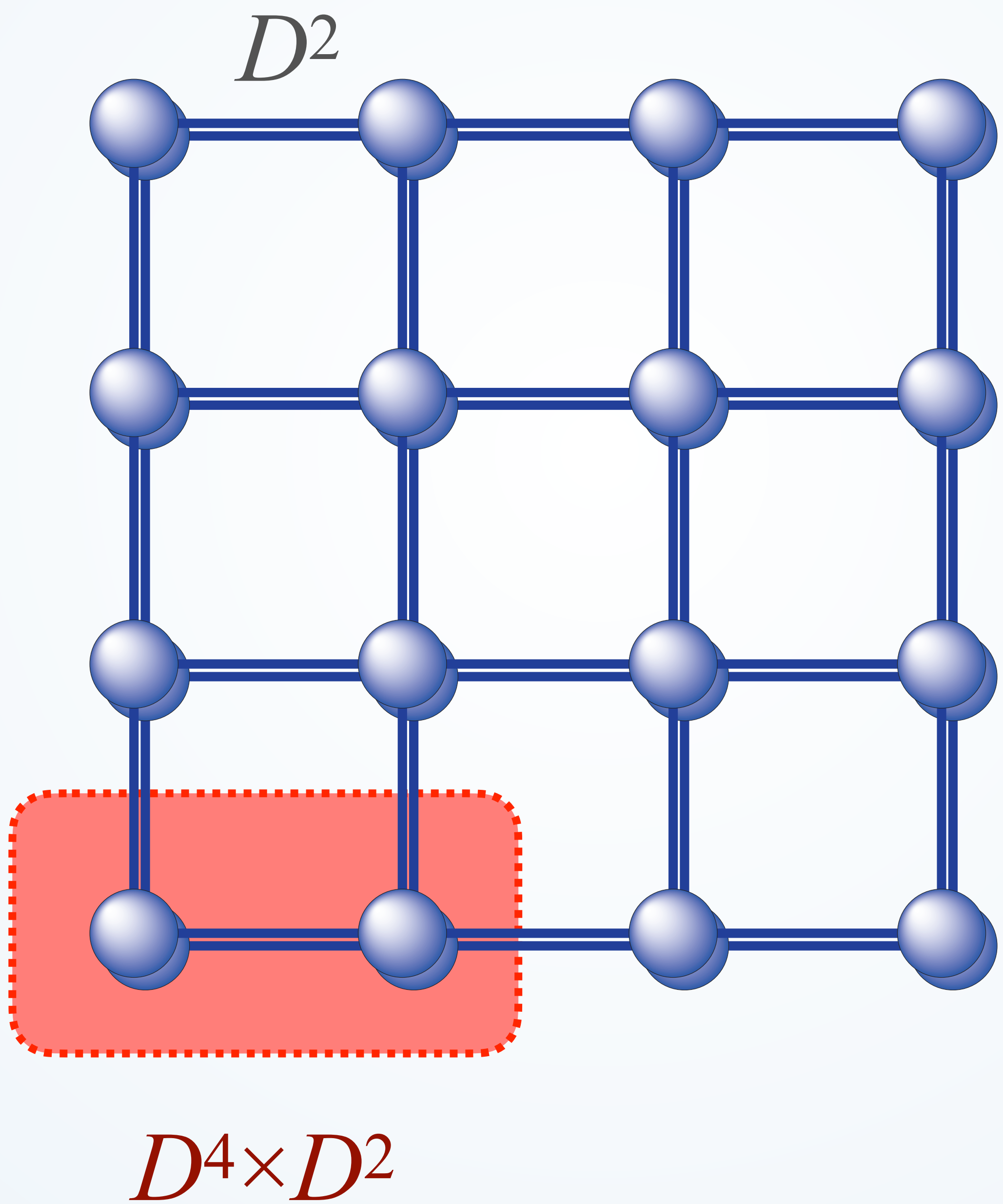
PEPS

Projected Entangled Pairs States



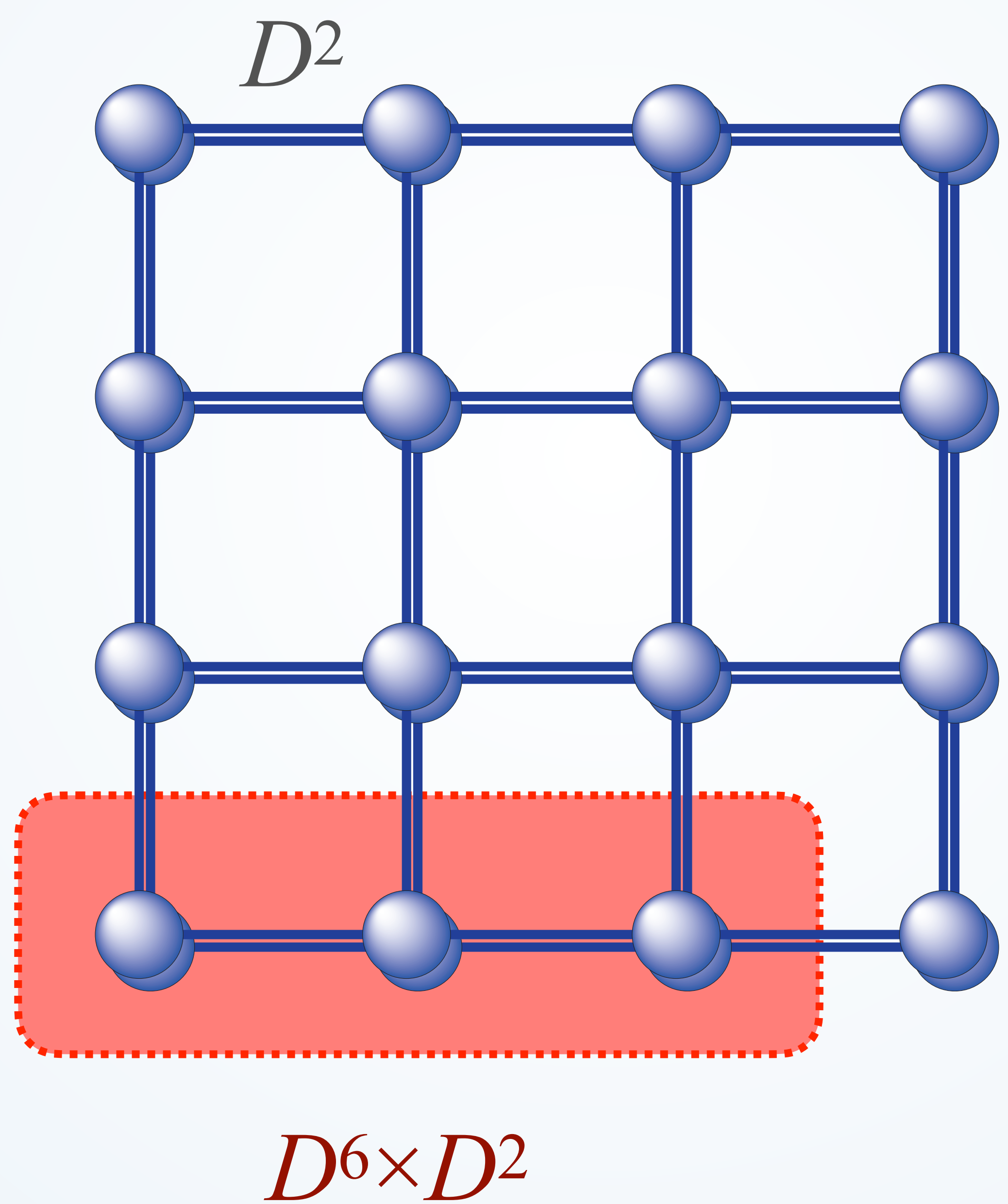
PEPS

Projected Entangled Pairs States



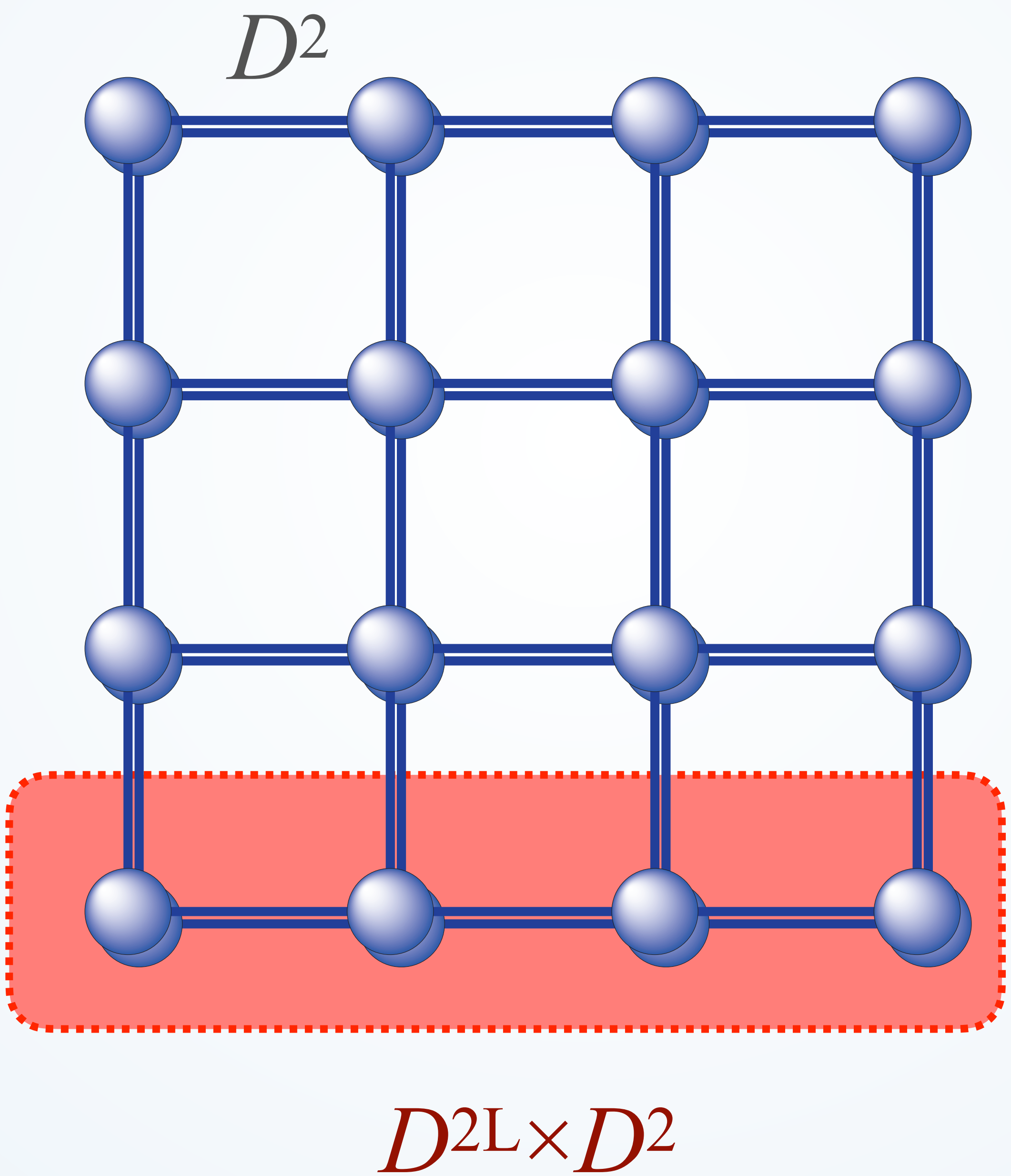
PEPS

Projected Entangled Pairs States



PEPS

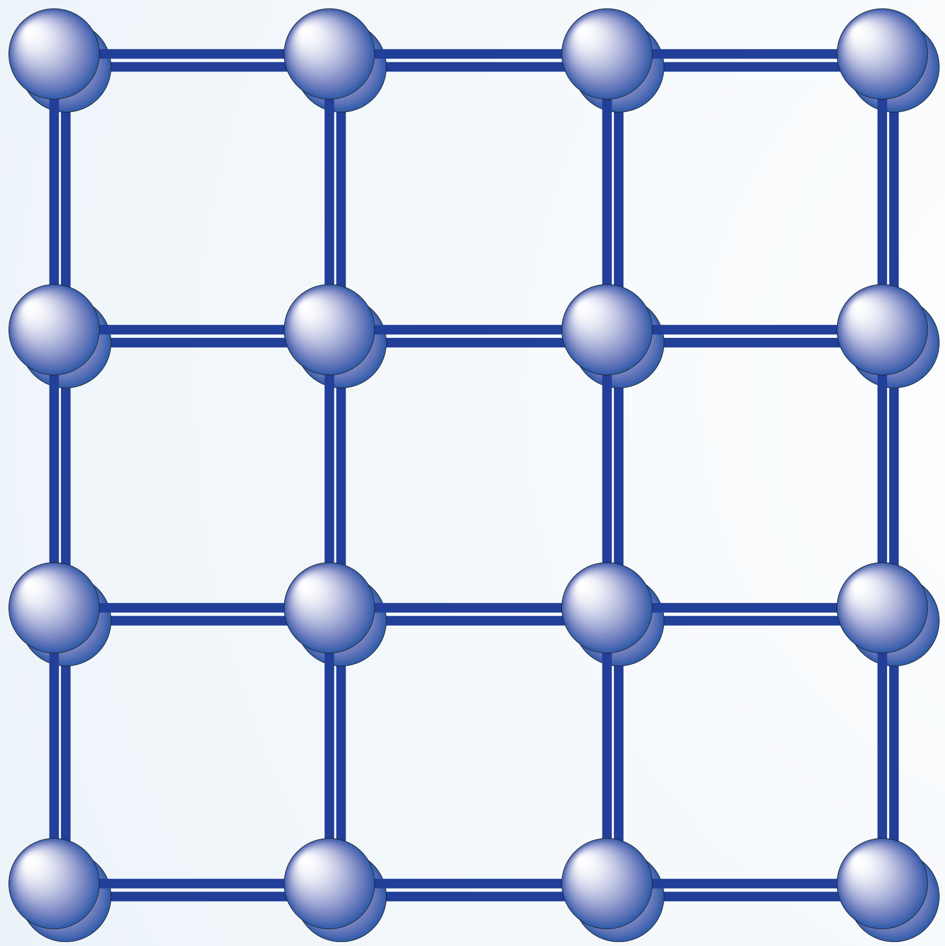
Projected Entangled Pairs States

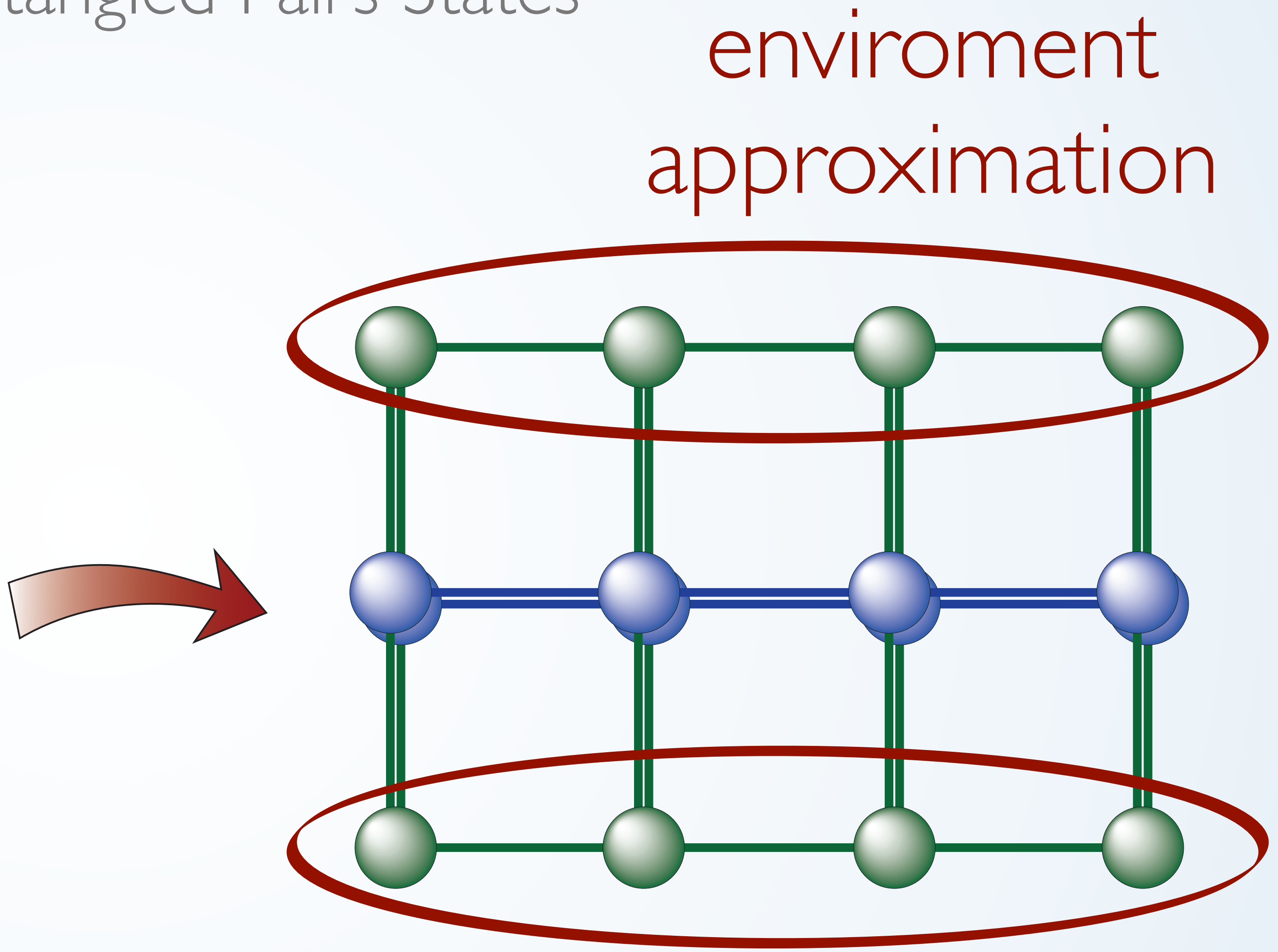


contracting
#P-complete

PEPS

Projected Entangled Pairs States





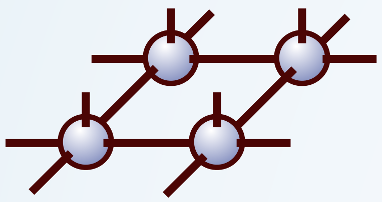
Needed for expectation values and tensor updates

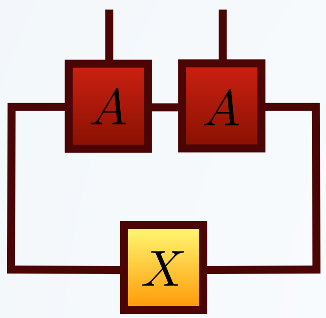
Best we can do: approximate (e.g. via MPO-MPS contractions)

PEPS

Projected Entangled Pairs States

local parent Hamiltonian





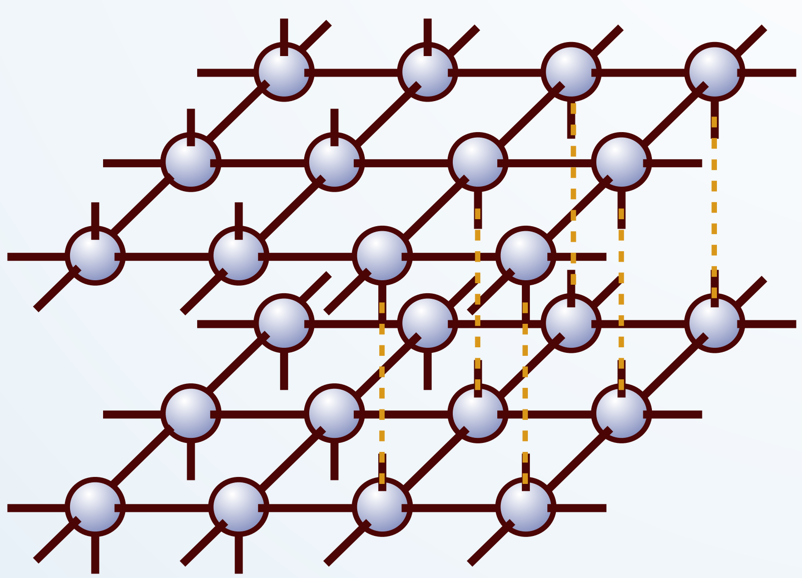
$$H = \sum_{i=1}^{N-1} (1 - \Pi_{S_2})$$

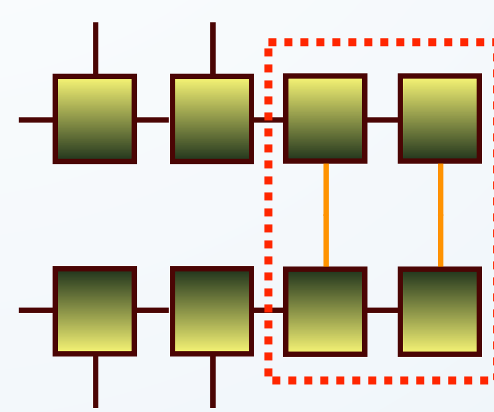
local, frustration-free

injectivity ⇒ unique ground state

bulk-boundary correspondence

holographic principle: boundary dof determine physics in bulk





half-system RDM

on virtual dof

map virtual to physical

PEPS

Projected Entangled Pairs States

Properties

no efficient calculation of expectation values

can hold algebraically decaying correlations

cannot be prepared efficiently

ground state of local frustration-free Hamiltonians

efficient approximation of thermal states

Hastings PRB 2006
Molnar et al PRB 2015