INTRODUCTION TO MPS

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In this lecture…

notes & biblio:

introducing Tensor Network States and MPS

TEBD: basic numerical algorithm for time evolution

Tutorial: files in

WHAT ARE TNS?

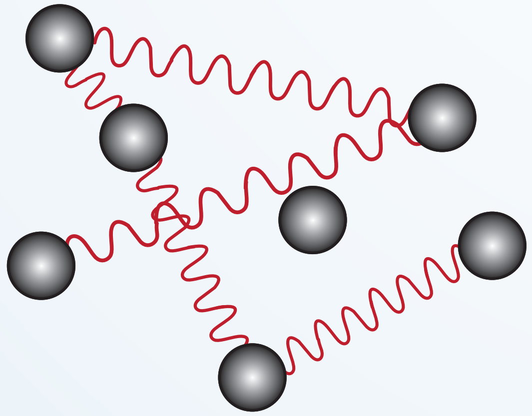
- TNS = Tensor Network States

Context: quantum many body systems

interacting with each other

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

N



Goal: describe interesting states

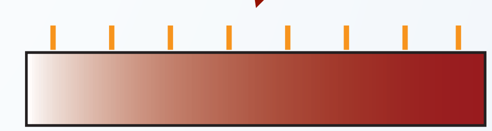
ground, thermal states

WHAT ARE TNS?

- TNS = Tensor Network States

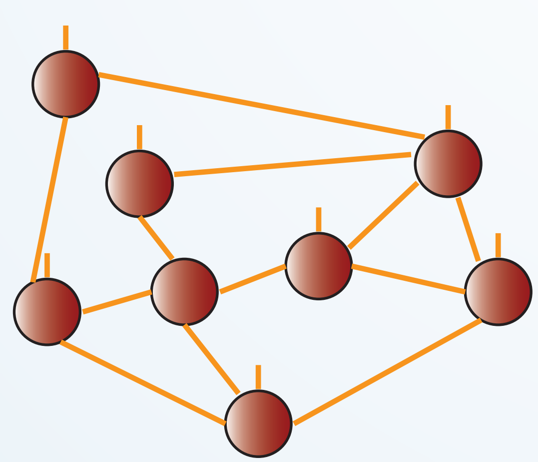
A general state of the N-body Hilbert space has exponentially many coefficients

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



N-legged tensor

d^N

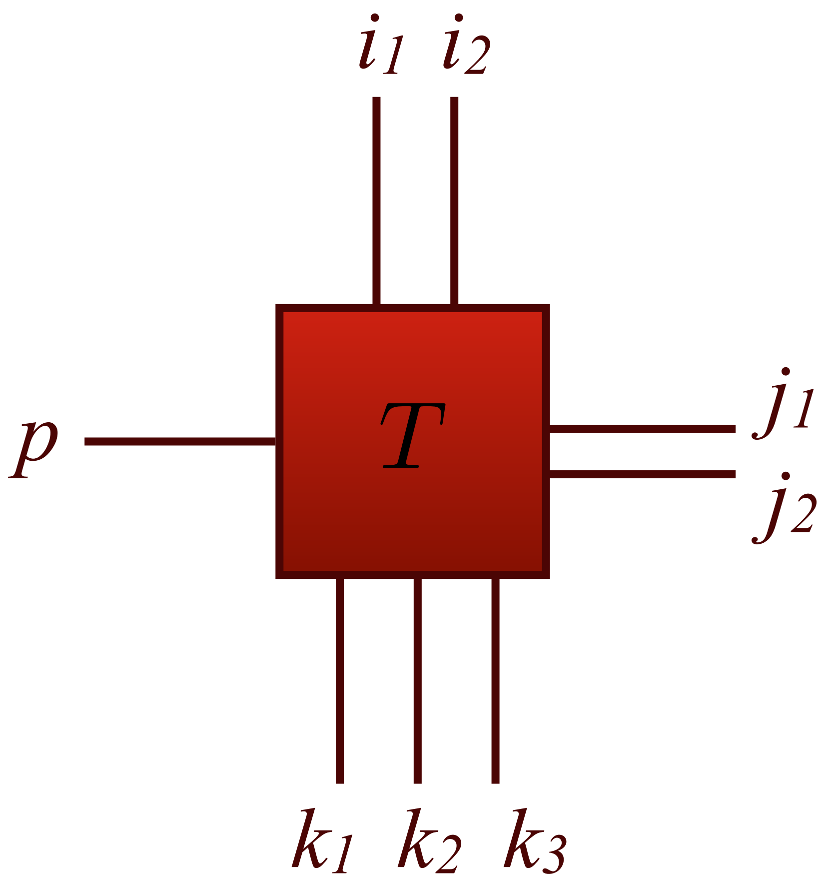


$\mathrm{poly}(N)$

A TNS has only a polynomial number of parameters pictorial representation

pictorial representation

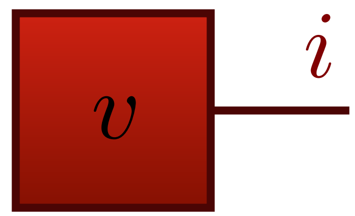
tensor = multidimensional array



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

pictorial representation

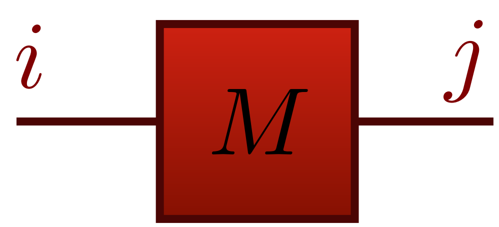
vector



v_i

$i = 1, \dots D$

matrix

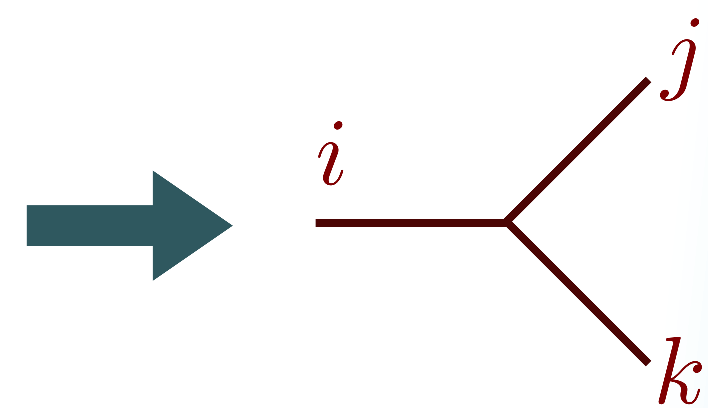


M_{ij}

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

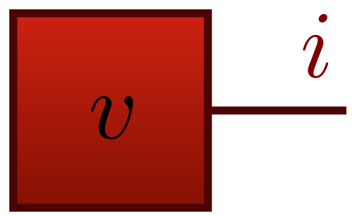
a special case

δ_{ij}

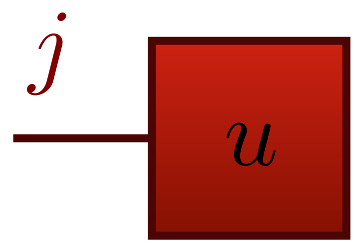


contractions

vector

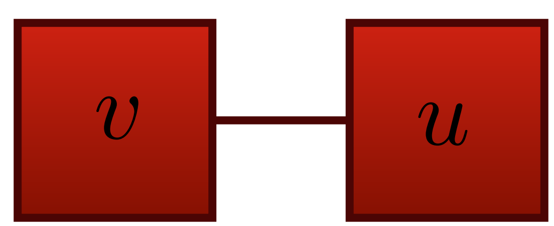


v_i $\quad$ $i = 1, \dots D$



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

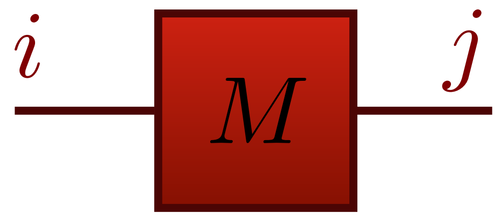
vector-vector



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

contractions

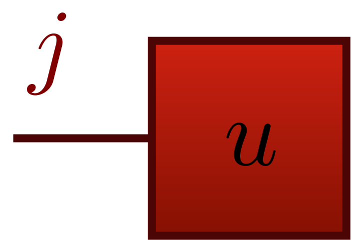
matrix



M_{ij}

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

vector



u_j

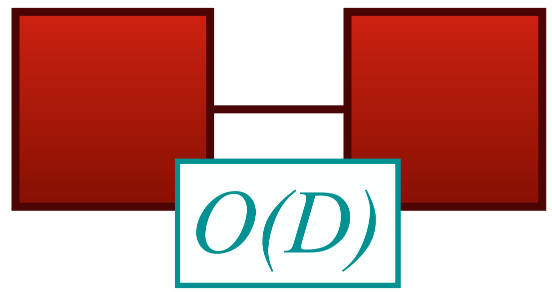
$j = 1, \dots D_2$

matrix-vector

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

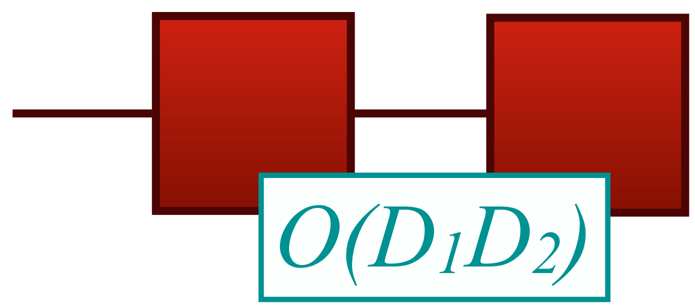
computational costs

vector-vector



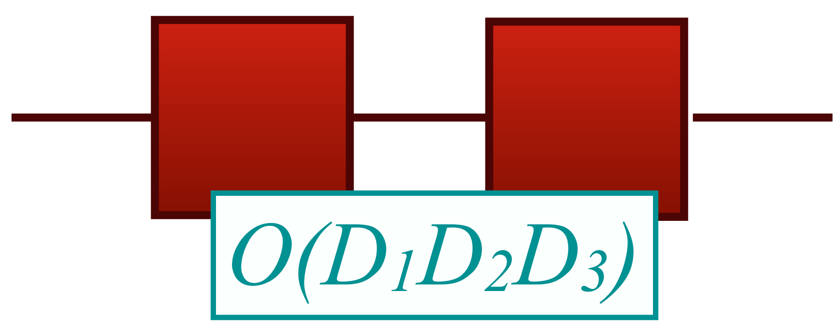
$$v \cdot u = \sum_i v_i u_i$$

matrix-vector



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

matrix-matrix

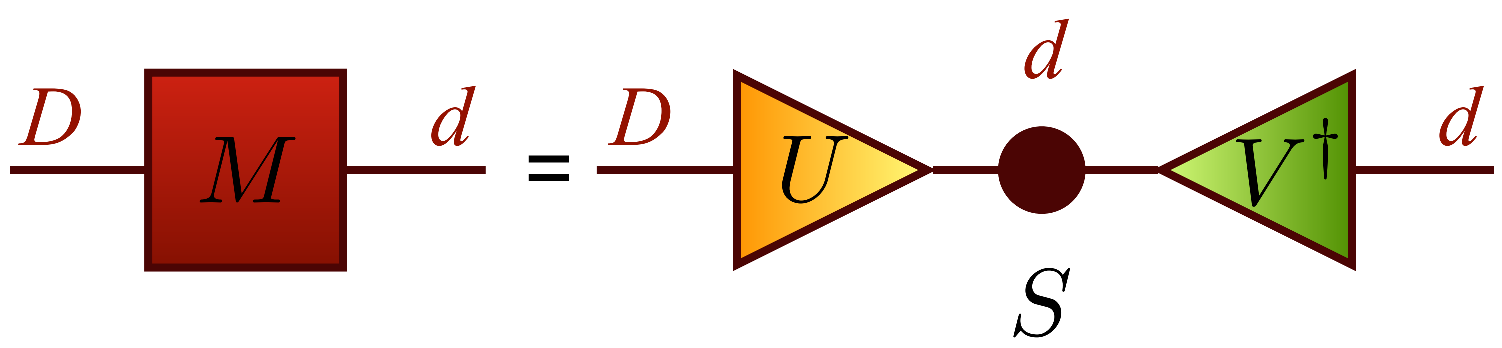


$$M \cdot N = \sum_j M_{ij} N_{jk}$$

in general: product of open and contracted dimensions

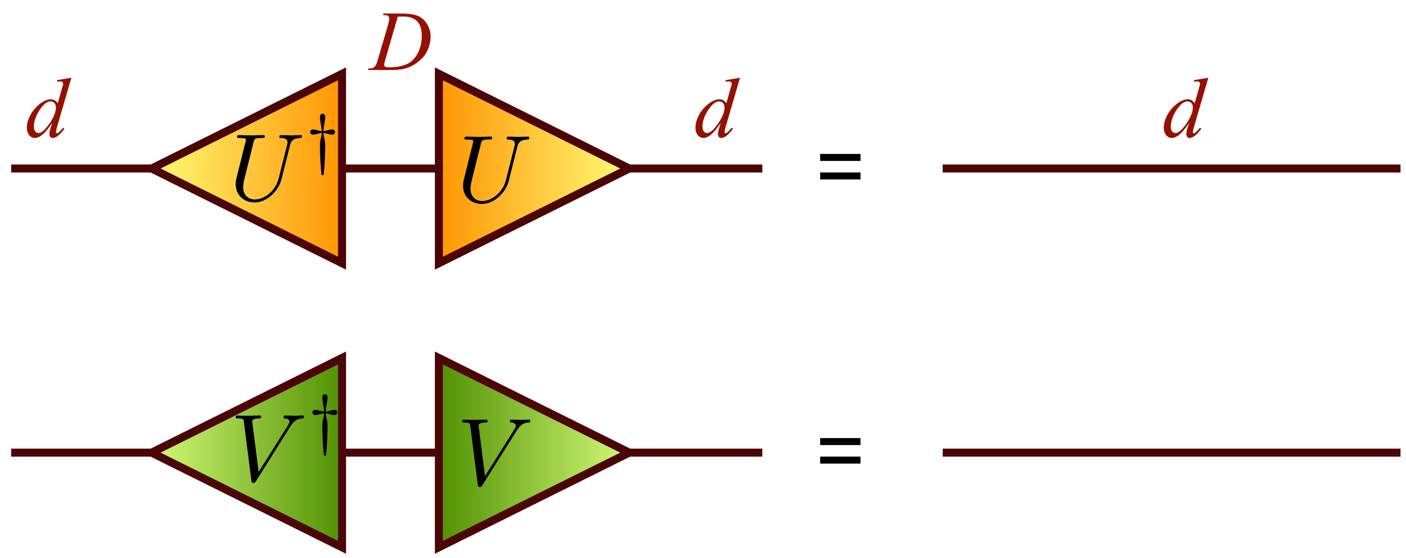
basic routines

SVD



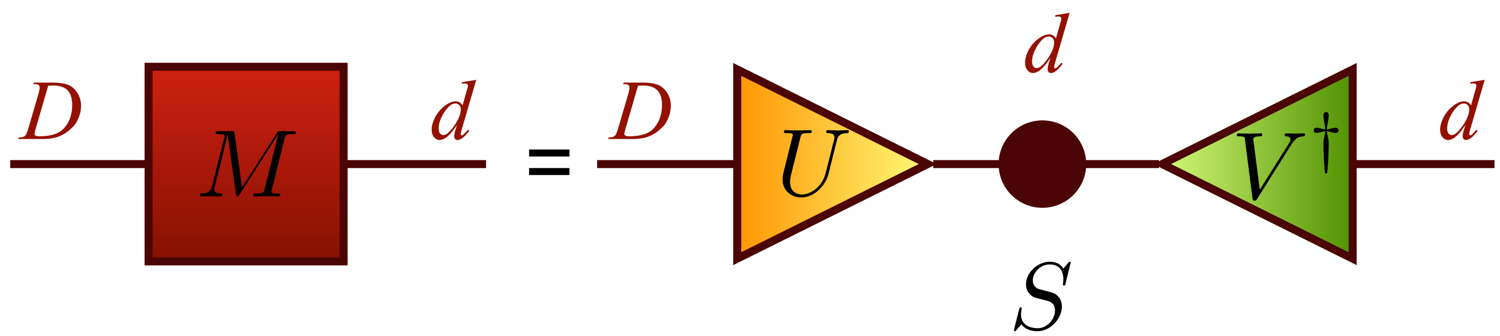
$M = USV^\dagger$

isometry



basic routines

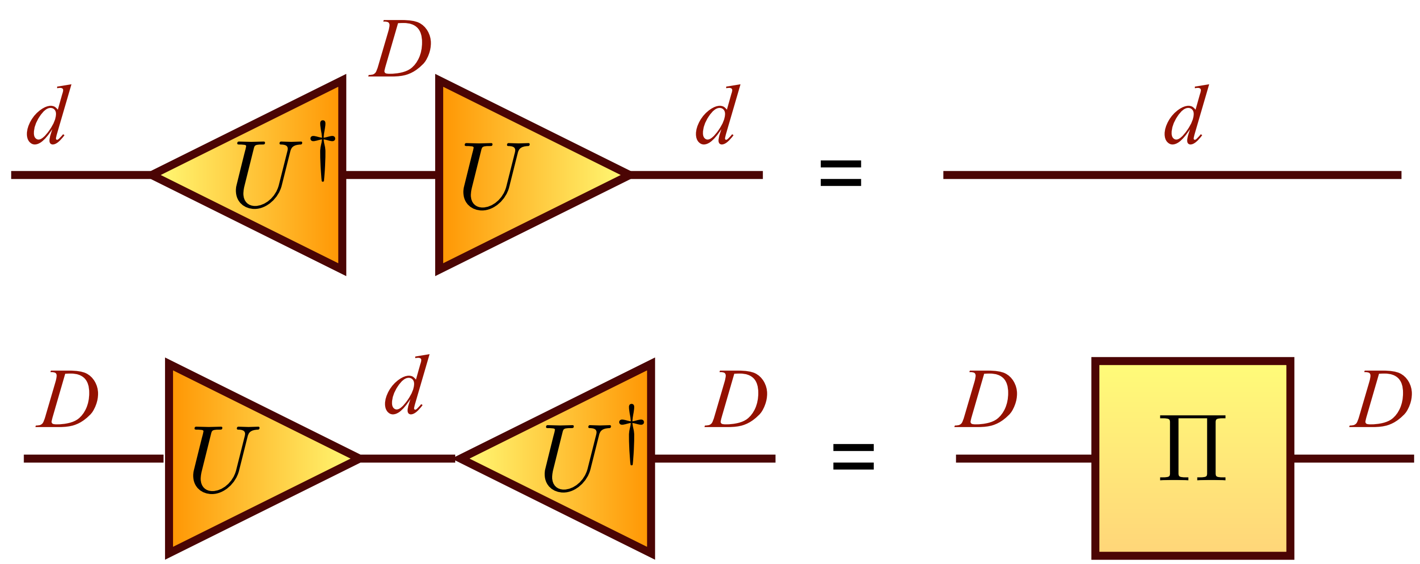
SVD



$$M = USV^\dagger$$

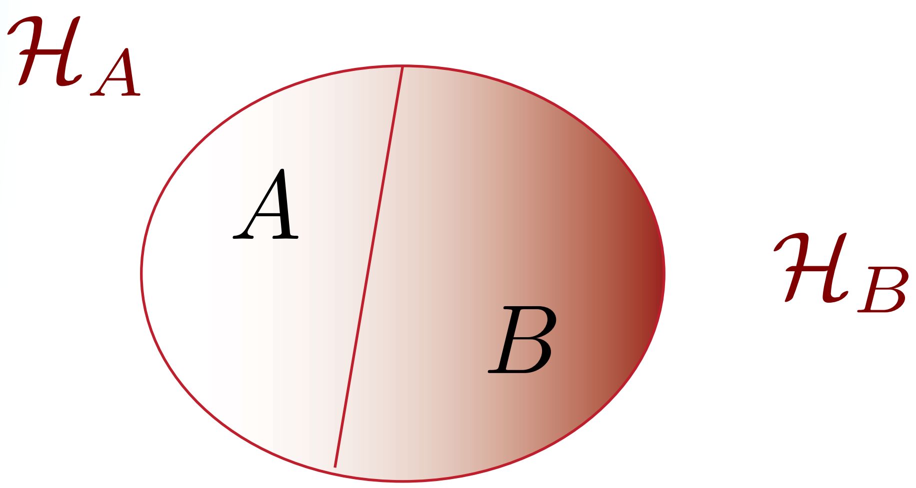
$\boxed{O(Dd^2)}$

isometry



Characterizing entanglement

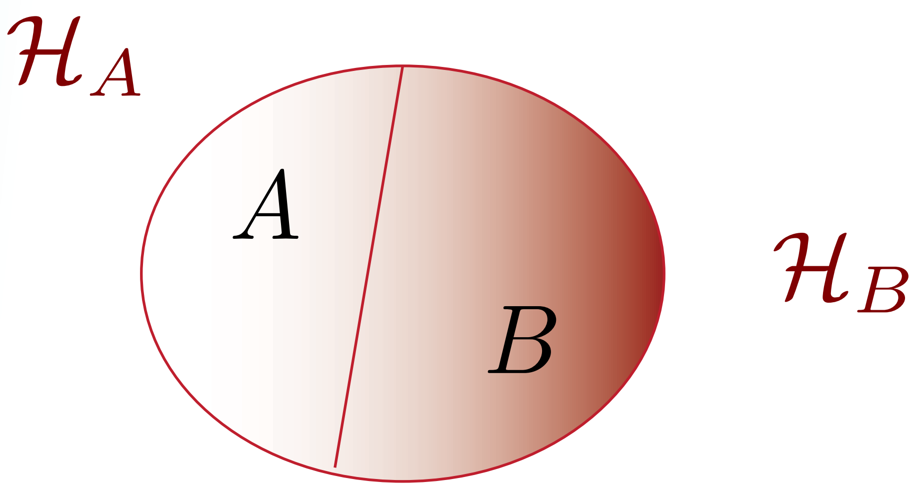
SVD ⇒ Schmidt decomposition



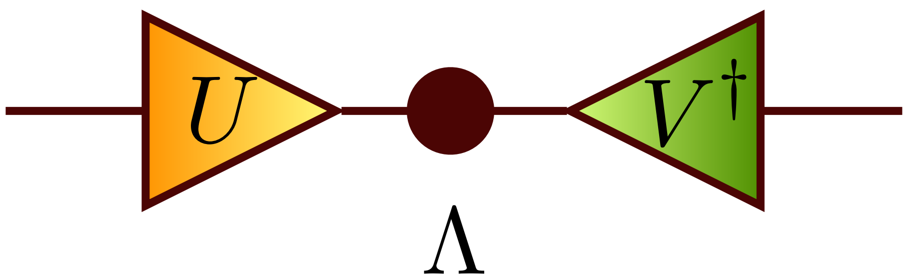
$$|\Psi\rangle = \sum_{ij} \Psi_{ij} |ij\rangle_{AB}$$

Characterizing entanglement

SVD ⇒ Schmidt decomposition



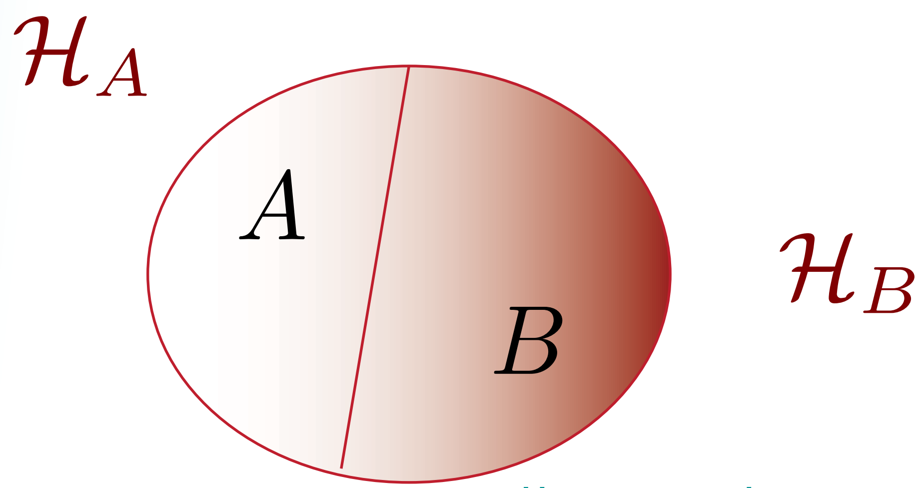
$$|\Psi\rangle = \sum_k \lambda_k \left(U_{ik}|i\rangle_A\right)\left(V^\dagger_{kj}|j\rangle_B\right)$$



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

Characterizing entanglement

SVD $\Rightarrow$ Schmidt decomposition

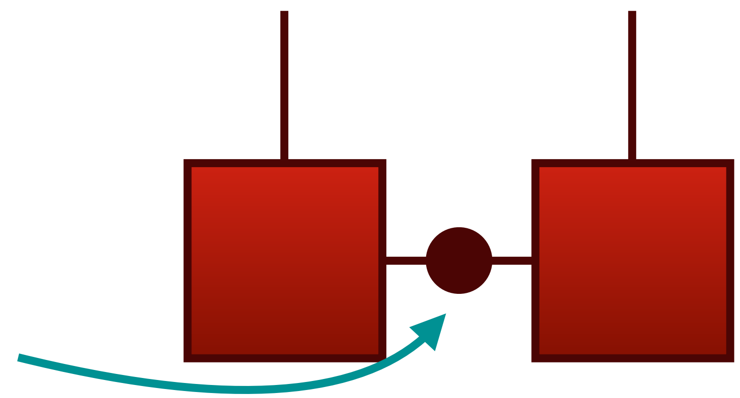


$$|\Psi\rangle = \sum_k \lambda_k |v_k\rangle_A |w_k\rangle_B$$

Schmidt coefficients

$$\sum_k \lambda_k^2 = 1$$

dimension of this index

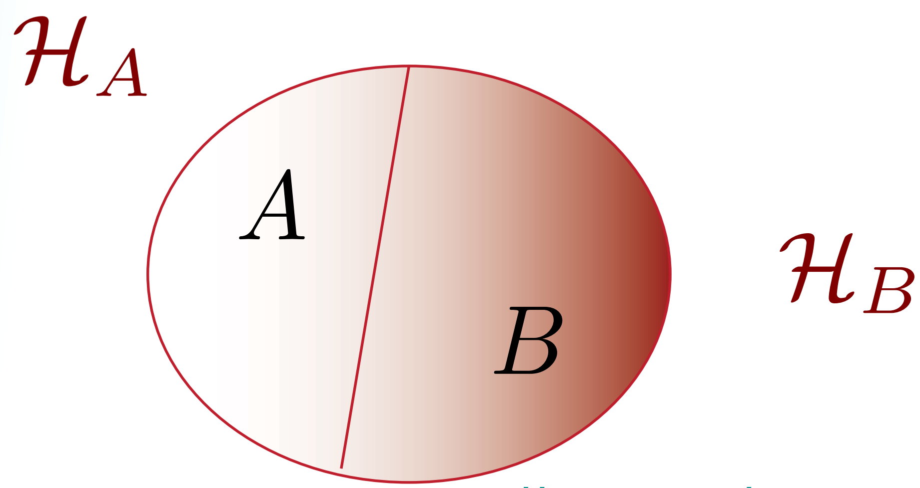


Schmidt rank: number of non-zero λ_k coefficients

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

Characterizing entanglement

SVD $\Rightarrow$ Schmidt decomposition



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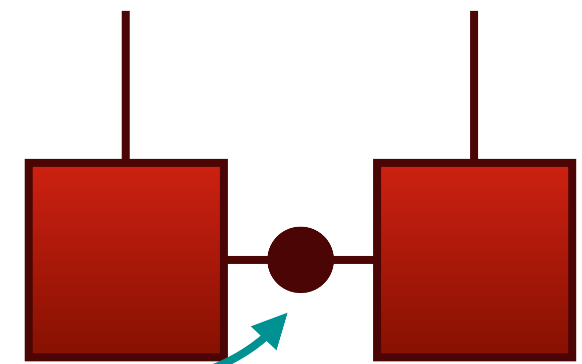
Schmidt coefficients

$$\sum_k \lambda_k^2 = 1$$



dimension of this index

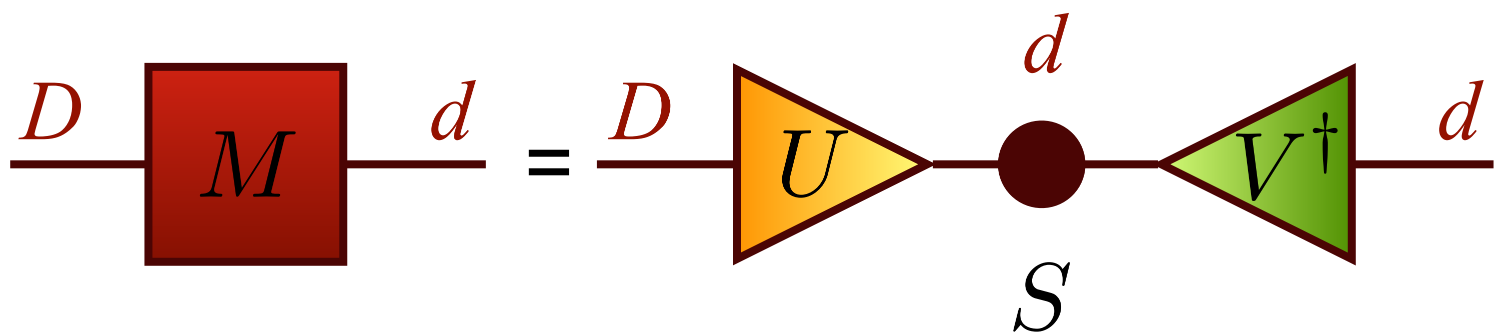
Schmidt rank: number of non-zero λ_k coefficients

$$|01\rangle \longrightarrow \{1,\, 0\}$$

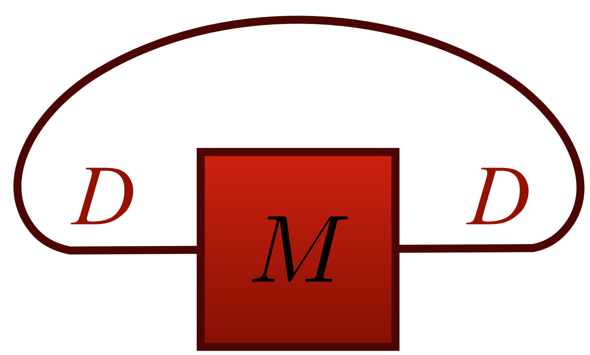
$$\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) \longrightarrow \{1/\sqrt{2},\, 1/\sqrt{2}\}$$

basic routines

SVD



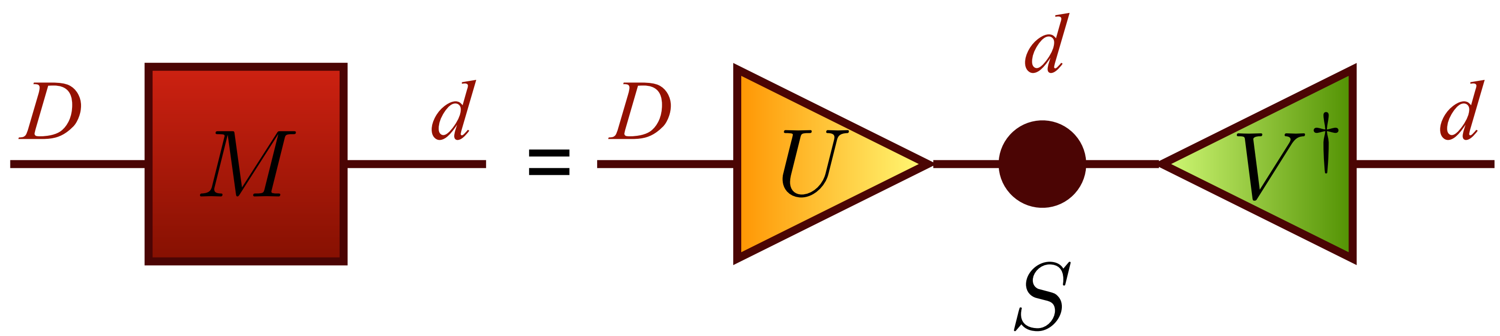
$$M = USV^\dagger$$



$$M_{ij}$$

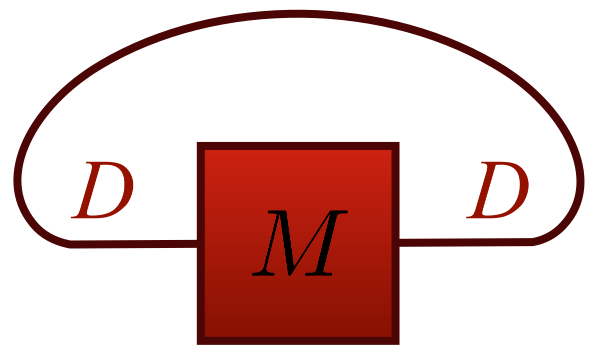
basic routines

SVD



$$M = USV^{\dagger}$$

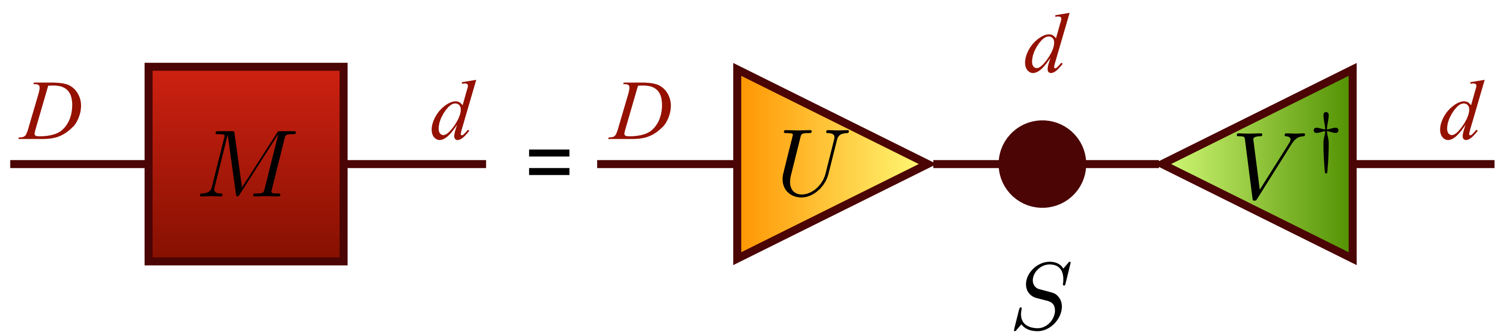
trace



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

basic routines

SVD



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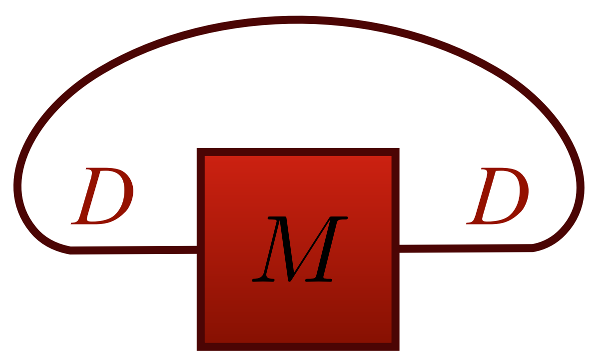

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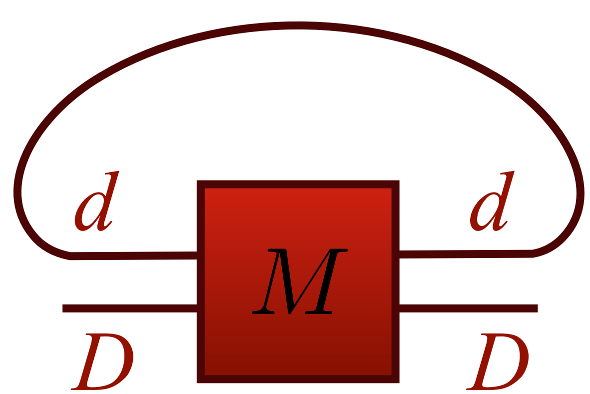
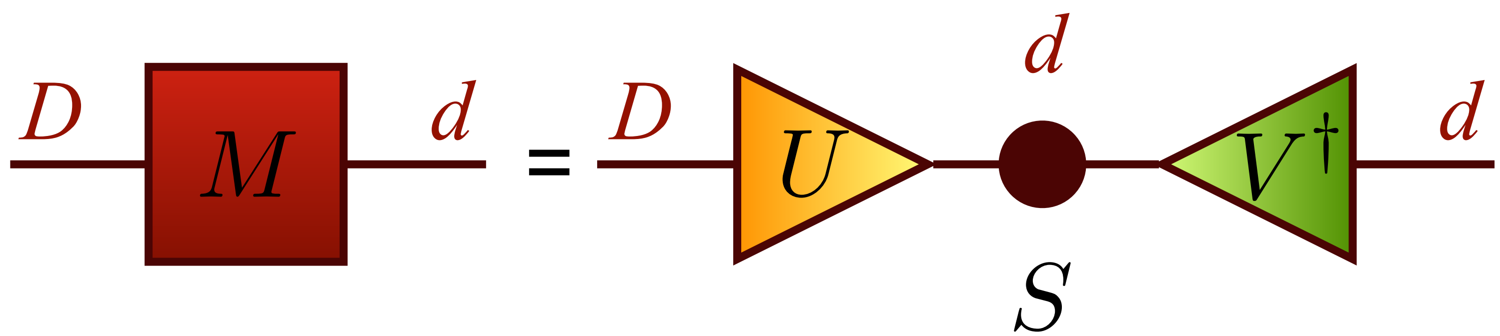


$$\sum_{ij} M_{ia,jb}\delta_{ij} = \sum_i M_{ia,ib}$$

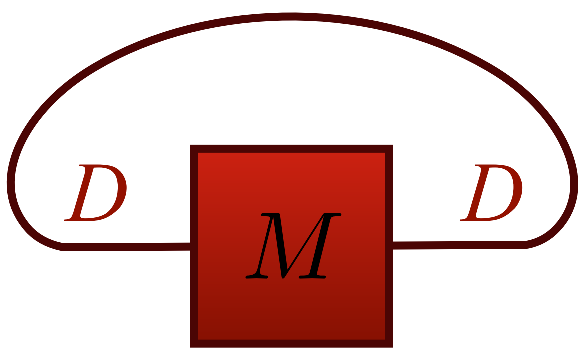
basic routines

SVD



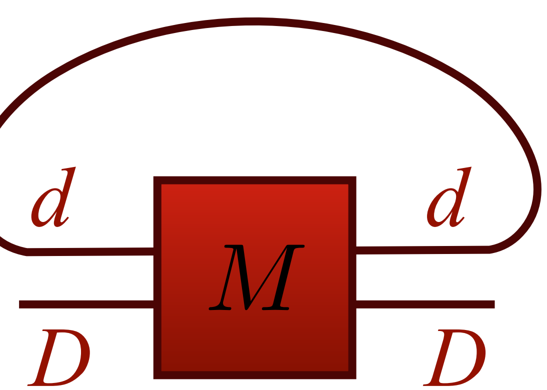
$$M = USV^\dagger$$

trace



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

partial trace



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

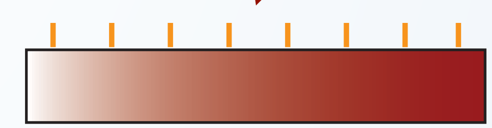
pictorial representation

WHAT ARE TNS?

- TNS = Tensor Network States

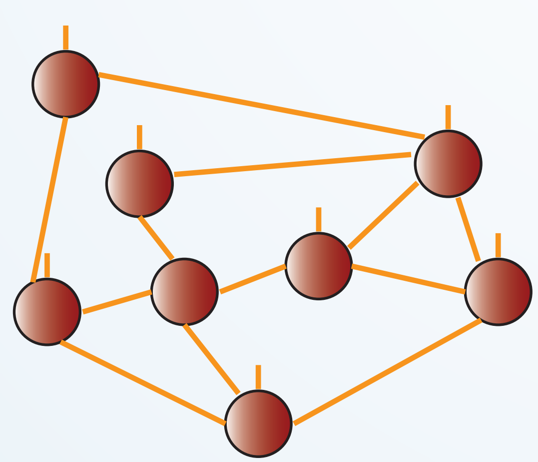
A general state of the N-body Hilbert space has exponentially many coefficients

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



N-legged tensor

d^N



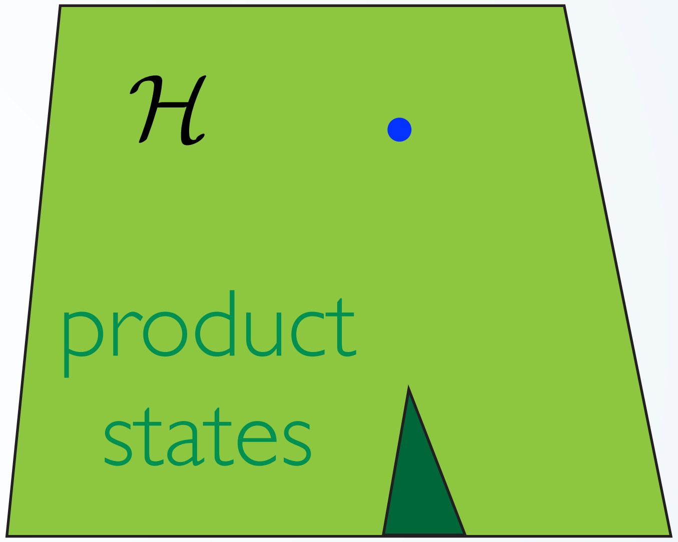
$\mathrm{poly}(N)$

A TNS has only a polynomial number of parameters

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

WHY SHOULD TNS BE USEFUL?

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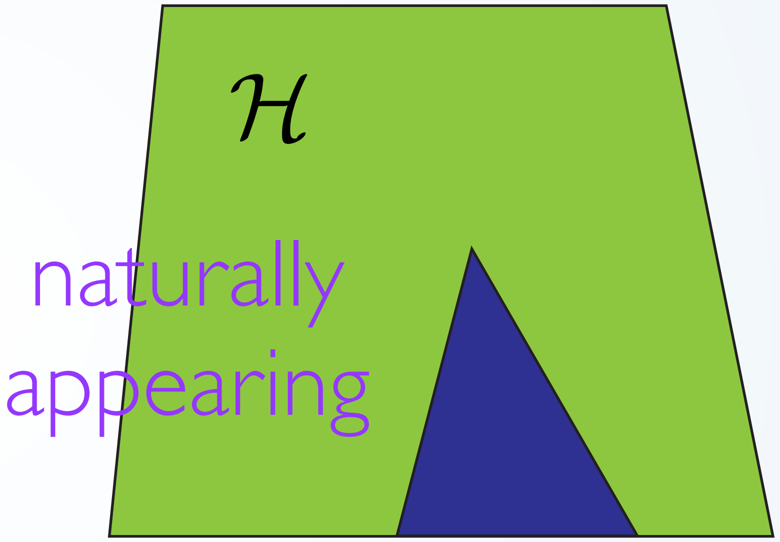


We look for the particular "*corner*" of the Hilbert space

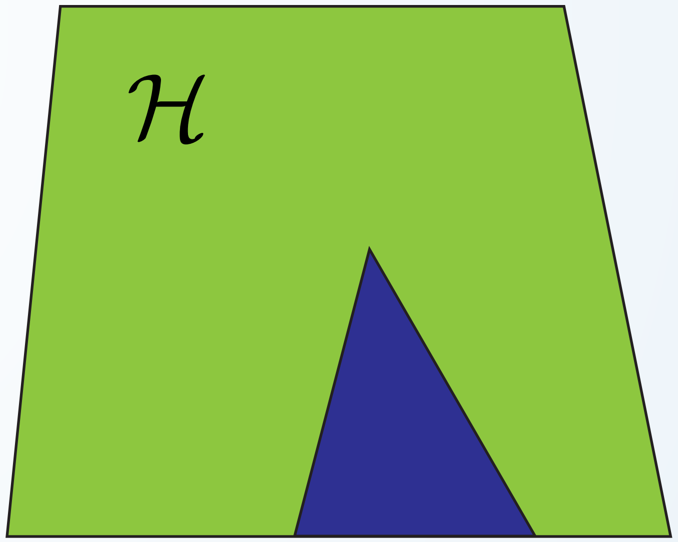
- TNS = Tensor Network States

WHY SHOULD TNS BE USEFUL?

The goal is to find good descriptions of physical states

WANTED

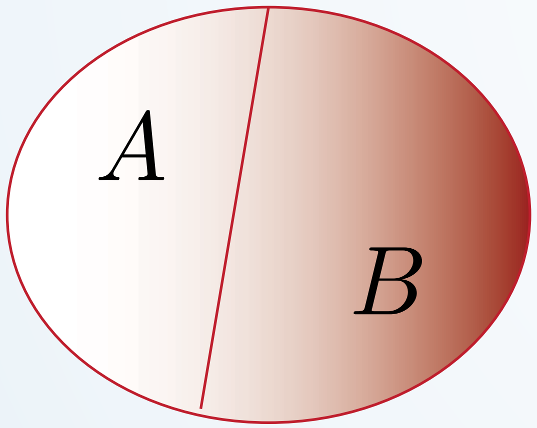
- ➡ efficient representation
- ➡ computable observables
- ➡ (variational) algorithms



FINDING A GOOD ANSATZ

Which properties characterize physically interesting states?

ENTANGLEMENT STRUCTURE



$|a\rangle \otimes |b\rangle$ product state

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

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

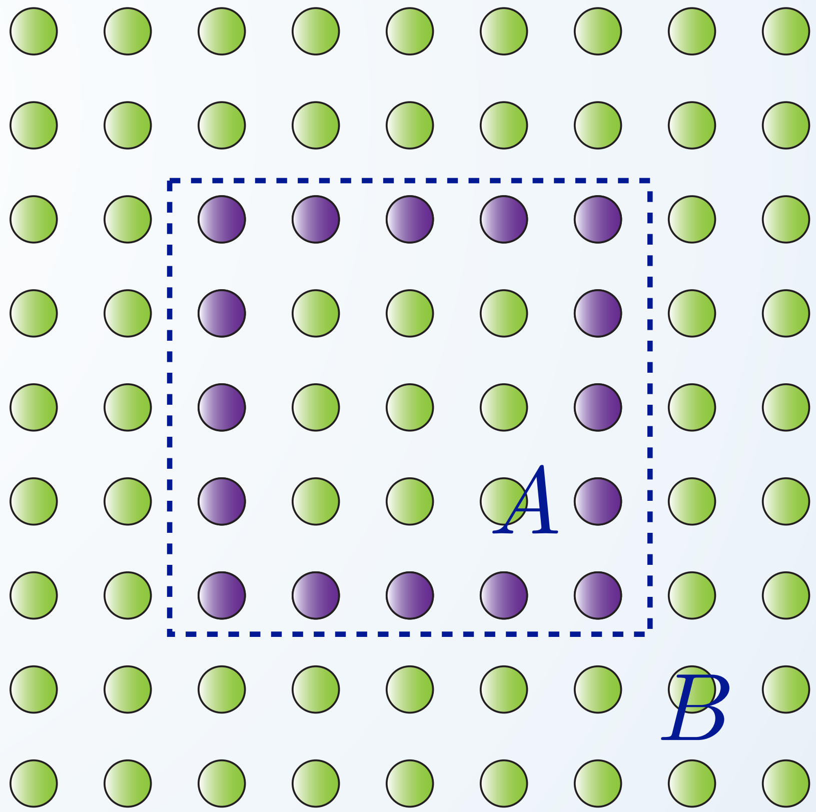
FINDING A GOOD ANSATZ

Which properties characterize ground states of relevant Hamiltonians?

Area law

finite range
gapped
Hamiltonians

states with
little entanglement



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

FINDING A GOOD ANSATZ

Which properties characterize ground states of relevant Hamiltonians?

Area law

local gapped 1D Hamiltonians

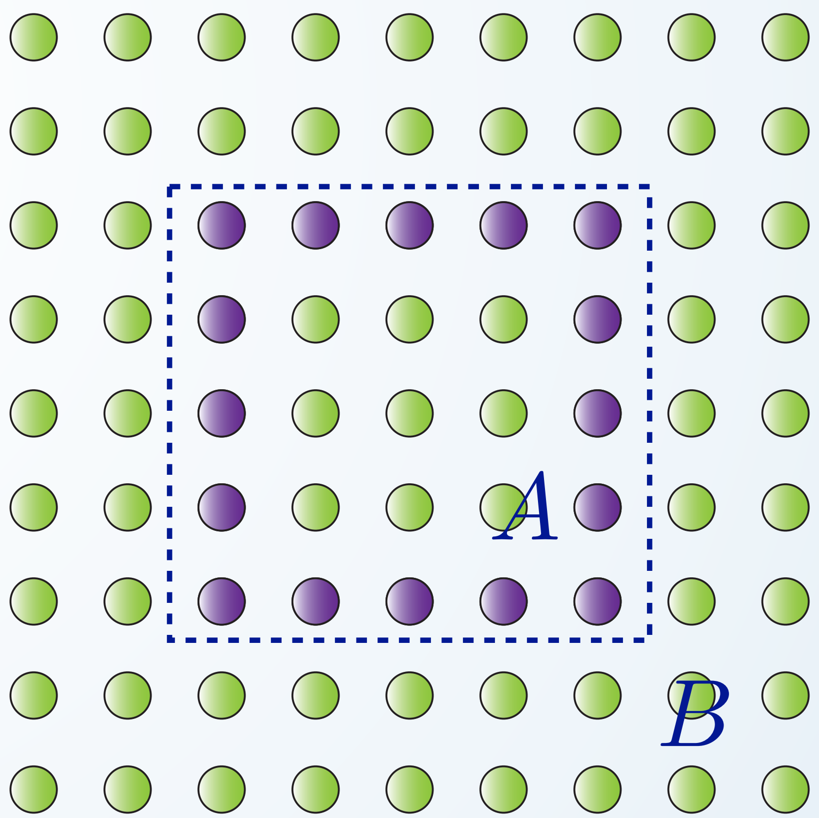
have ground states

with area law of entanglement

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

in 1D critical systems, logarithmic corrections

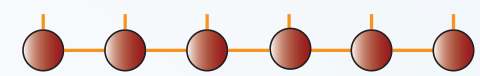
$S_{A\max} \propto |\delta A| \log A$ Calabrese, Cardy 2004



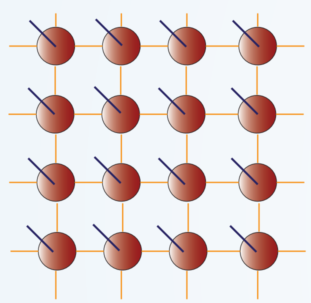
satisfied at finite temperature Wolf, Verstraete, Hastings, Cirac, PRL 2008

MPS & PEPS

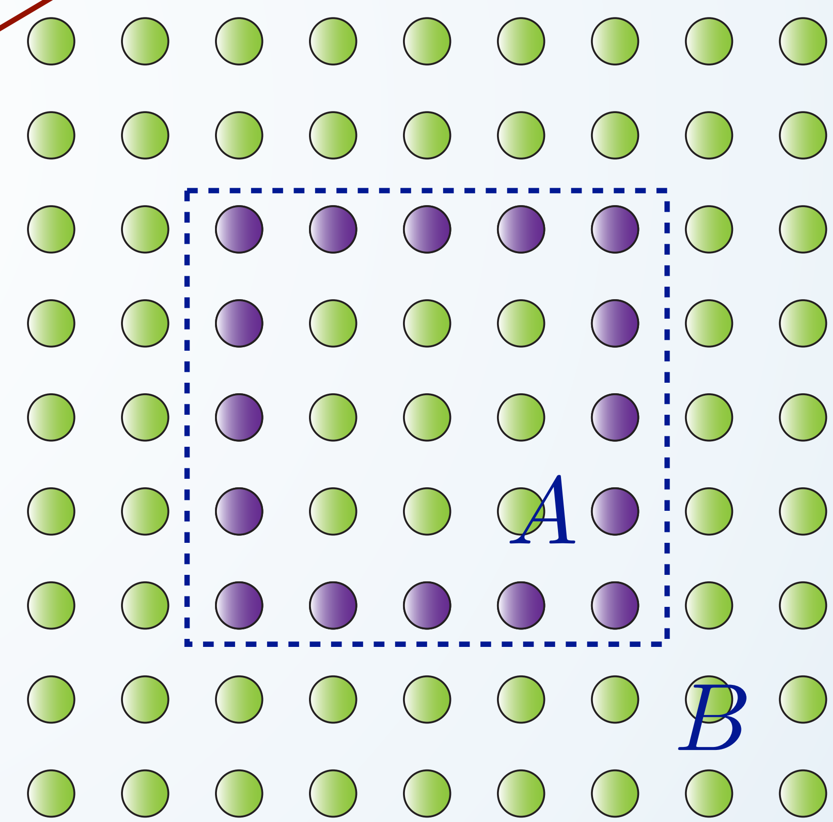
- MPS = Matrix Product States



- PEPS = Projected Entangled Pairs States



Area law



Ansätze satisfying
the area law
by construction

TNS = entanglement based ansatz

MPS

Matrix Product States

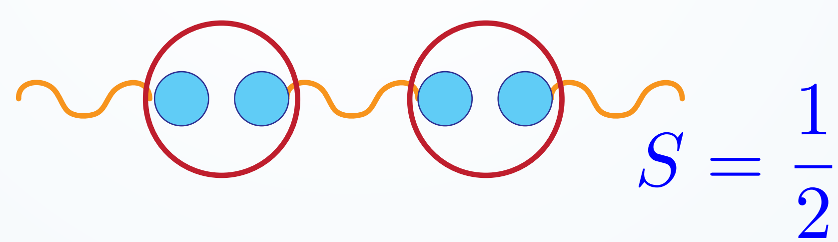
A bit of history...

Matrix Product States

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)

A bit of history...

Matrix Product States

AKLT exactly solvable spin model

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)

A bit of history...

Matrix Product States

AKLT exactly solvable spin model

Affleck, Kennedy, Lieb, Tasaki, PRL 1987

↓

Finitely correlated states

Fannes, Nachtergaele, Werner, CMP 1992

DMRG algorithm

White, PRL 1992

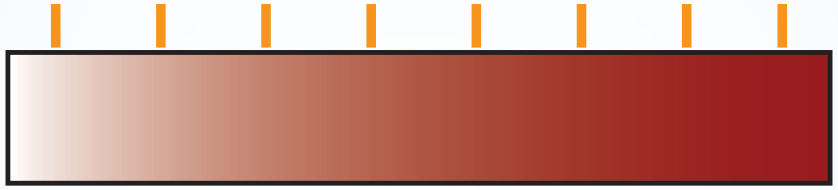
DMRG variational over MPS

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

Quantum Information perspective

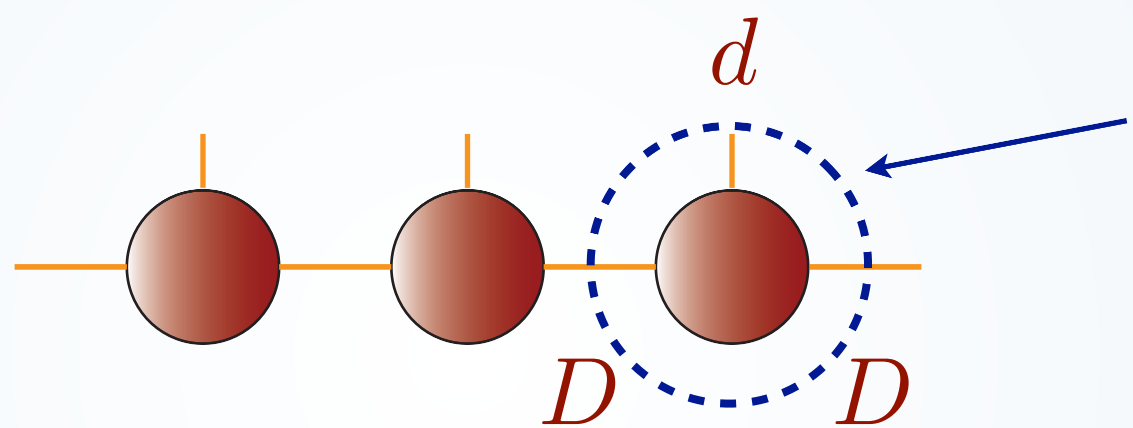
Vidal, PRL 2003
Verstraete, Porras, Cirac, PRL 2004

Matrix Product States



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

Matrix Product States

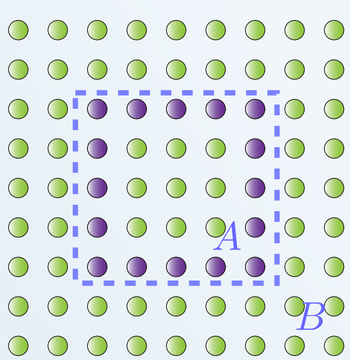


$A^{i}_{\alpha\beta}$

number of parameters

NdD^2

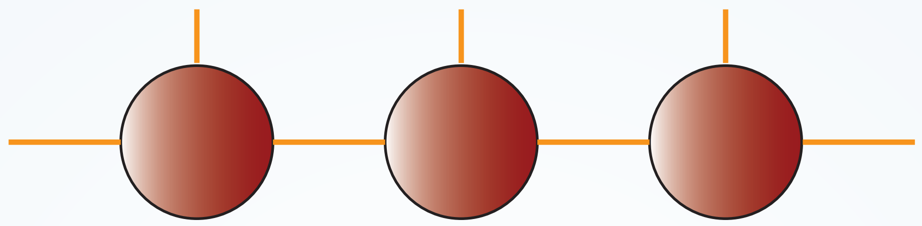
$$|\Psi\rangle = \sum_{i_1 \ldots i_N} \mathrm{tr}(A_1^{i_1} A_2^{i_2} \ldots A_N^{i_N}) |i_1 \ldots i_N\rangle$$



Area law by construction

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

MPS EXAMPLE



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

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

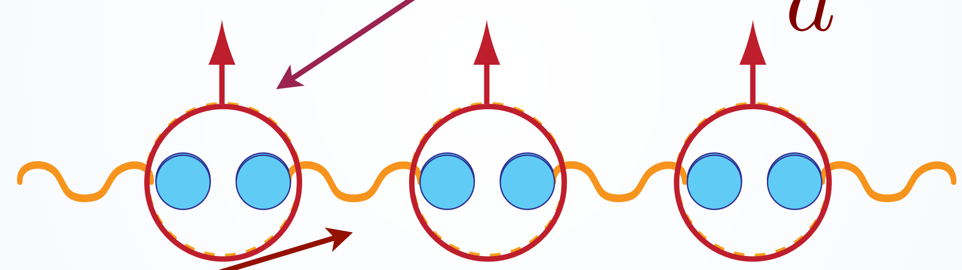
$$|100\ldots\rangle + |010\ldots\rangle + |001\ldots\rangle + \ldots$$

$$D = 2$$

Matrix Product States

project onto the physical degrees of freedom

d



maximally entangled

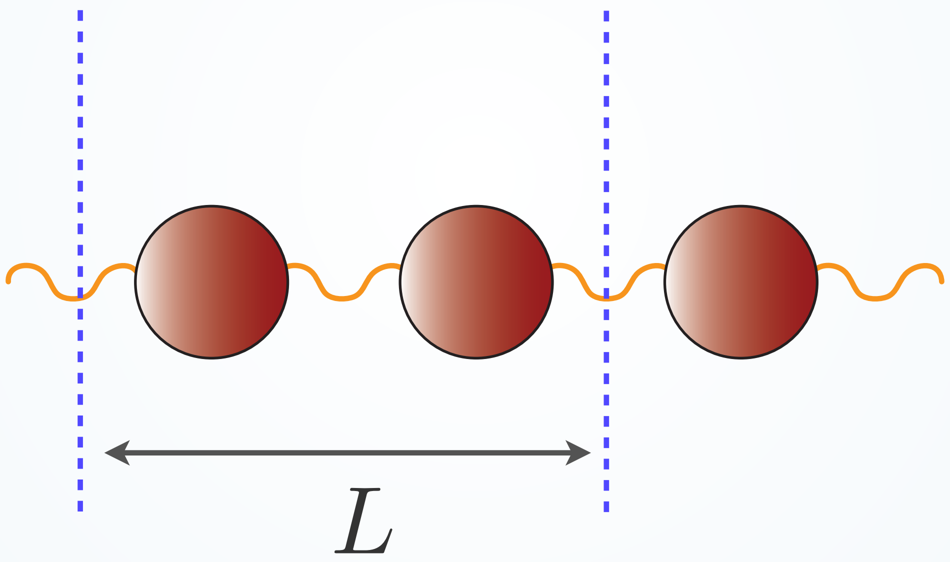
$$\sum_{\alpha=1}^{D} |\alpha\rangle|\alpha\rangle$$

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

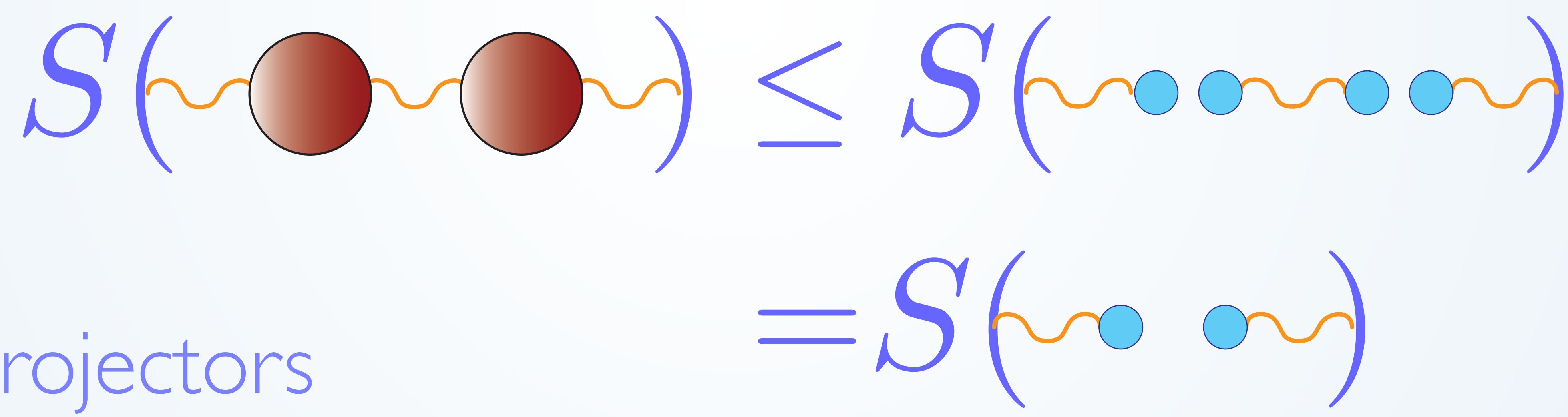
virtual particles

D

Area law by construction



Area law by construction



$$= 2 \log D$$

local projectors
cannot increase
the entropy

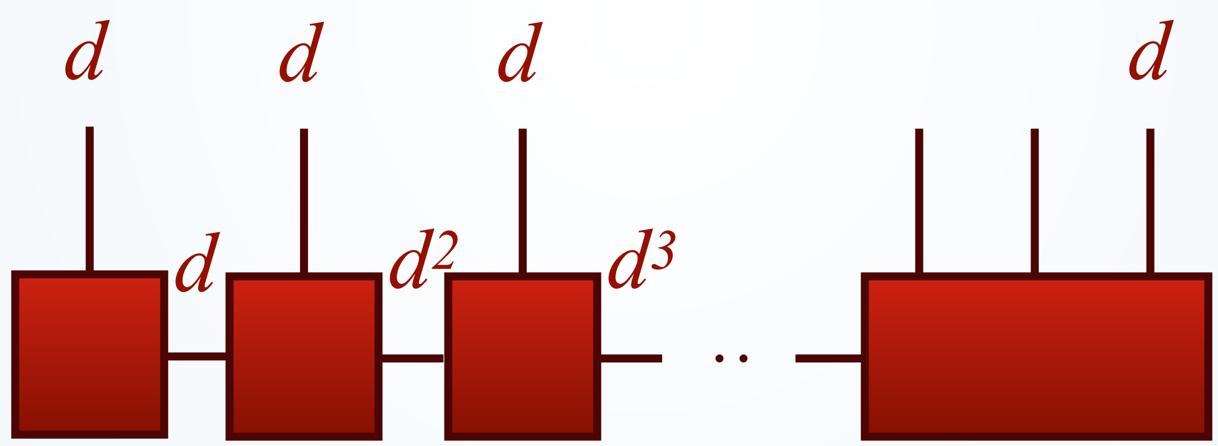
SOME OTHER PROPERTIES

MPS PROPERTIES

any state can be written as MPS

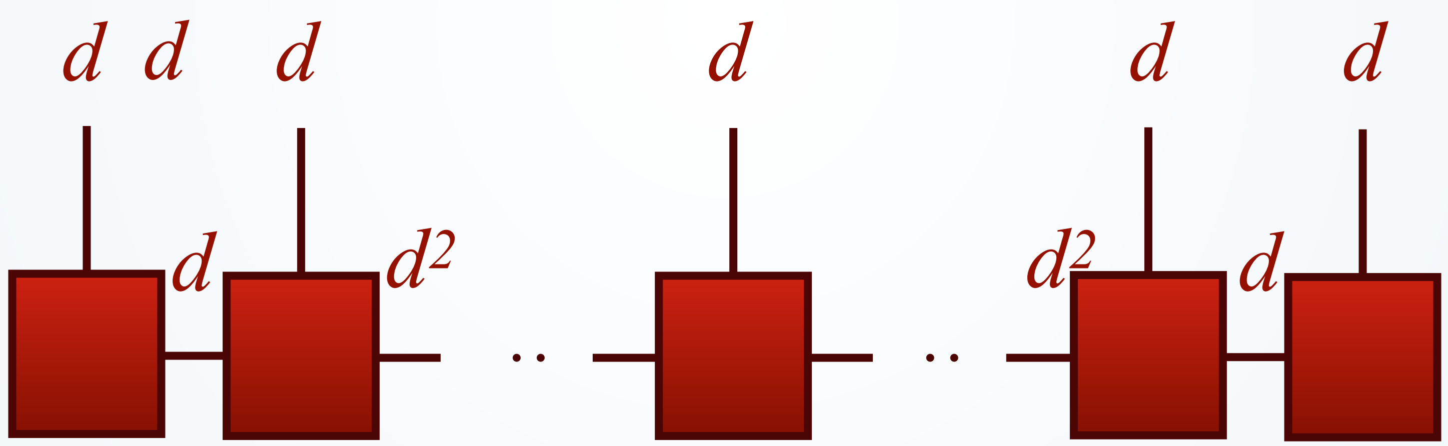
MPS PROPERTIES

any state can be written as MPS



MPS PROPERTIES

any state can be written as MPS



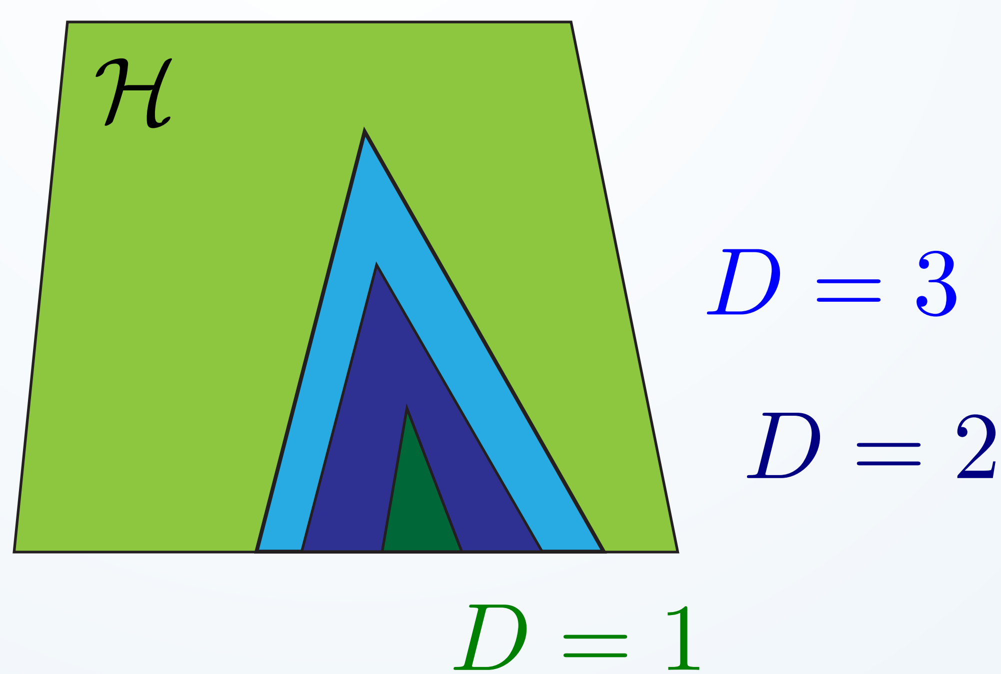
$$D \leq d^{N/2}$$

MPS PROPERTIES

MPS are a complete family

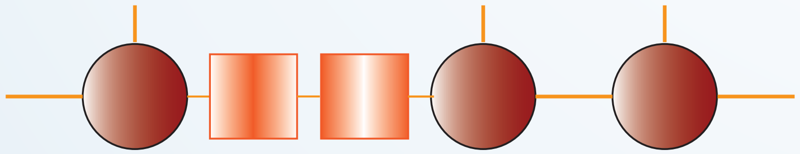
increasing the bond dimension, they can describe any state of the Hilbert space

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



MPS PROPERTIES

$X \cdot X^{-1}$



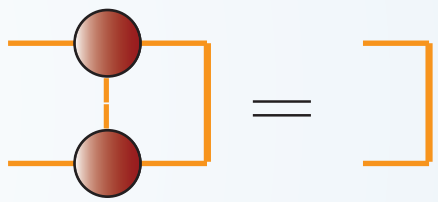
gauge freedom

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

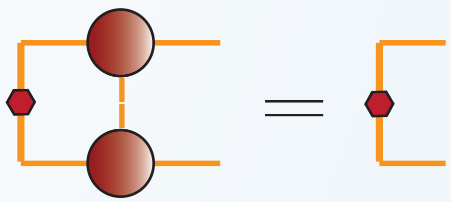
MPS PROPERTIES

canonical form

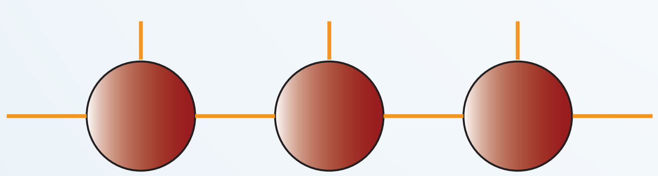
$$\sum_i A^{[m]i} A^{[m]i\dagger} = 1$$



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



unique
imposed locally

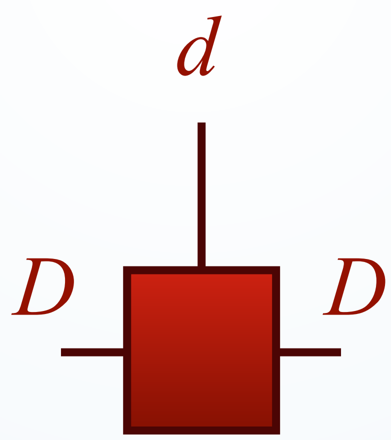


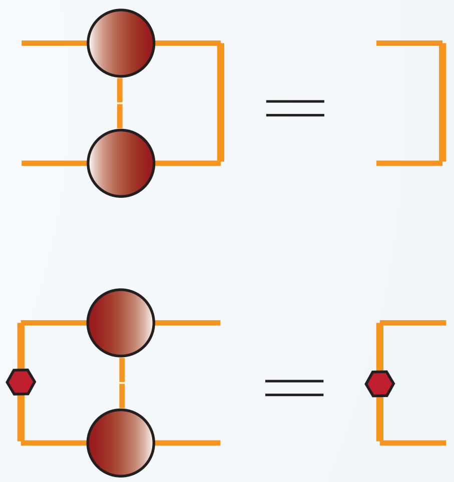
gauge freedom

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

MPS PROPERTIES

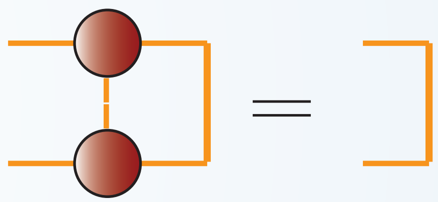
finding the canonical form

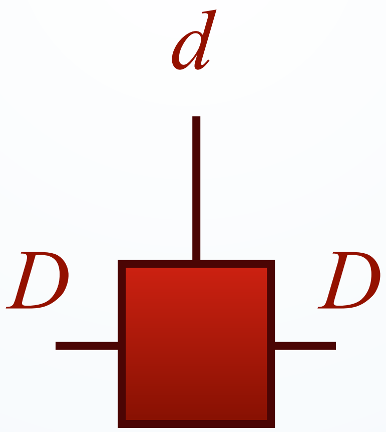




MPS PROPERTIES

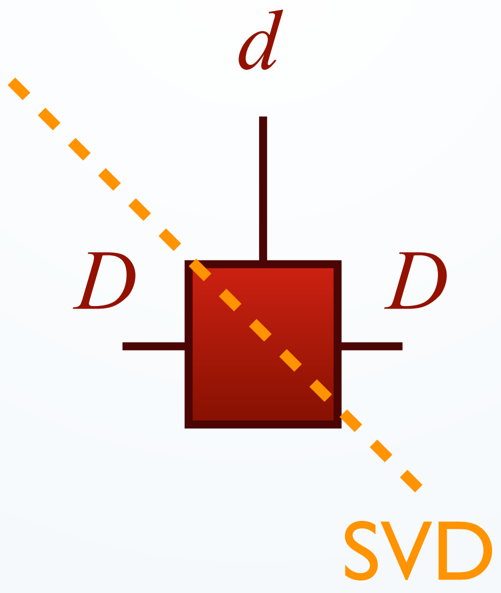
finding the canonical form

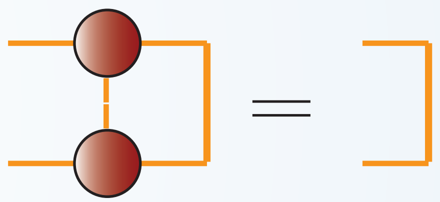




MPS PROPERTIES

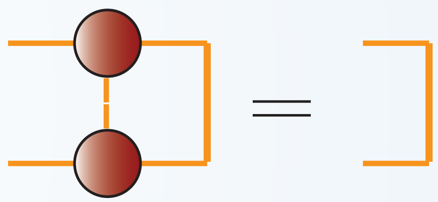
finding the canonical form

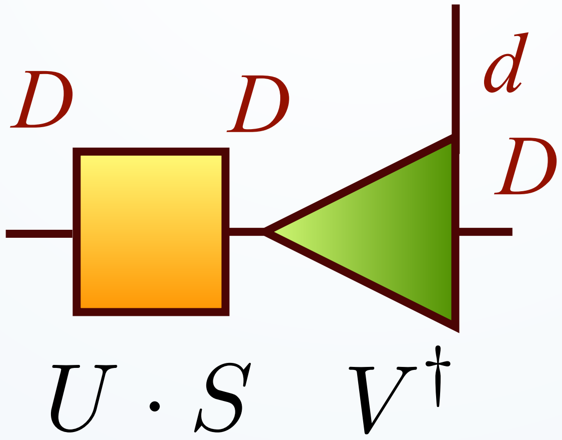


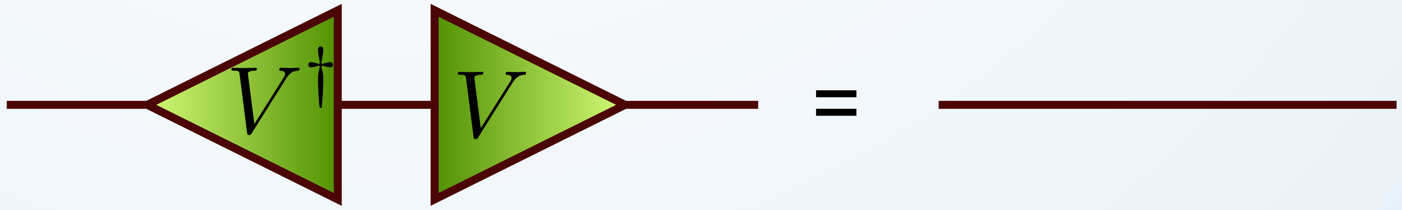


MPS PROPERTIES

finding the canonical form

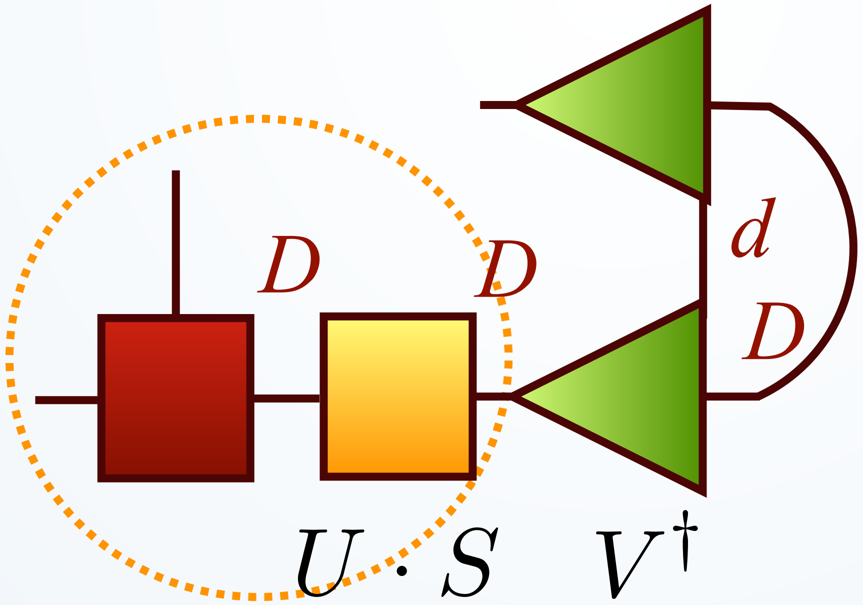


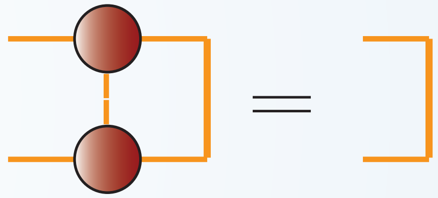


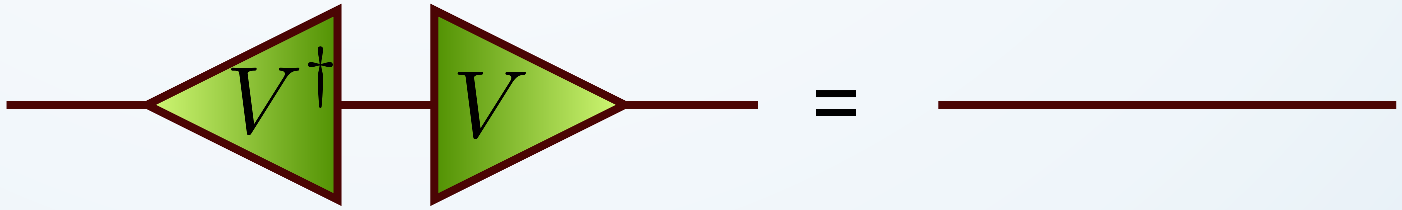


MPS PROPERTIES

finding the canonical form

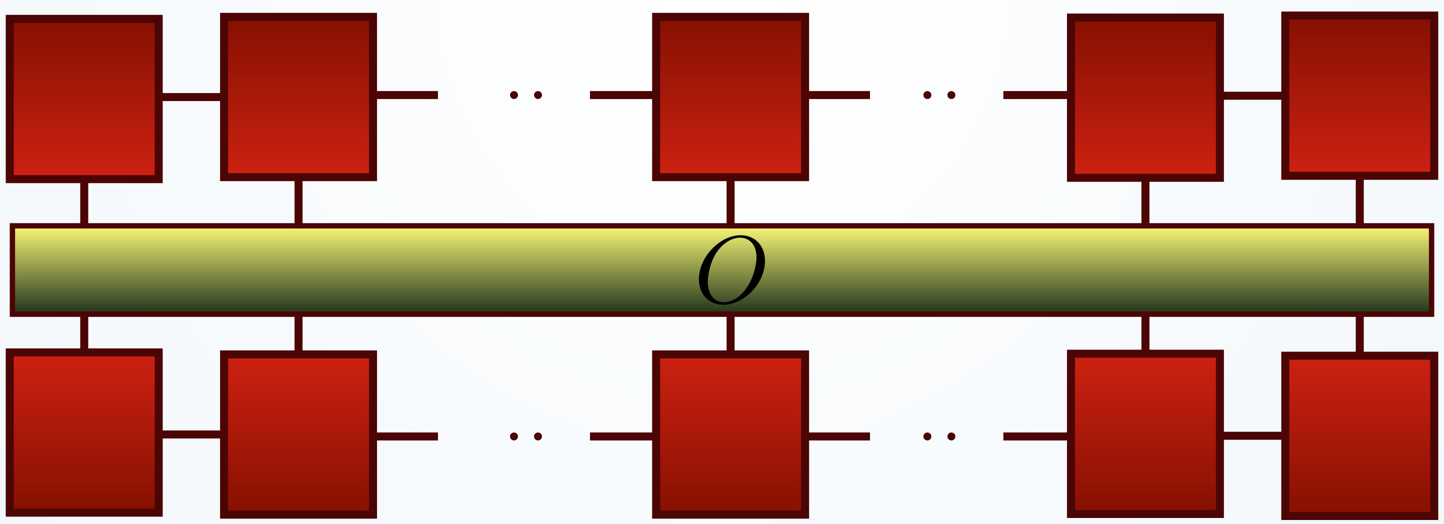






MPS PROPERTIES

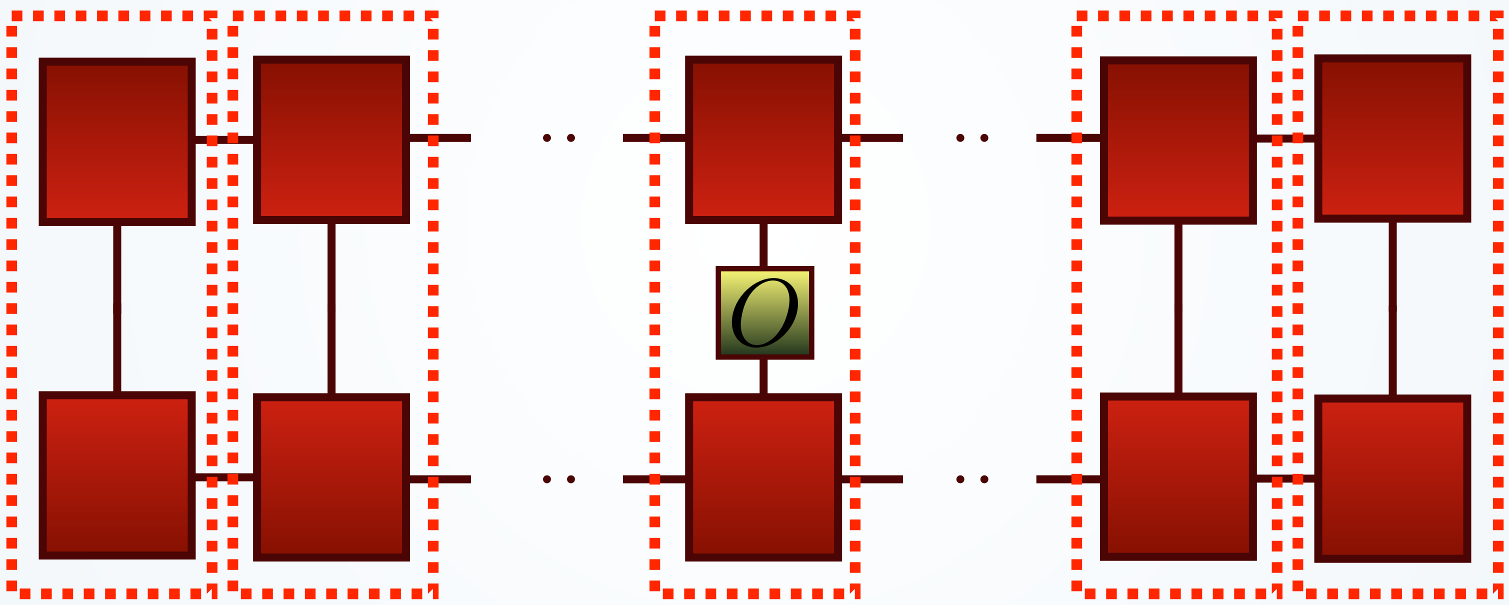
Efficient expectation values



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

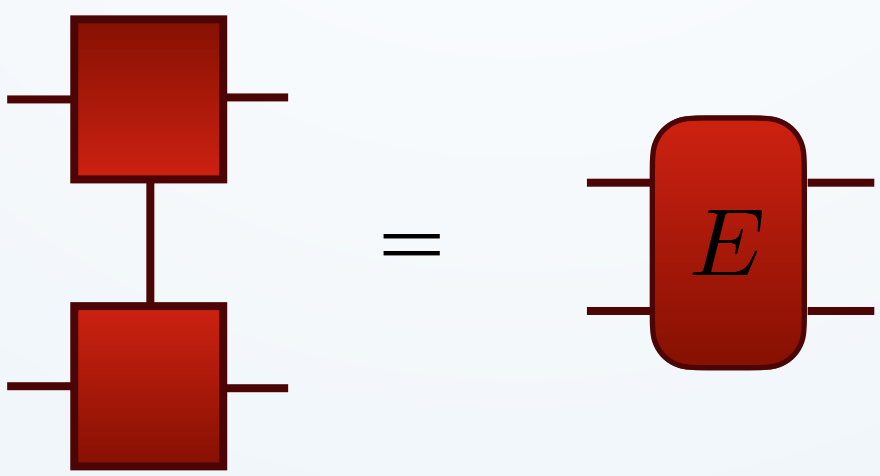
MPS PROPERTIES

Efficient expectation values



transfer operator

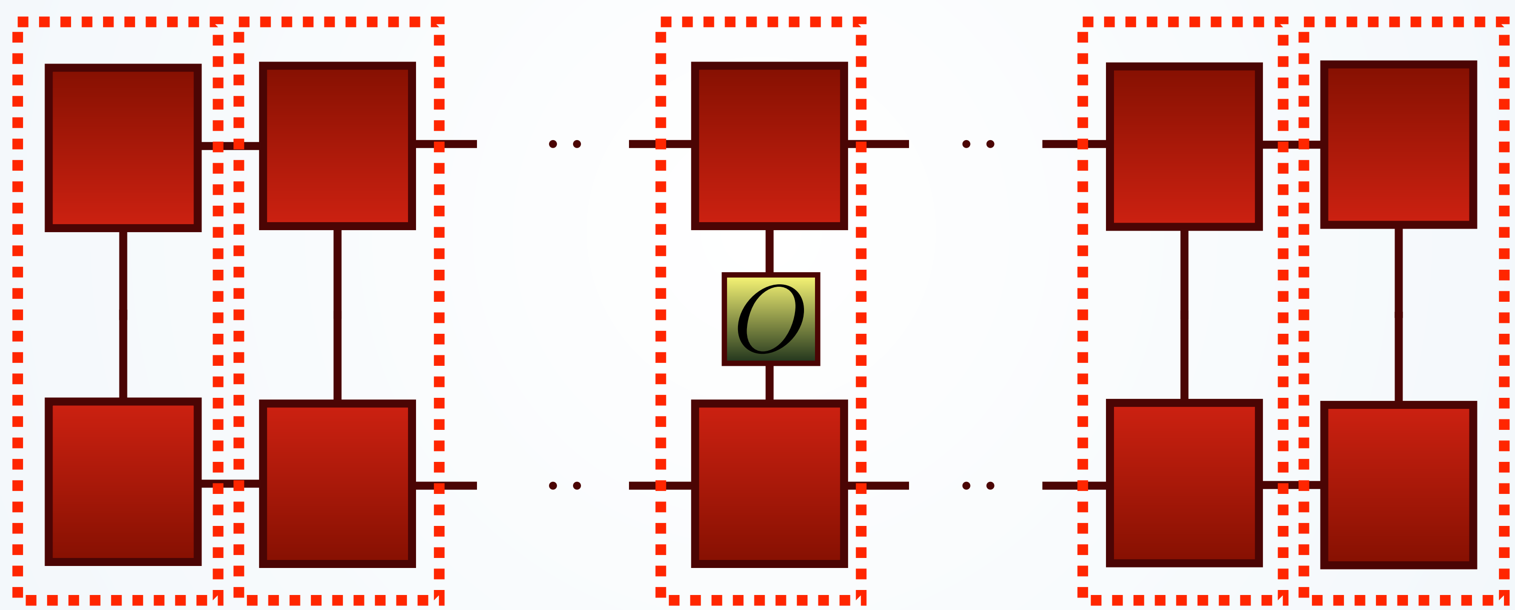
$D^2 \times D^2$ matrix



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

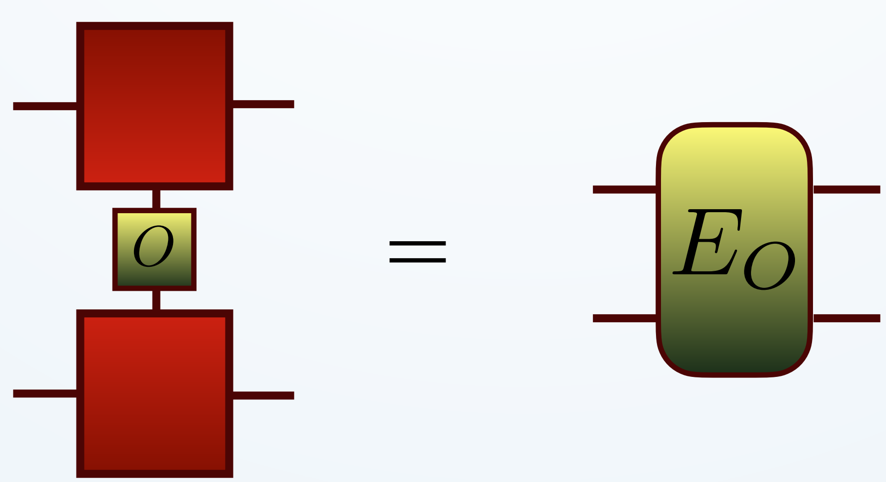
MPS PROPERTIES

Efficient expectation values



transfer operator

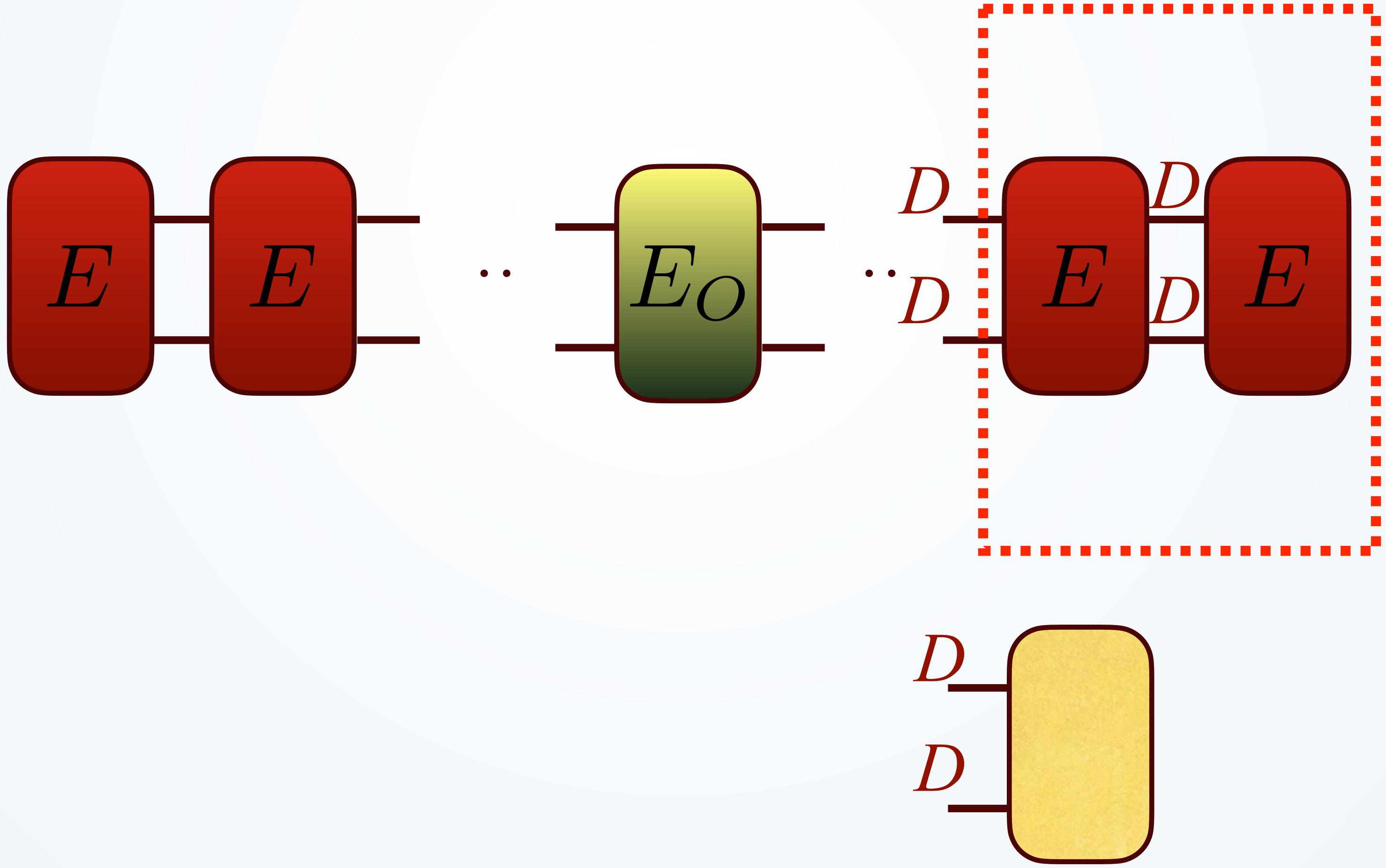
$D^2 \times D^2$ matrix



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

MPS PROPERTIES

Efficient expectation values

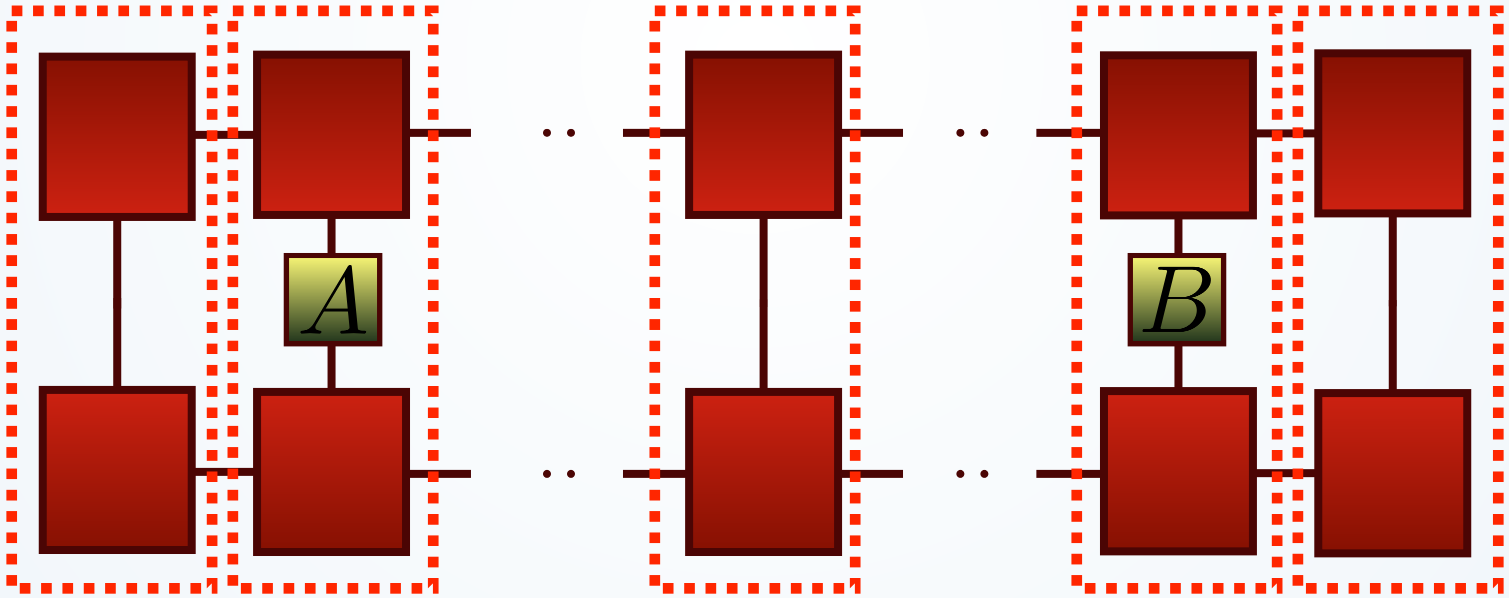


$O(D^4)$

MPS PROPERTIES

Exponentially decaying correlations

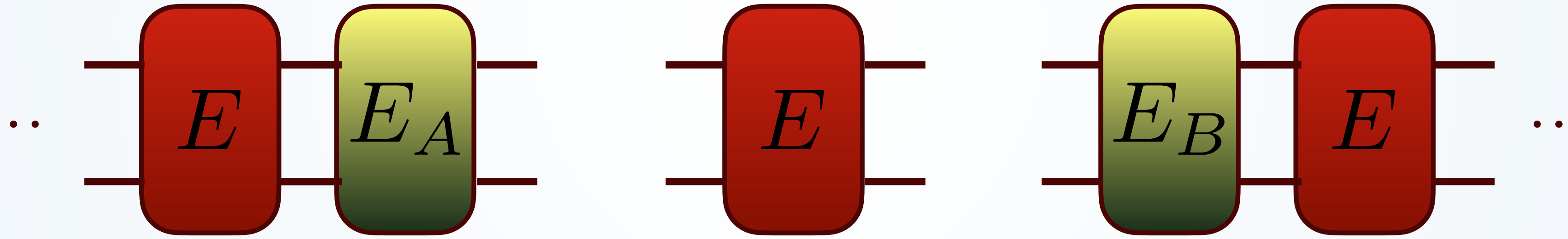
$$\langle A^{[p]} B^{[p+x]} \rangle - \langle A^{[p]} \rangle \langle B^{p+x} \rangle$$



MPS PROPERTIES

Exponentially decaying correlations

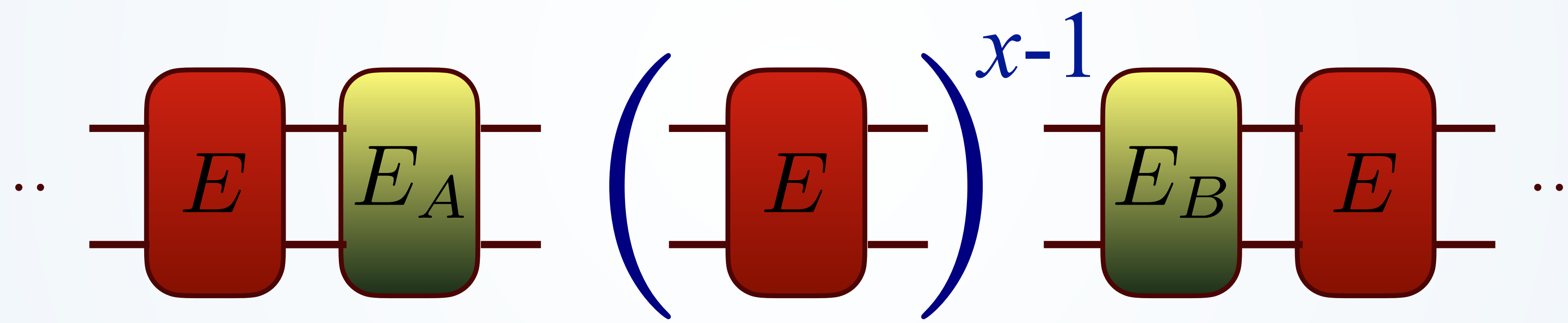
$$\langle A^{[p]} B^{[p+x]} \rangle$$



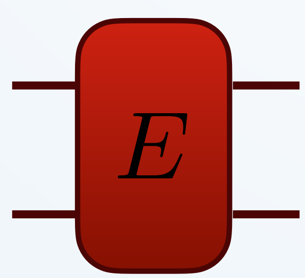
MPS PROPERTIES

Exponentially decaying correlations

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



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

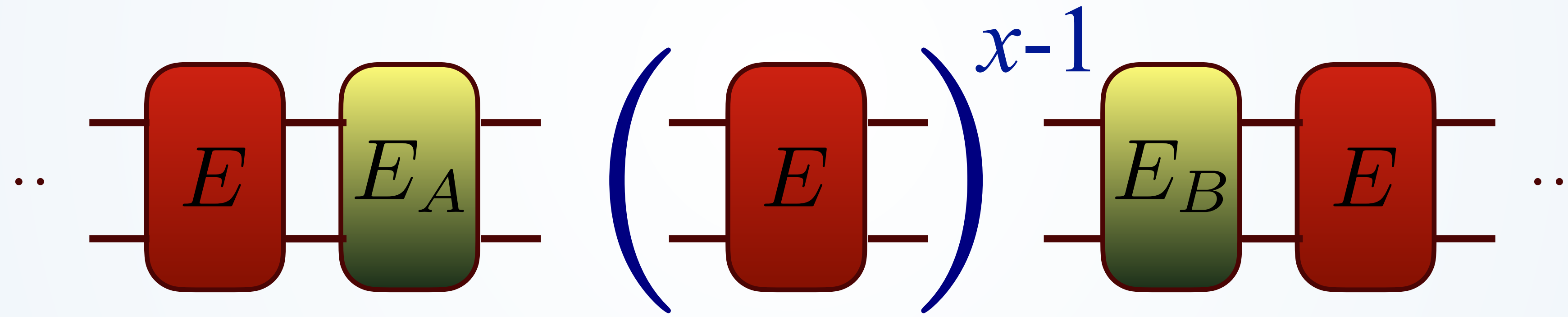


$$E = \sum_i A^{i*} \otimes A^i = \sum_k \lambda_k |R_k\rangle\langle L_k|$$

MPS PROPERTIES

Exponentially decaying correlations

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



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

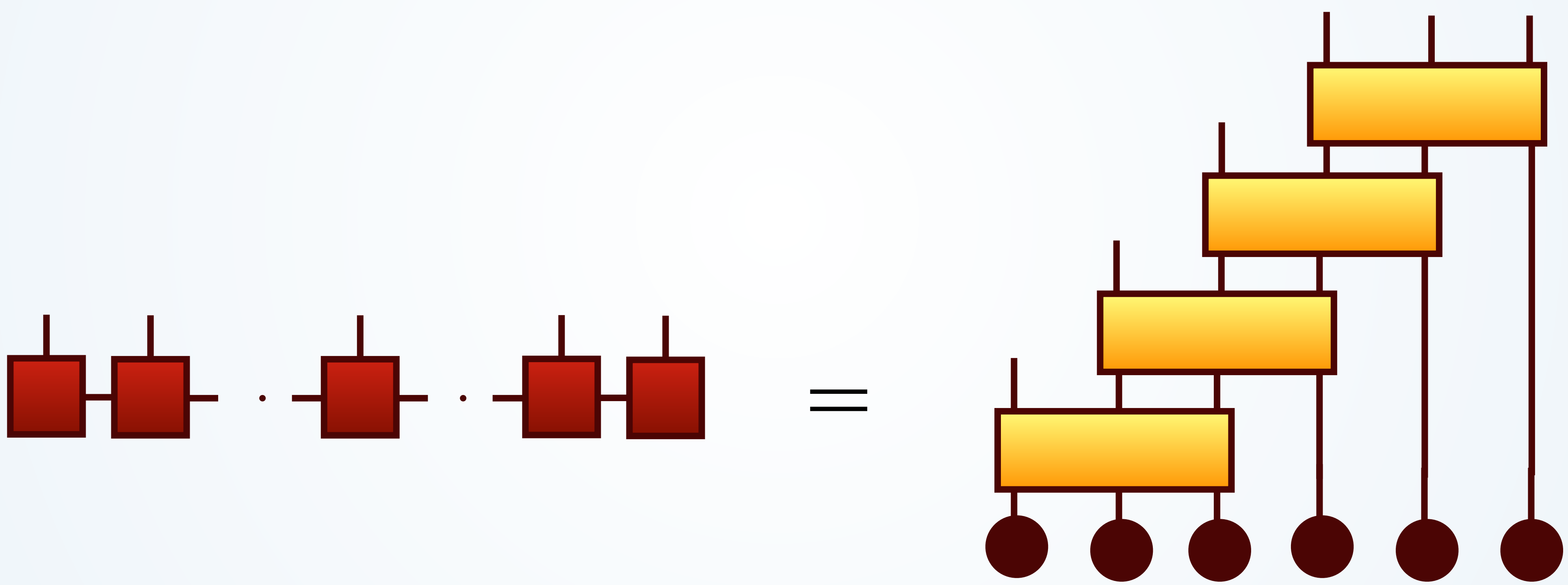
normalize

disconnected component

exponential decrease

MPS PROPERTIES

Efficient preparation



equivalent to an ancilla with dimension D

MPS PROPERTIES

Approximate ground states efficiently

$|\Psi\rangle$  $|\Psi_D\rangle$

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

truncation per link

squared Schmidt values

quality of approximation depends on how fast
Schmidt values decay

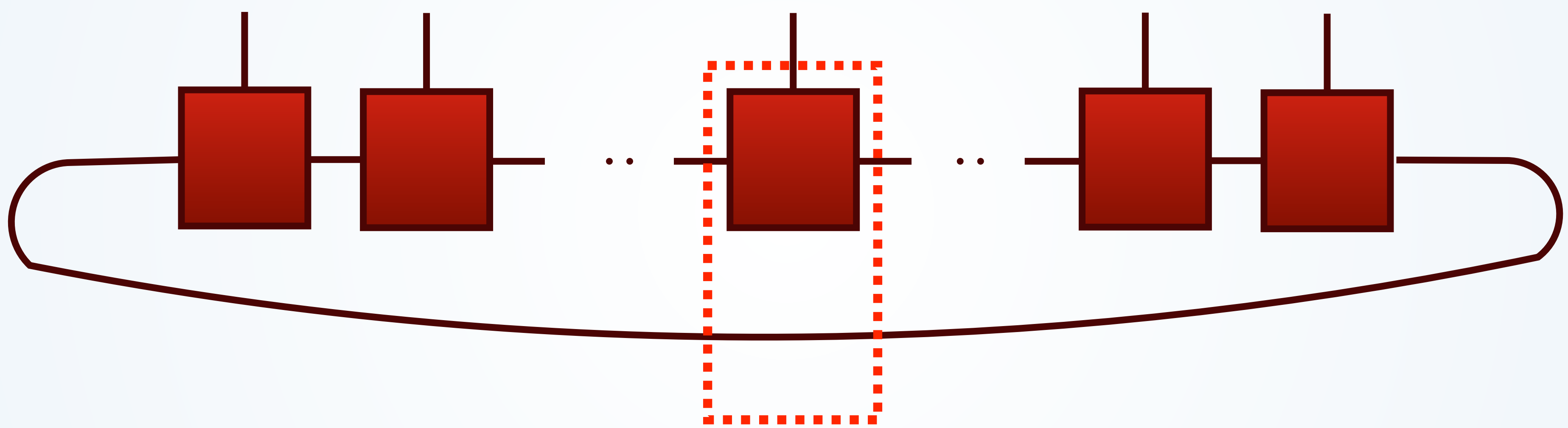
for ground states of local
gapped 1D Hamiltonians

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

Hastings JStatMech 2007

MPS PROPERTIES

Also periodic boundary conditions



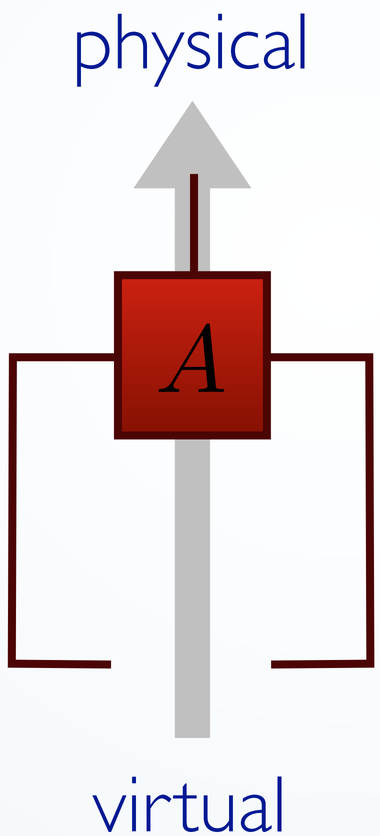
more expensive (still efficient) contractions $\mathbf{O}(D^5)$

could be written as OBC with D^2

(twice the entropy at half chain)

MPS PROPERTIES

Def: injectivity



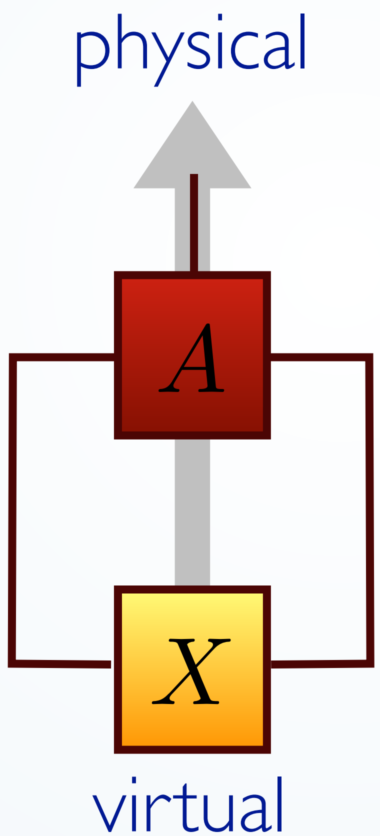
$$\Gamma(X) : \mathbb{C}^{D\times D} \to \mathbb{C}^d$$

generic property

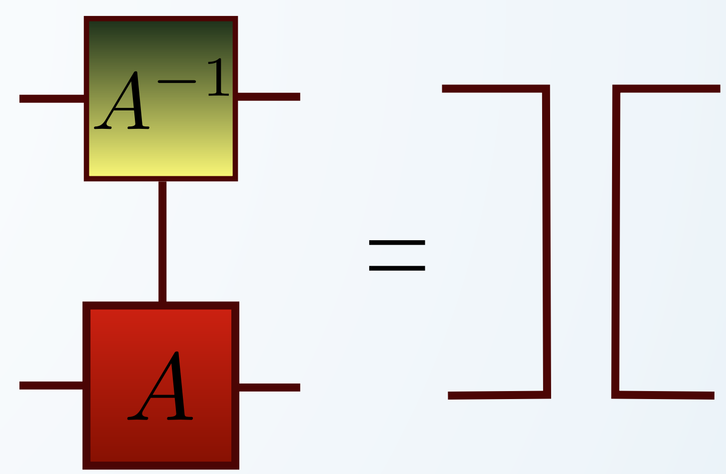
MPS PROPERTIES

Def: injectivity

$$\Gamma(X) : \mathbb{C}^{D\times D} \to \mathbb{C}^d$$



$\Leftrightarrow$



generic property

injective

only 0 mapped to 0

∃ inverse

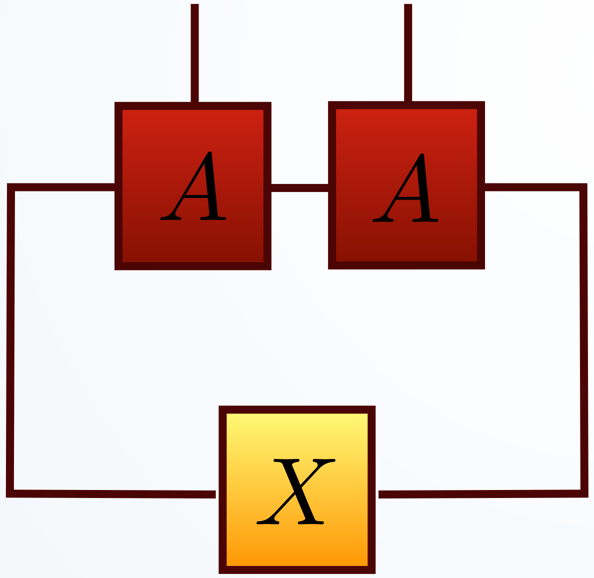
all boundary accessible from physical

MPS PROPERTIES

local parent Hamiltonian

Generalization of AKLT construction

S_2



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

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

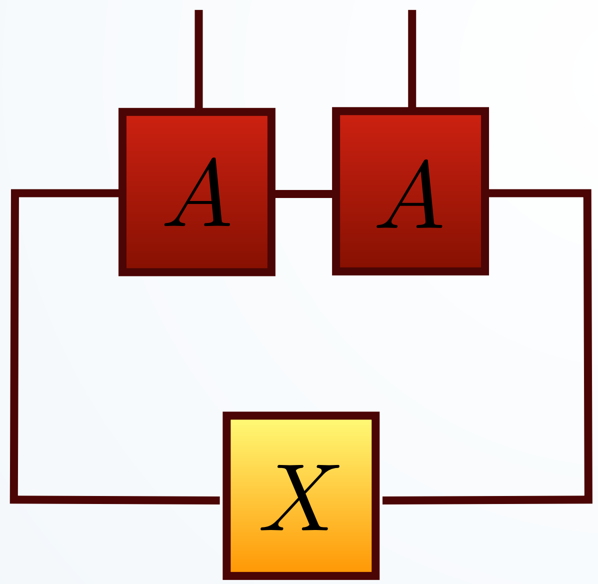
local, frustration-free

MPS 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

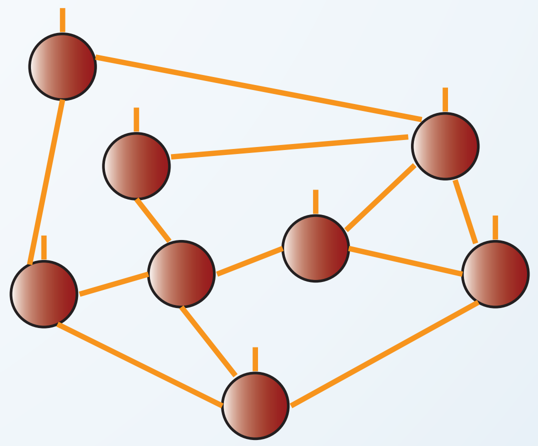
fundamental physical concept

invariant Hamiltonian → symmetric (covariant) eigenstate

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

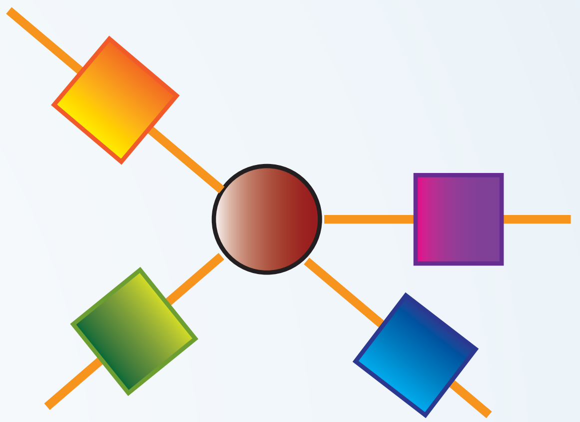
restrict effective Hilbert space to given quantum numbers

role of tensors symmetry?



MPS PROPERTIES

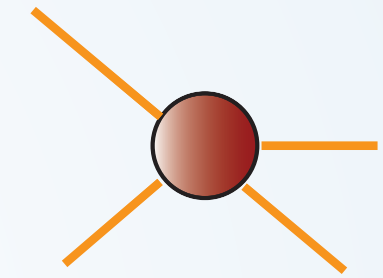
Tensors can be symmetric ⇒ state invariant



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

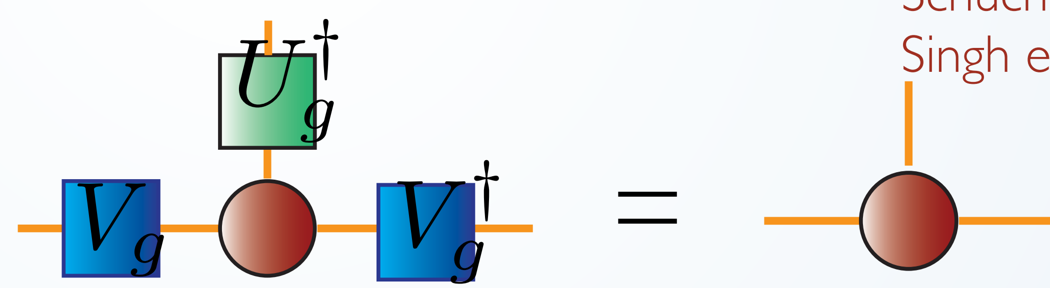
Tensors can be symmetric ⇒ state invariant



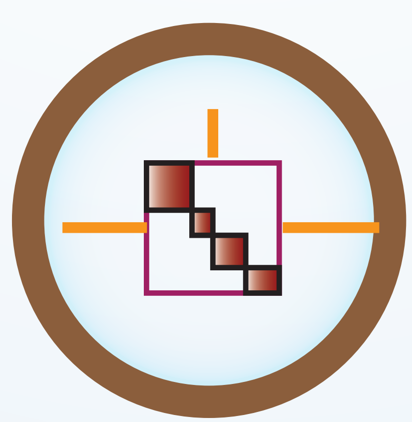
For MPS and PEPS, there is a canonical form

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 ⇔



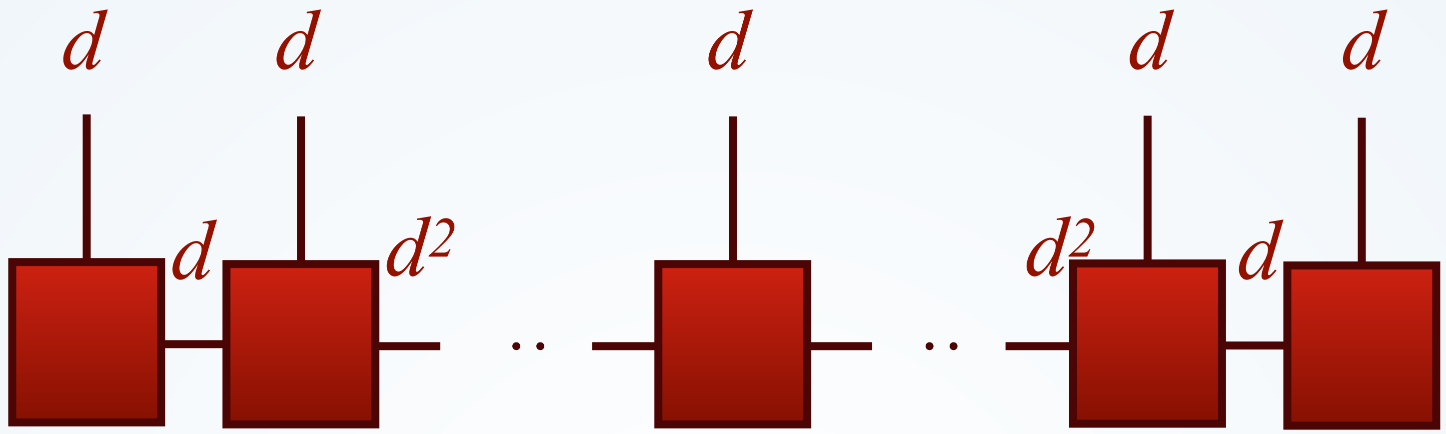
In general: structure of tensor → symmetry properties



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

Recap...

MPS

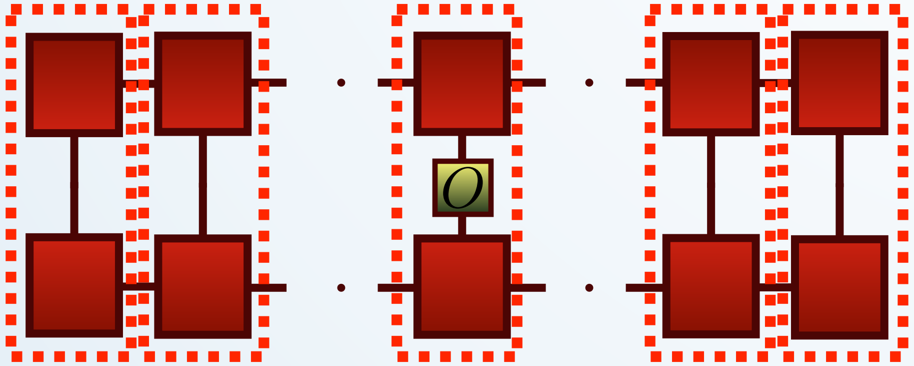


complete family $D \leq d^{N/2}$

good approximation of ground states

gapped finite range Hamiltonian ⇒
area law (ground state)

efficient calculation of expectation values



exponentially decaying correlations

canonical form

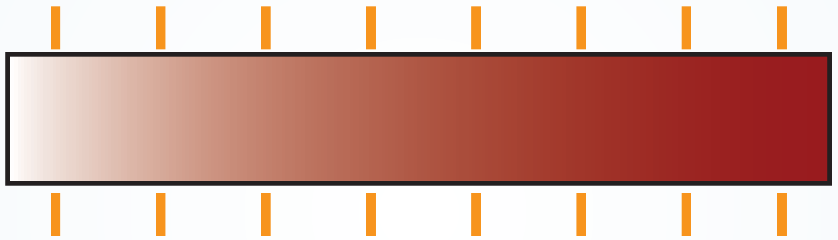
MPO

Matrix Product Operators

MPO

Matrix Product Operator

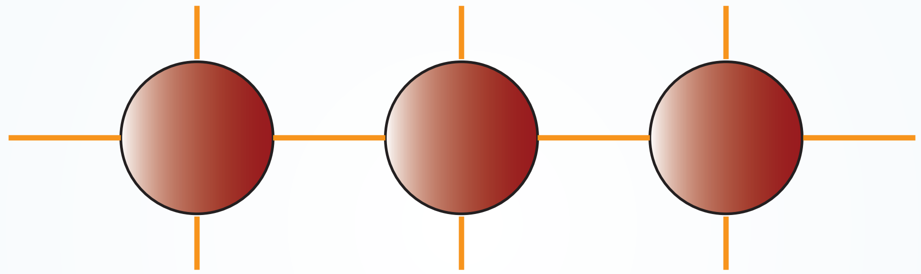
Same kind of ansatz for operators



MPO

Matrix Product Operator

Same kind of ansatz for operators



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

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 $\longrightarrow$ recognize regular expressions

$$(0*)1(0*)$$

accept	reject
1000	0000
0100	1100
0010	1010
0001	$\ldots$

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

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

MPO

local Hamiltonians are simple MPOs

finite state automata ⟶ recognize regular expressions

FSA = computational model

$(0*)1(0*)$

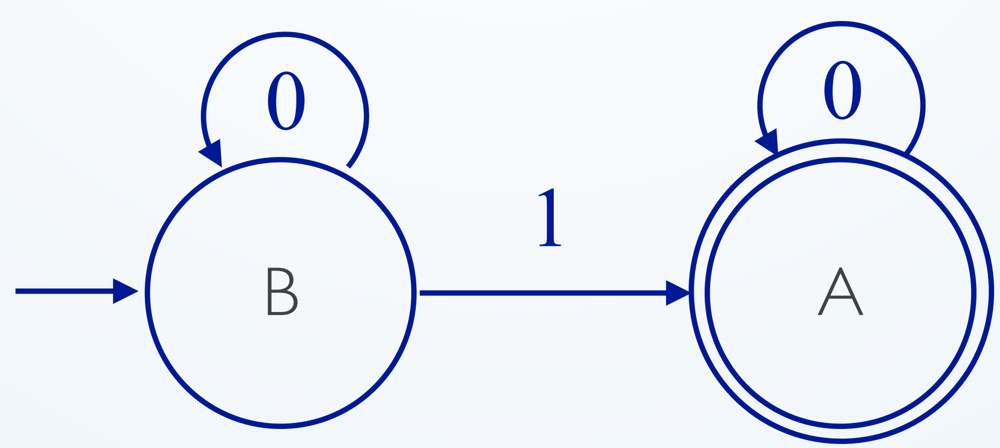
S states $S_0, S_f \in S$

B: before 1

A: after 1

Σ input alphabet 0, 1

$S \times \Sigma \to S$ transitions

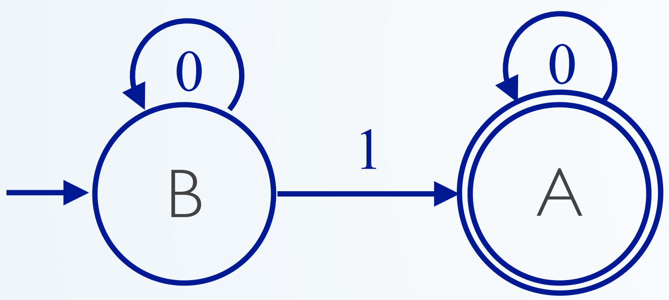


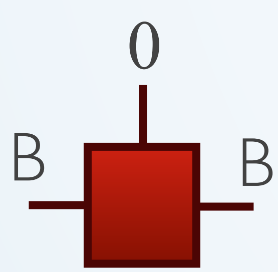
MPO

Matrix Product Operator

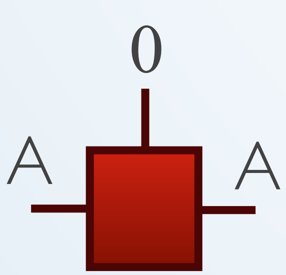
local Hamiltonians are simple MPOs

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



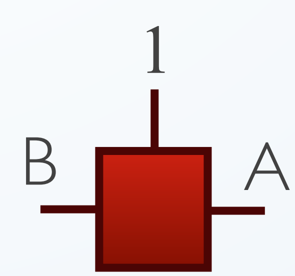


$= 1$



$= 1$

$$\begin{array}{cc} B & A \\ \end{array}$$
$$M^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



$= 1$

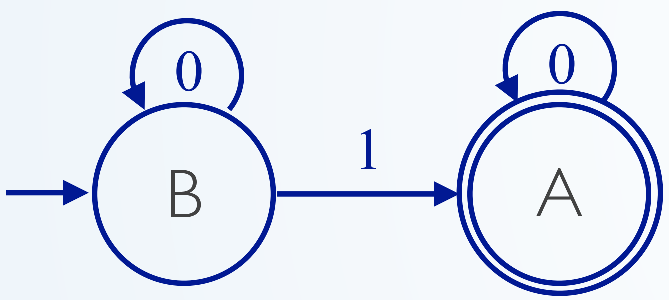
$$M^1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$

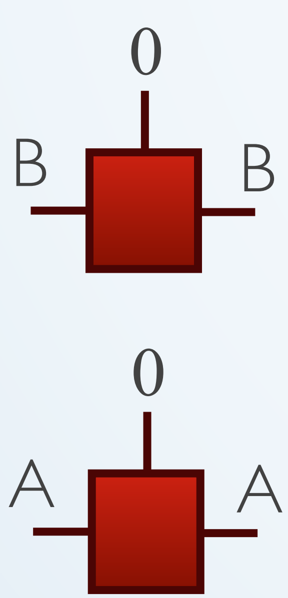
MPO

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

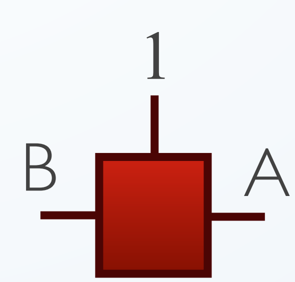




$= 1$

$= 1$

$$M^0 = \begin{array}{cc} \mathrm{B} & \mathrm{A} \\ \end{array} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



$= 1$

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

boundaries M_L, M_R

MPO

Matrix Product Operator

local Hamiltonians are simple MPOs

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

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

expressed as operator(vector) valued matrix

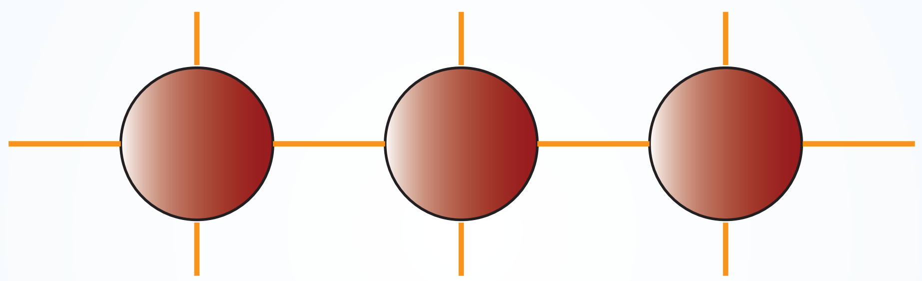
$$M = \begin{pmatrix} |0\rangle & |1\rangle \\ 0 & |0\rangle \end{pmatrix} \qquad M = \begin{pmatrix} \mathbb{I} & \sigma_x \\ 0 & \mathbb{I} \end{pmatrix}$$

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

MPO

Matrix Product Operator

an ansatz for density matrices



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*?

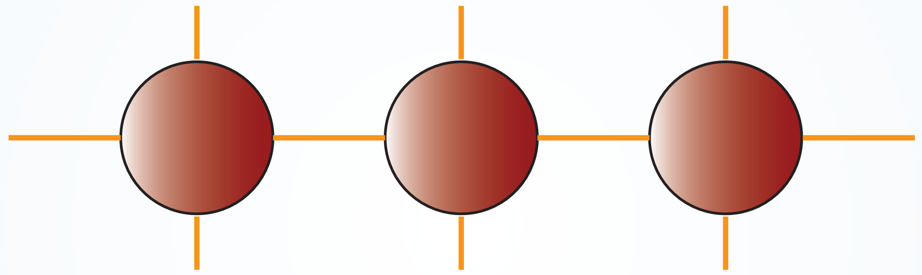
$\rho = \rho^\dagger$ $\quad$ $\mathrm{tr}\rho = 1$ $\quad$ $\rho \geq 0$

not all MPO satisfy them!

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*?

$\rho = \rho^\dagger$ ✓

$\mathrm{tr}\rho = 1$ ✓

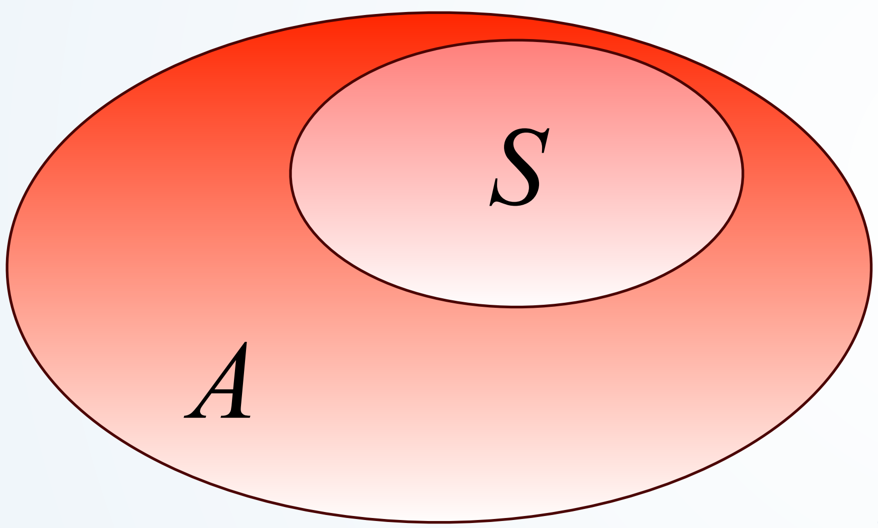
$\rho \geq 0$ ✗

there is a way

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 $\mathbf{A}$ $\quad d_A \leq d_S$

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

orthogonal

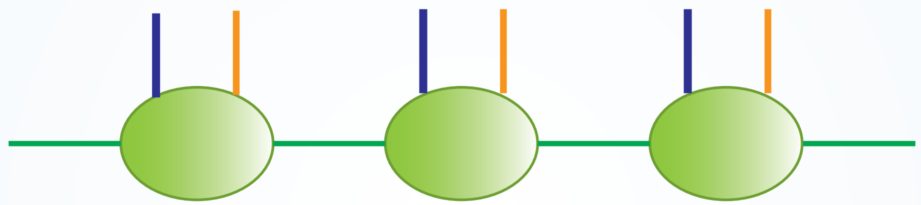
$$\rho_S = \mathrm{tr}\left(|\Psi_{SA}\rangle\langle\Psi_{SA}|\right)$$

unitary freedom on ancilla

MPO

Matrix Product Operator

purification



need some properties

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

can we impose them *locally*?

$\rho = \rho^\dagger$ ✓

$\mathrm{tr}\rho = 1$ ✓

$\rho \geq 0$

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

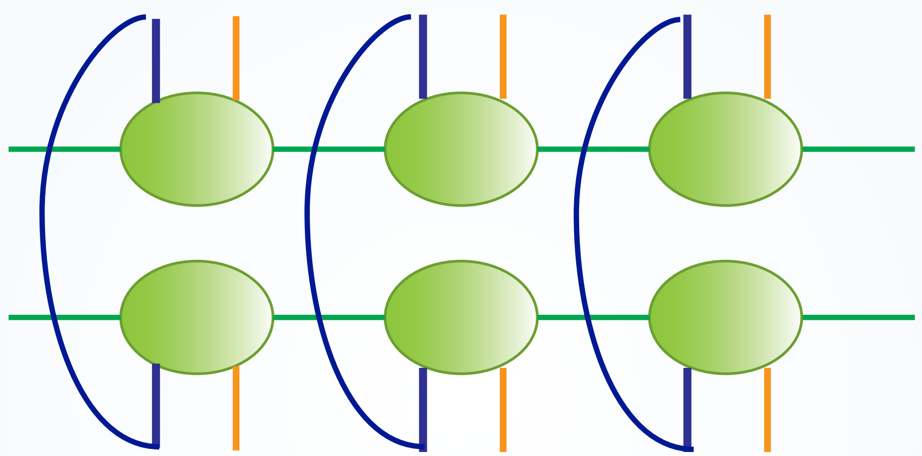
Verstraete et al., PRL 2004

Zwolak and Vidal, PRL 2004

MPO

Matrix Product Operator

purification



need some properties

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

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$\rho = \rho^\dagger$ ✔ $\qquad$ $\mathrm{tr}\rho = 1$ ✔ $\qquad$ $\rho \geq 0$

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

Verstraete et al., PRL 2004

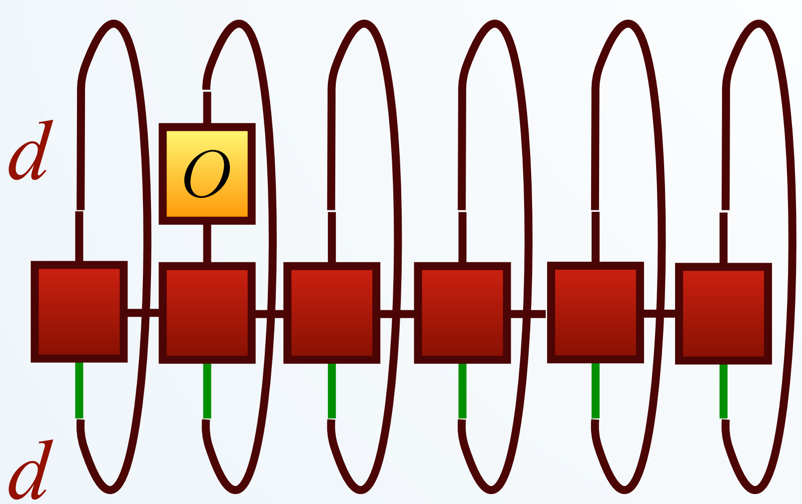
Zwolak and Vidal, PRL 2004

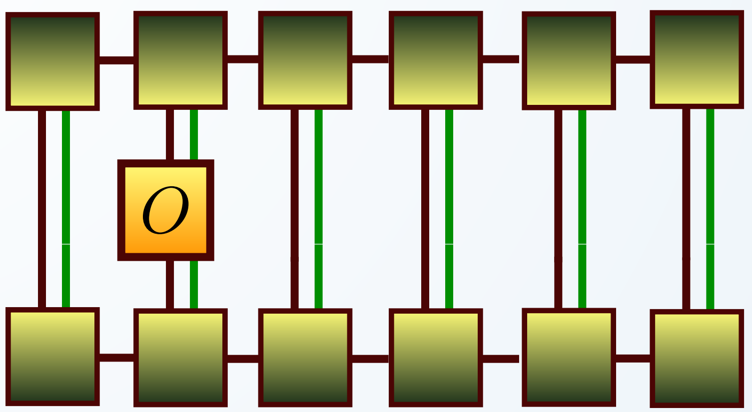
MPO

Matrix Product Operator

expectation values

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





TEBD: time evolution and more

Mari-Carmen Bañuls

Max Planck Institut
of Quantum Optics
(Garching)

ICCUB 27.9.2021

Simplest time evolution algorithms with MPS

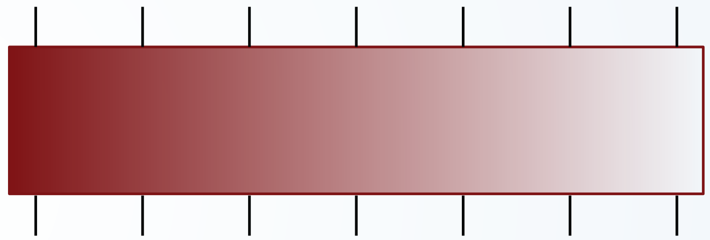
TEBD, t-DMRG, tMPS

photo: Alejandro Piñero Amerio @ Unsplash

BASIC ALGORITHMS

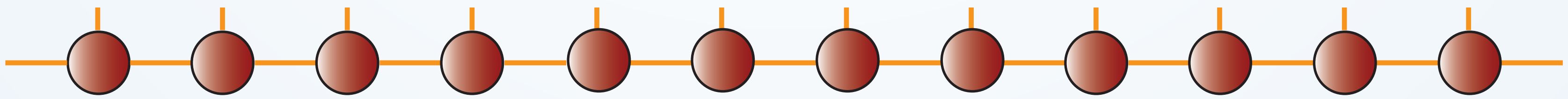
simulate time evolution

$U(t)$



initial MPS

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



TEBD, t-DMRG, tMPS

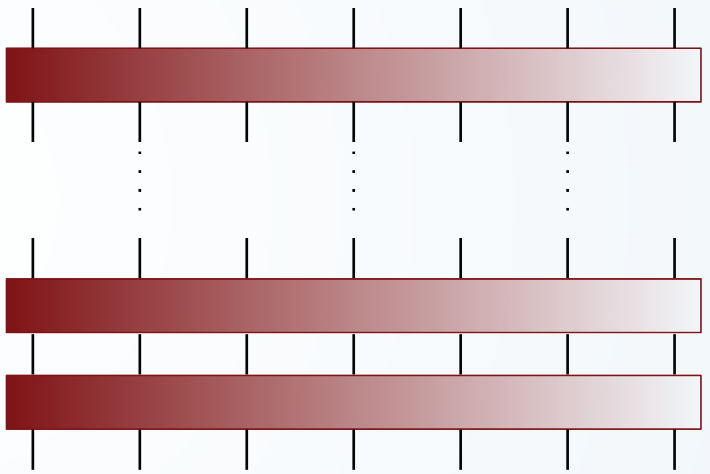
Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

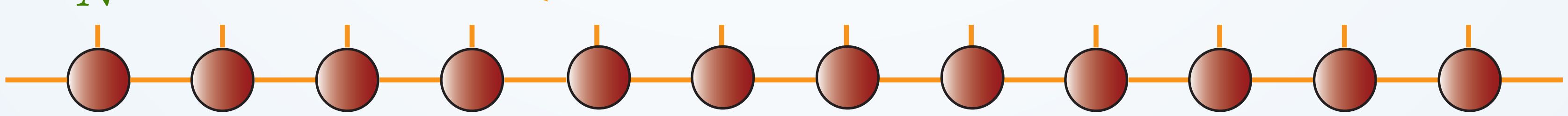
simulate time evolution

$$U(t) \to [U(\delta)]^M$$



initial MPS

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



TEBD, t-DMRG, tMPS

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

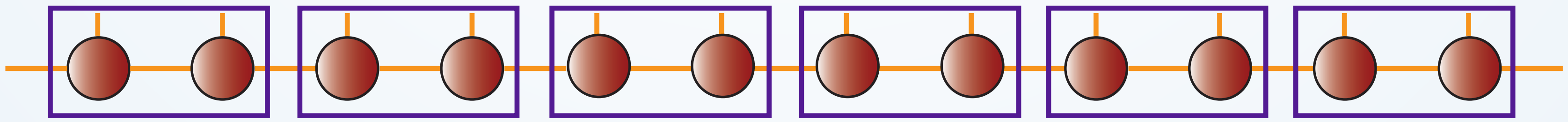
simulate time evolution

$$U(t) \to [U(\delta)]^M$$

$$H = \boxed{H_e} + H_o$$

apply evolution step

Suzuki-Trotter expansion



TEBD, t-DMRG, tMPS

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

simulate time evolution

$$U(t) \rightarrow [U(\delta)]^M$$

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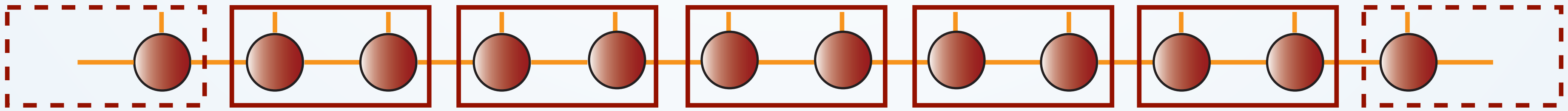


TEBD, t-DMRG, tMPS

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

simulate time evolution

$$U(t) \to [U(\delta)]^M$$

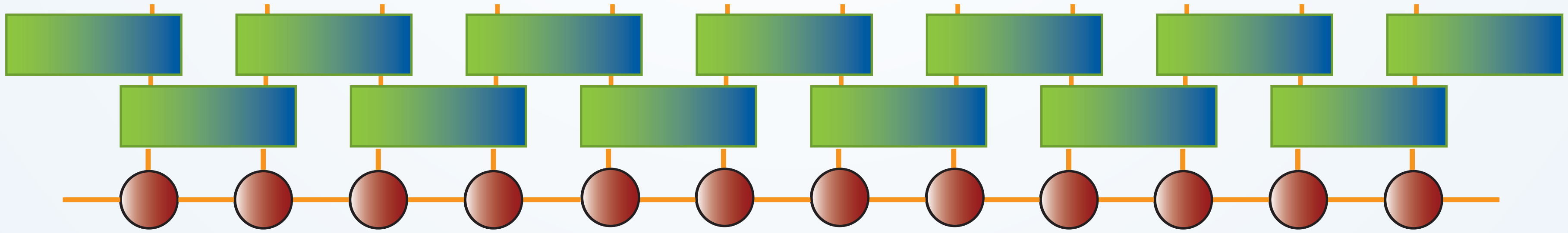
apply evolution step

$$H = H_e + H_o$$

Suzuki-Trotter expansion

$$U(\delta) \approx e^{-iH_e\delta} e^{-iH_o\delta}$$

as local terms!



TEBD, t-DMRG, tMPS

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

simulate time evolution

$$U(t) \to [U(\delta)]^M$$

apply evolution step

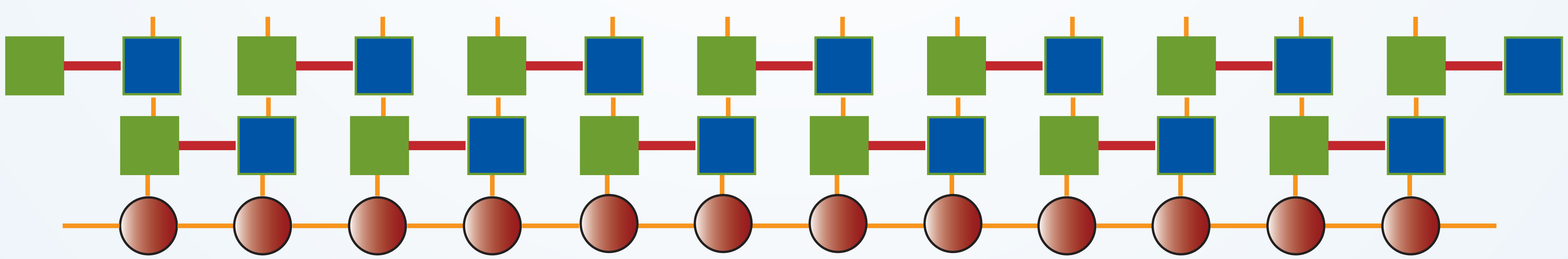
$$H = H_e + H_o$$

Suzuki-Trotter expansion

$$U(\delta) \approx e^{-iH_e\delta} e^{-iH_o\delta}$$

as local terms!

MPOs



TEBD, t-DMRG, tMPS

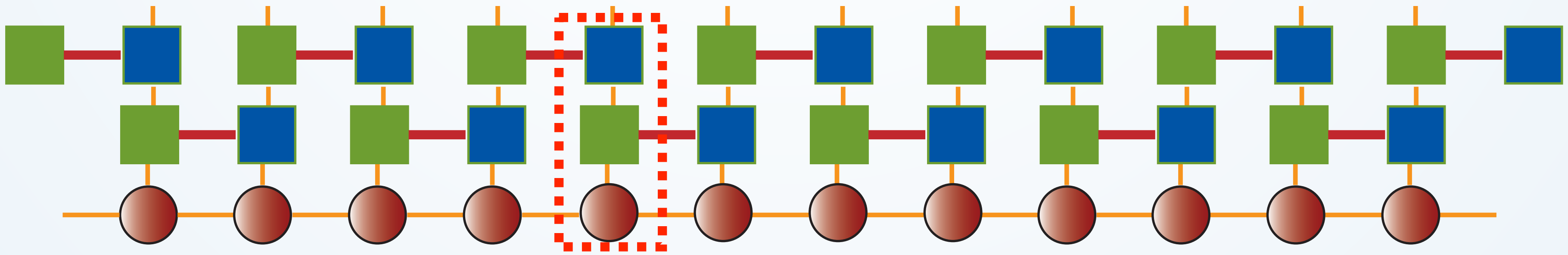
Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

simulate time evolution

truncate bond
dimension



TEBD, t-DMRG, tMPS

Vidal, PRL 2003, 2004

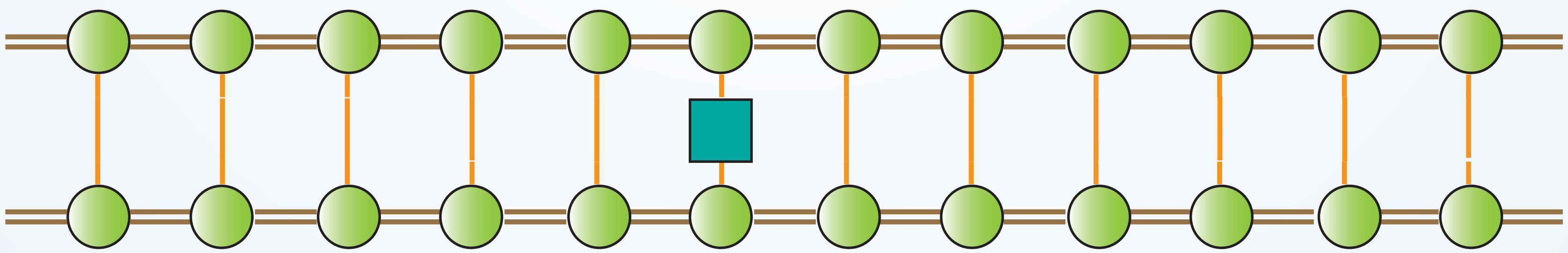
Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

simulate time evolution

works for real and imaginary time

imaginary time for ground states,
thermal equilibrium



compute observables

TEBD, t-DMRG, tMPS

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

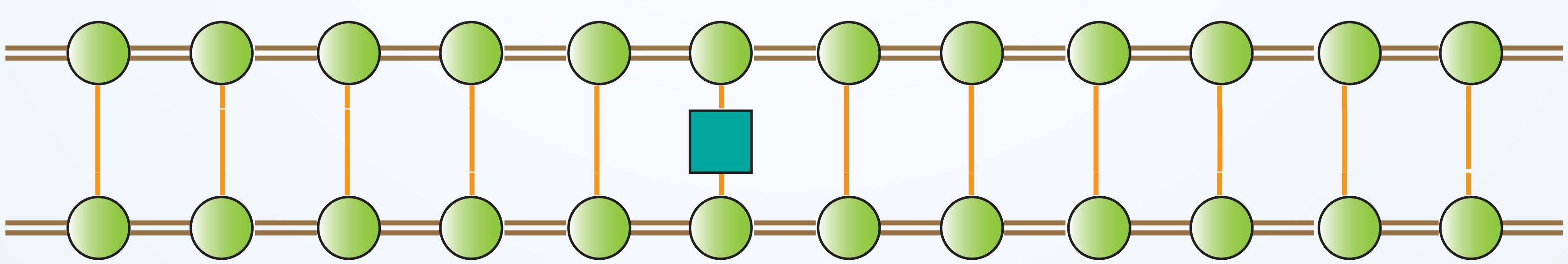
BASIC ALGORITHMS

simulate time evolution

works for real and imaginary time

imaginary time for ground states,
thermal equilibrium

truncation schemes



compute observables

TEBD, t-DMRG, tMPS

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

approximate action of local operators

local truncation

variational truncation

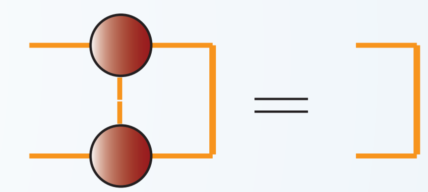
basis of most common evolution algorithms

disclaimer: also other algorithms exist

BASIC ALGORITHMS

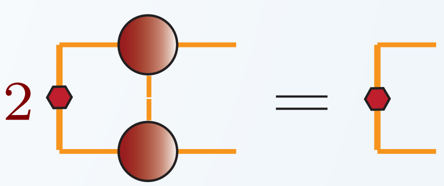
local truncation: TEBD

recall canonical form



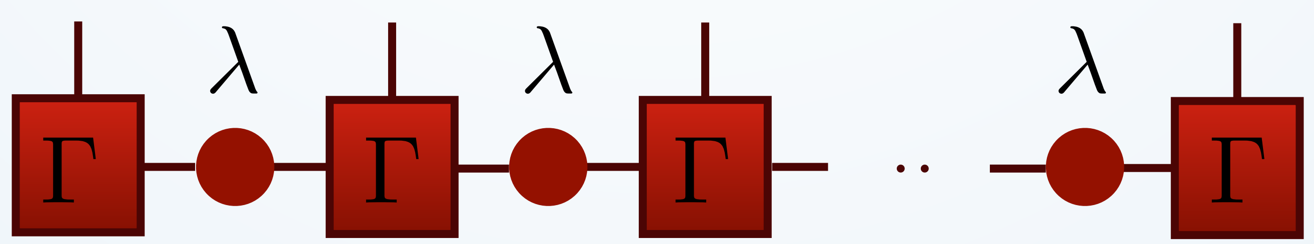
Schmidt values

$$\Lambda^{[k]} = {\lambda^{[k]}}^2$$



can be made explicit

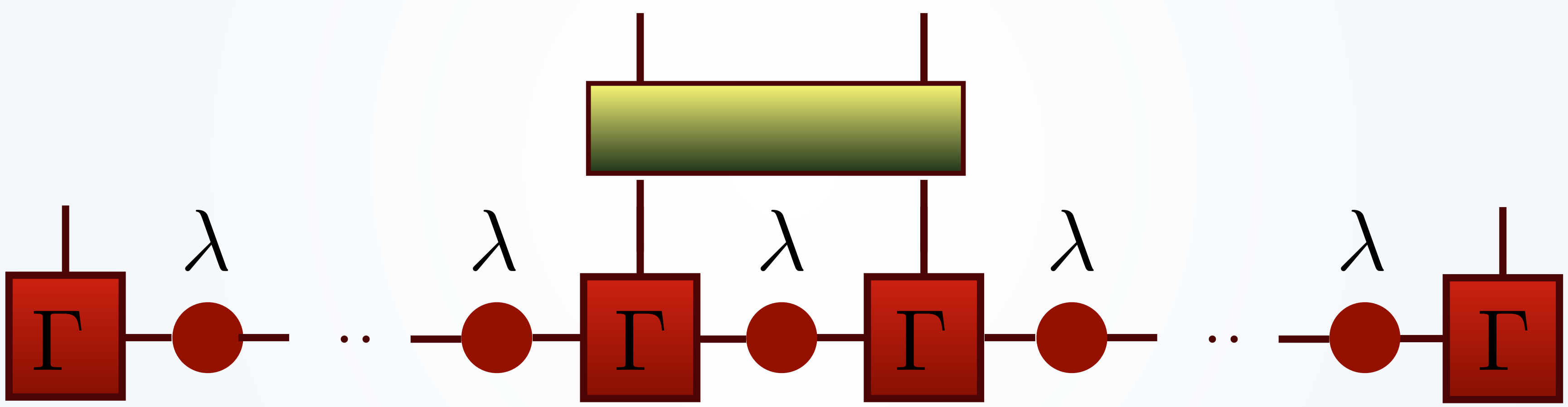
$$A^{[k]} = \Gamma^{[k]} \lambda^{[k]}$$



Vidal, PRL 2003, 2004

BASIC ALGORITHMS

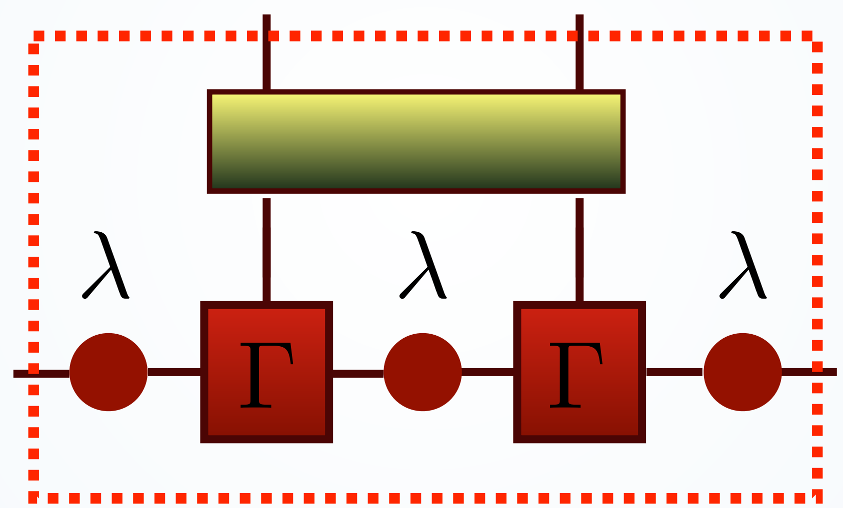
local truncation: TEBD

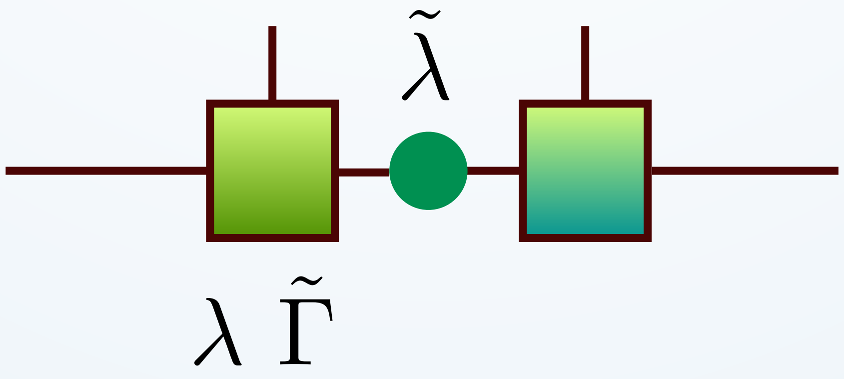


Vidal, PRL 2003, 2004

BASIC ALGORITHMS

local truncation: TEBD

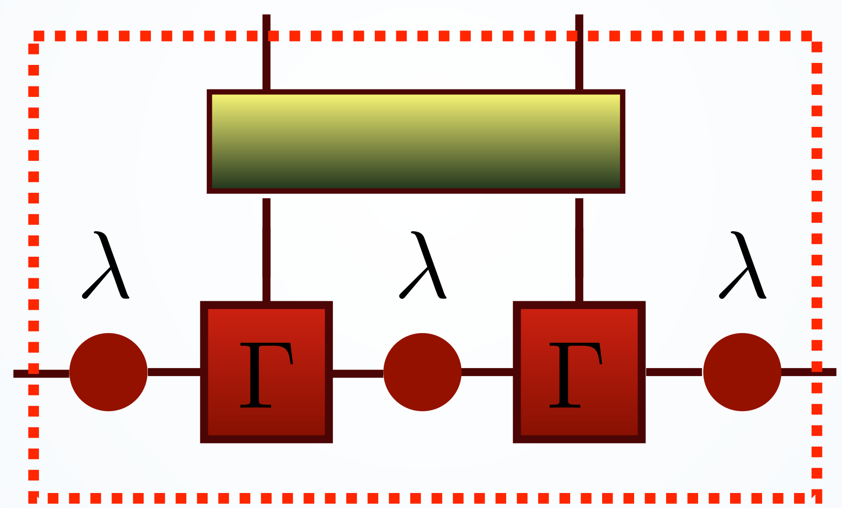




Vidal, PRL 2003, 2004

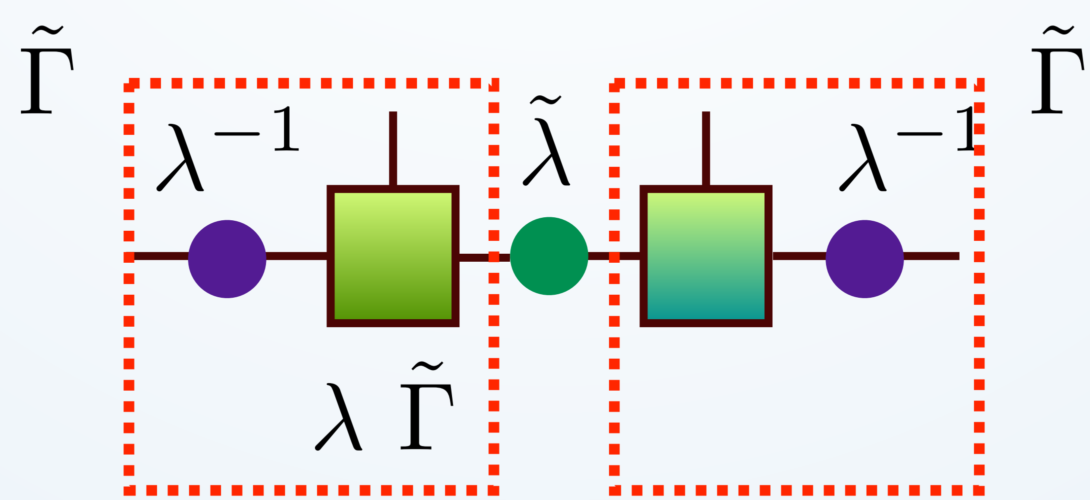
BASIC ALGORITHMS

local truncation: TEBD



unitary gate
⇒canonical form preserved

up to truncation



also possible in the TD limit

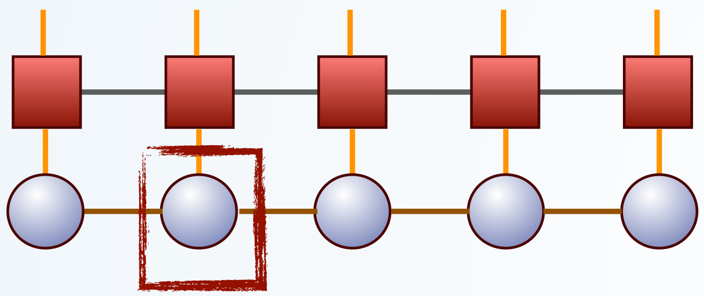
canonical form lost

Vidal, PRL 2003, 2004

BASIC ALGORITHMS

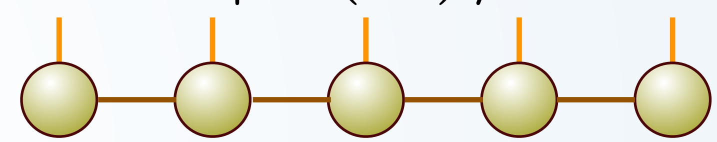
global truncation

$|\Phi_0\rangle$



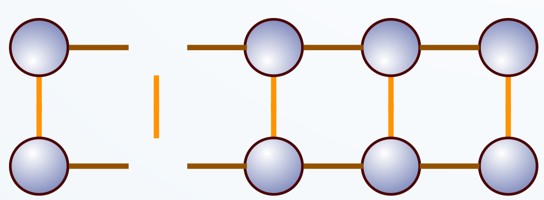
$\approx$

$|\Psi(A)\rangle$

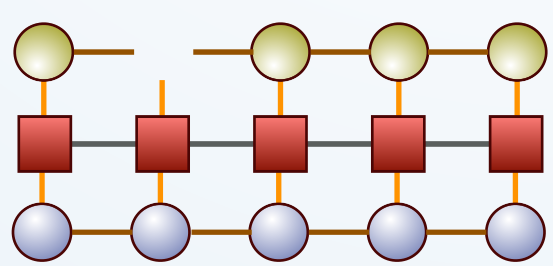


$$\min_{\{A\}} \| |\Psi\rangle - O|\Phi_0\rangle \|^2 \longrightarrow \min_{A} (\bar{A} N_{\mathrm{eff}} A - \bar{A} M - \bar{M} A + \mathrm{const})$$

N_{eff}



M



$$N_{\mathrm{eff}} A = M$$

BASIC ALGORITHMS

imaginary time evolution ⇒ ground state

$$\lim_{\tau\to\infty} e^{-\tau H}|\Phi_0\rangle \to |E_{\min}\rangle$$

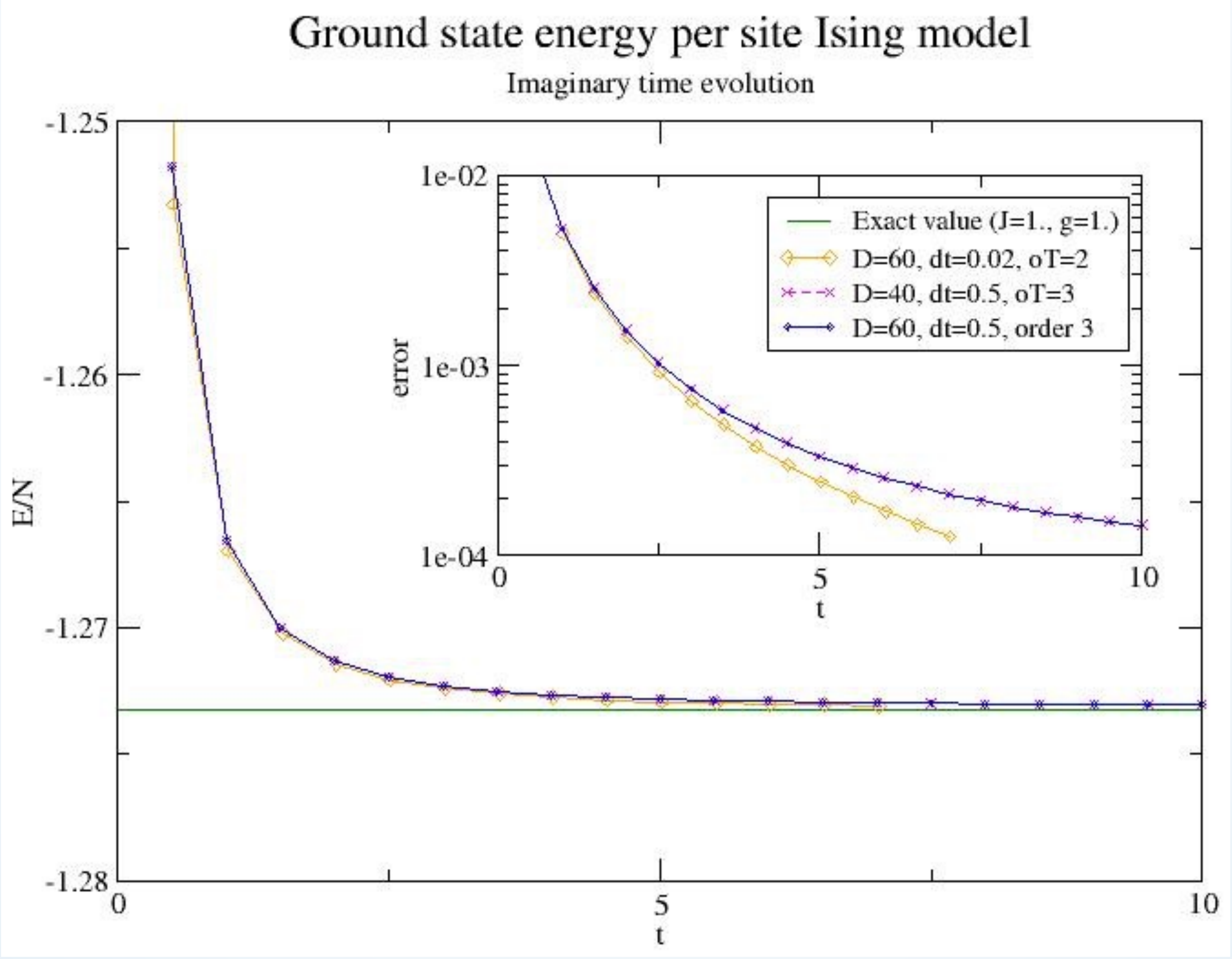
$$|\Phi_0\rangle = \sum c_n|E_n\rangle$$

$$e^{-\tau H}|\Phi_0\rangle = \sum c_n e^{-\tau E_n}|E_n\rangle$$

$$e^{-\tau H}|\Phi_0\rangle \propto c_0|E_0\rangle + \sum_{n>0} c_n e^{-\tau(E_n-E_0)}|E_n\rangle$$

BASIC ALGORITHMS

imaginary time evolution ⇒ ground state



BASIC ALGORITHMS

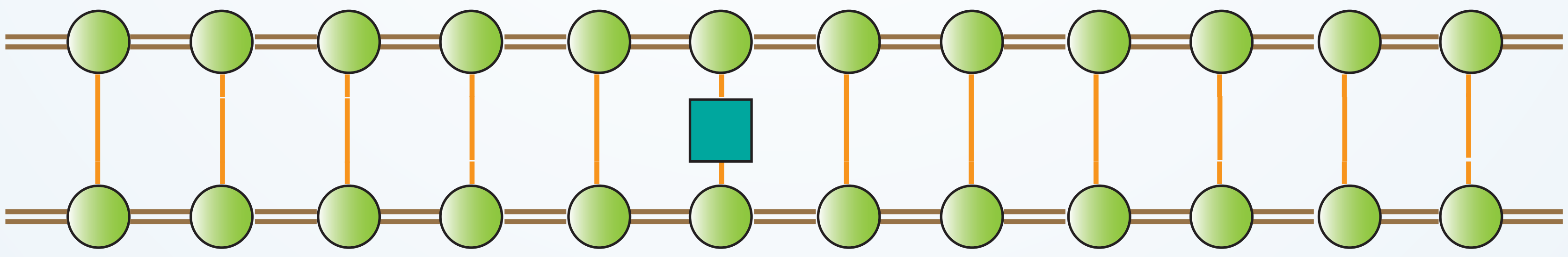
simulate time evolution

works for real and imaginary time

imaginary time for ground states,
thermal equilibrium

but out of equilibrium entanglement can grow fast!

Osborne, PRL 2006
Schuch et al., NJP 2008

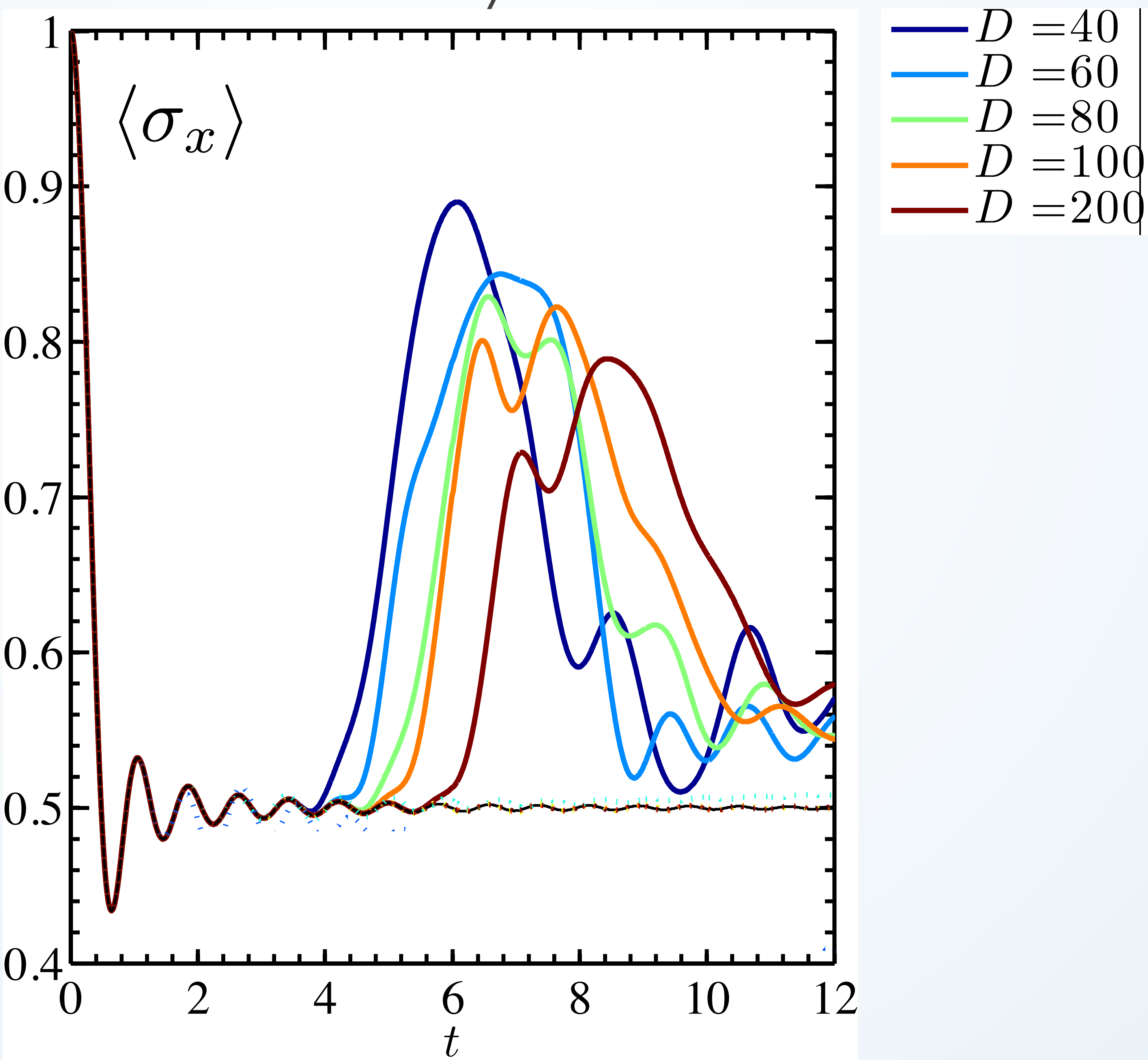


compute
observables

TEBD
t-DMRG

BASIC ALGORITHMS

real time dynamics

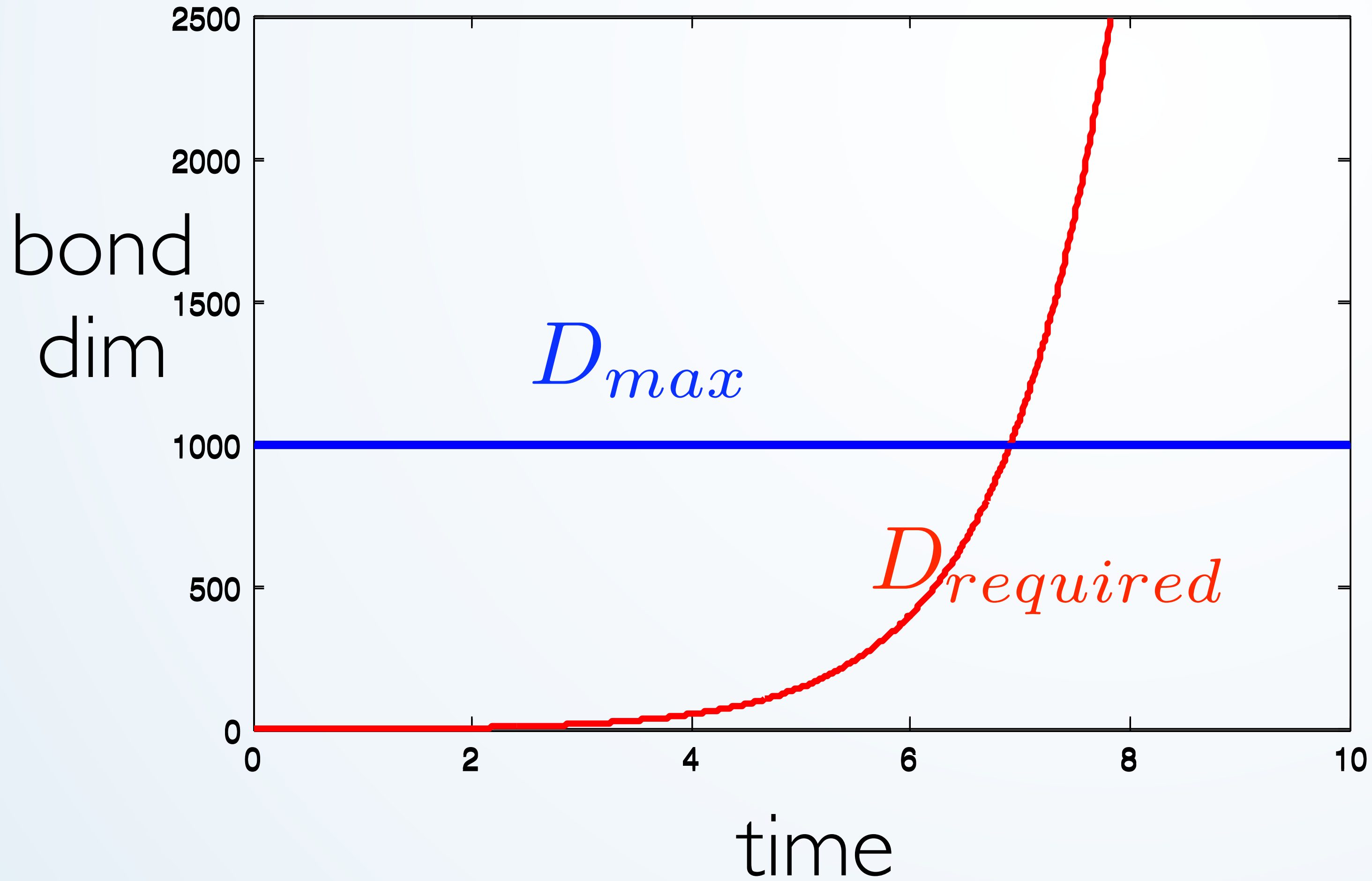


ENTANGLEMENT AND TIME EVOLUTION

ENTANGLEMENT GROWTH

Entropy of evolved state may grow linearly

Osborne, PRL 2006
Schuch et al., NJP 2008



required bond for fixed precision

$$D \sim e^{\alpha t}$$

limits the simulation of out of equilibrium many physical situations (in closed and open quantum systems) can be successfully studied!

short times, adiabatic, low energy can work well

García-Ripoll, NJP 2006
Wall, Carr NJP 2012
Paeckel et al arXiv:1901.05824

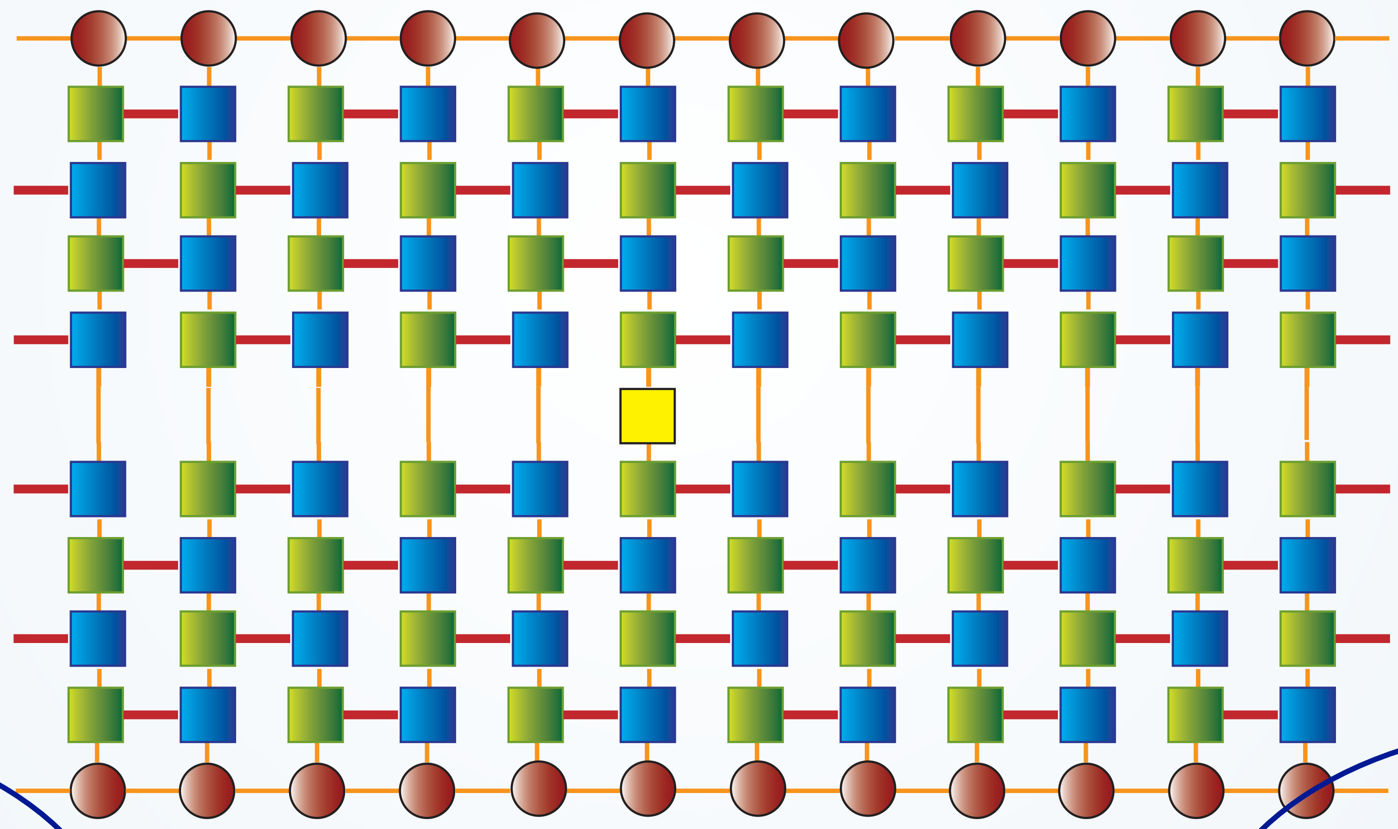
SOME ALTERNATIVES

avoid representing the state as MPS

ALTERNATIVELY...

time dependent observables as TN

problem is contracting the network



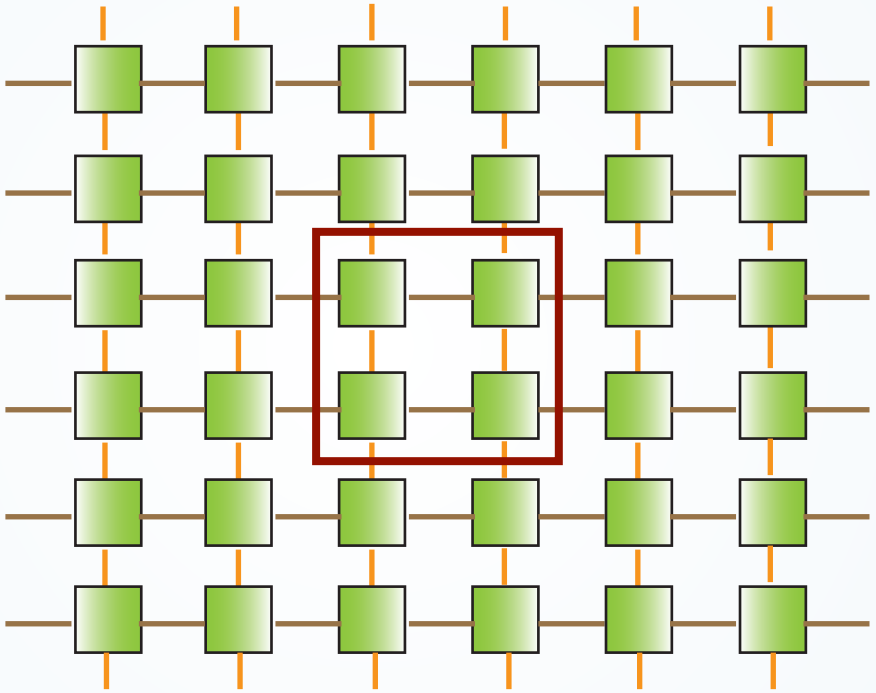
TN describe observables, not states

key: *entanglement* in TN

exact contraction not possible
#P complete

tensor networks may describe partition functions (observables)

need to contract a TN

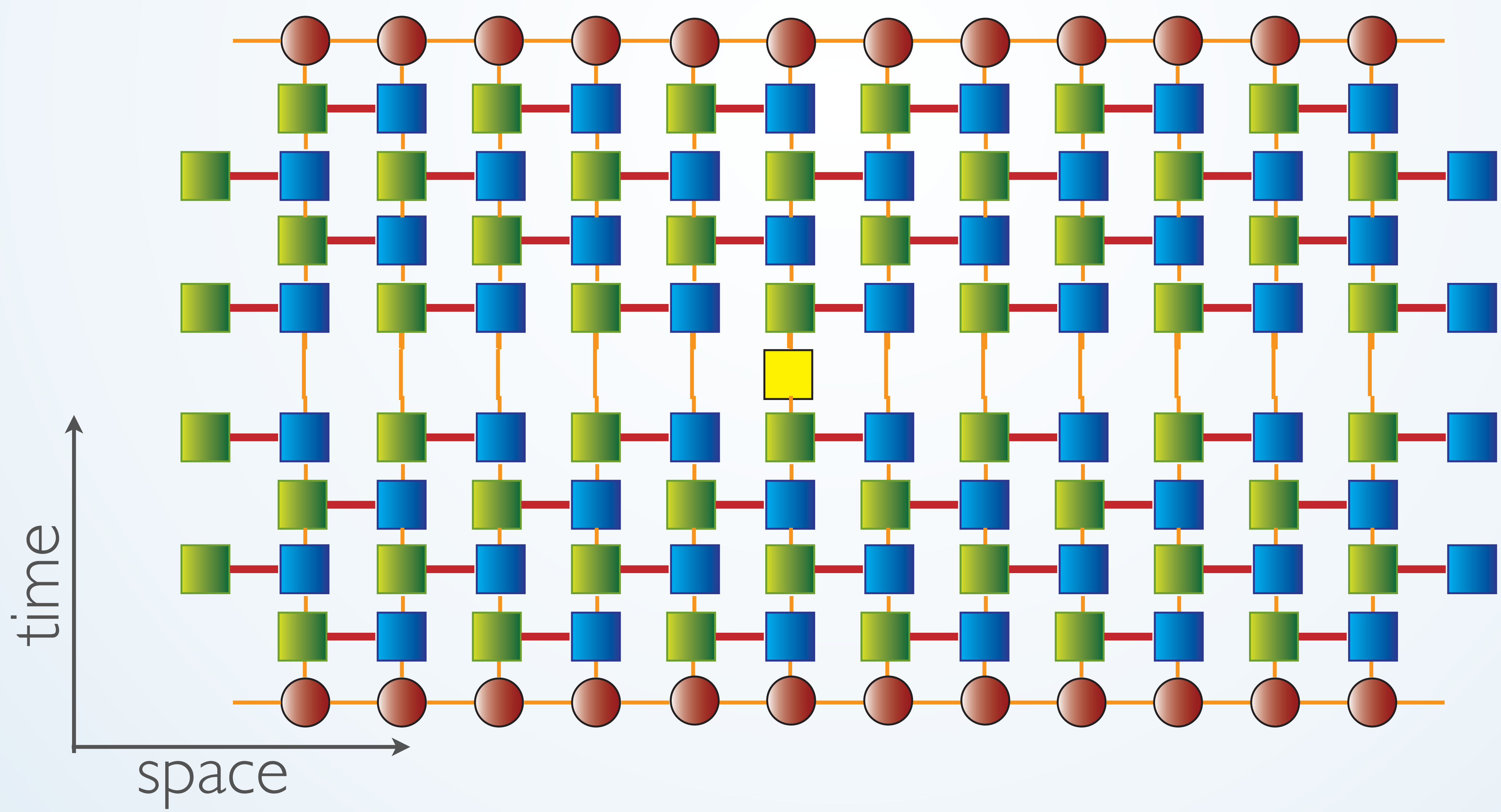


TRG approaches

Nishino, JPSJ 1995
Levin & Wen PRL 2008
Xie et al PRL2009; Zhao et al PRB 2010

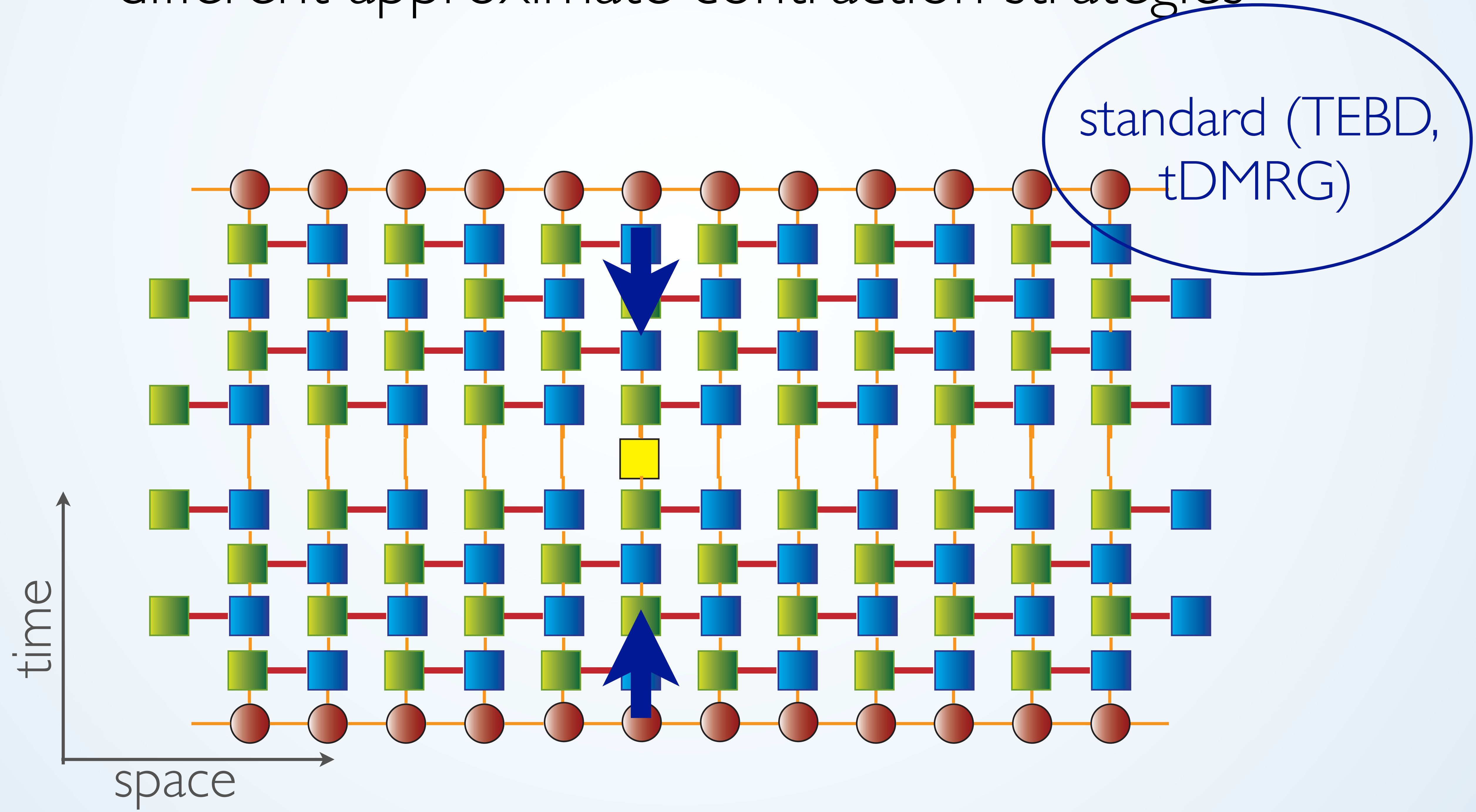
OBSERVABLE AS TN

different approximate contraction strategies



OBSERVABLE AS TN

different approximate contraction strategies

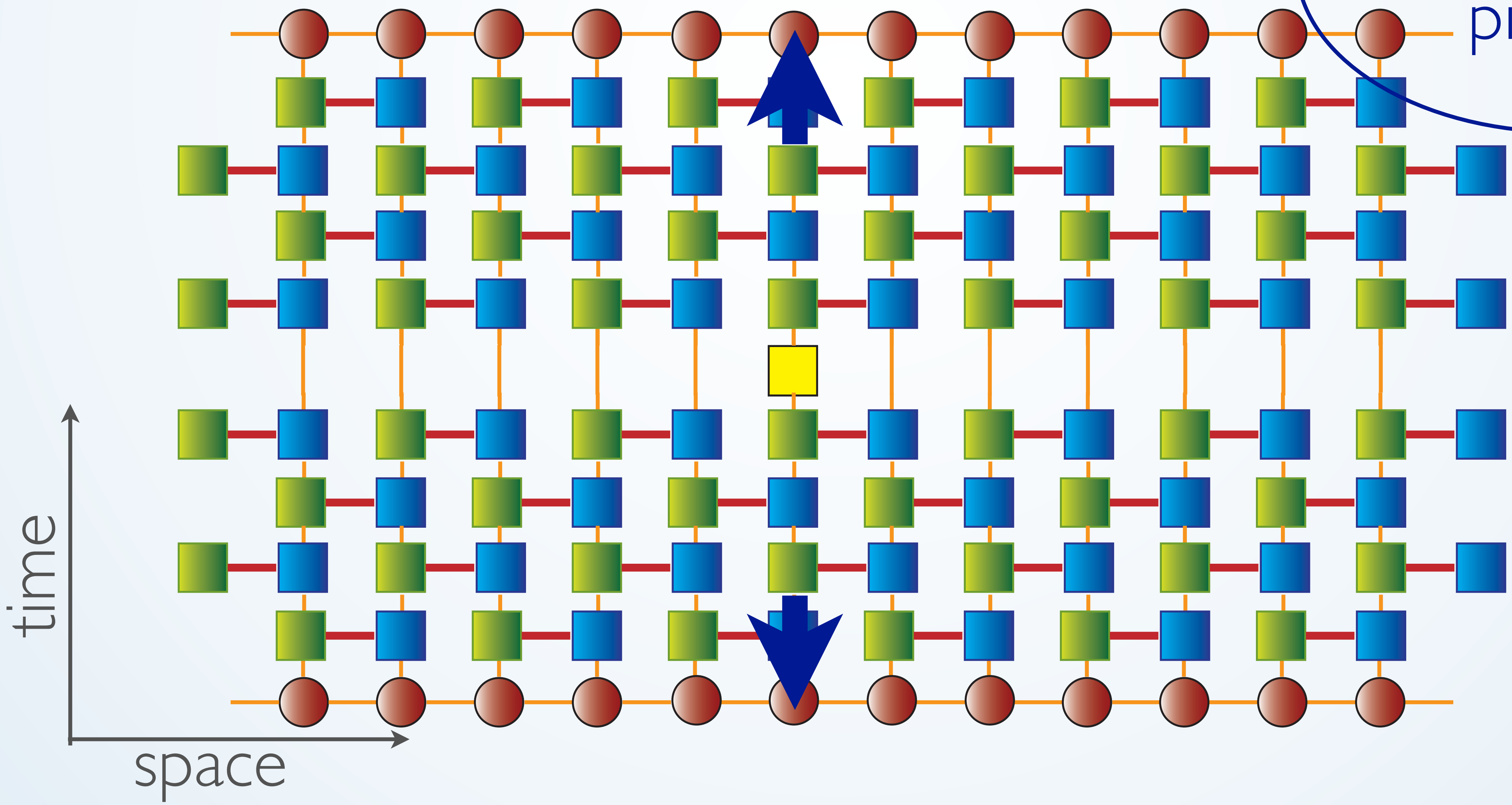


OBSERVABLE AS TN

different approximate contraction strategies

evolved operator as MPO

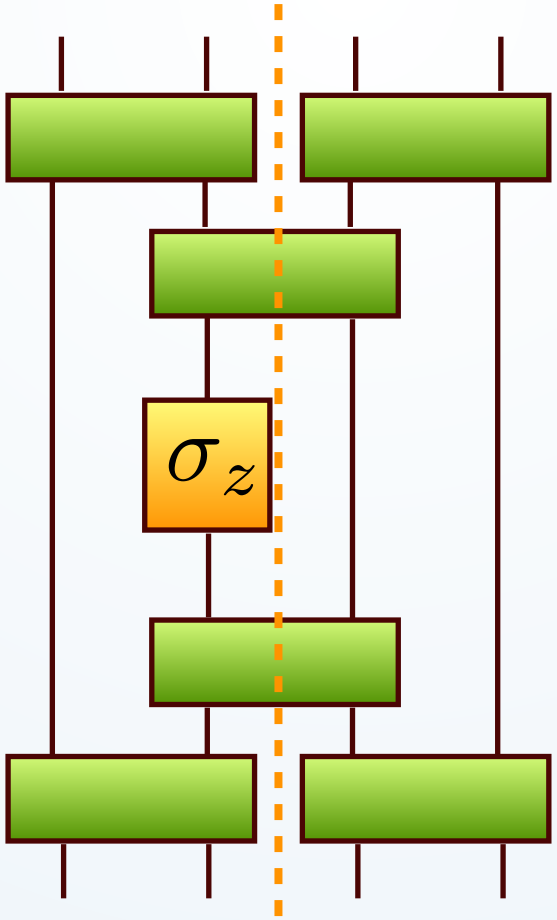
Heisenberg picture



EVOLVING OPERATORS

Heisenberg picture DMRG

$$\frac{dO}{dt} = i[H, O] \quad \rightarrow \quad O(t) = e^{iHt} O(0) e^{-iHt}$$

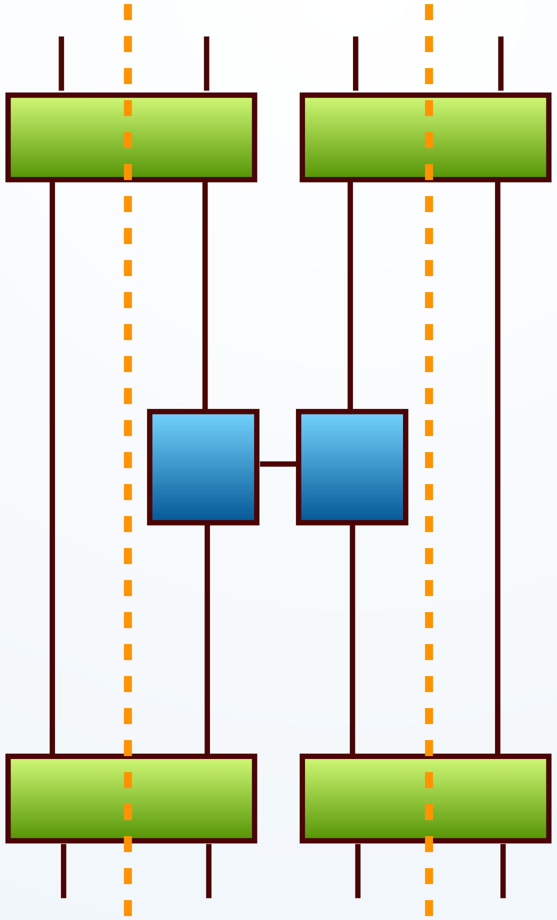


truncation as in TEBD

EVOLVING OPERATORS

Heisenberg picture DMRG

$$\frac{dO}{dt} = i[H, O] \quad \rightarrow \quad O(t) = e^{iHt} O(0) e^{-iHt}$$

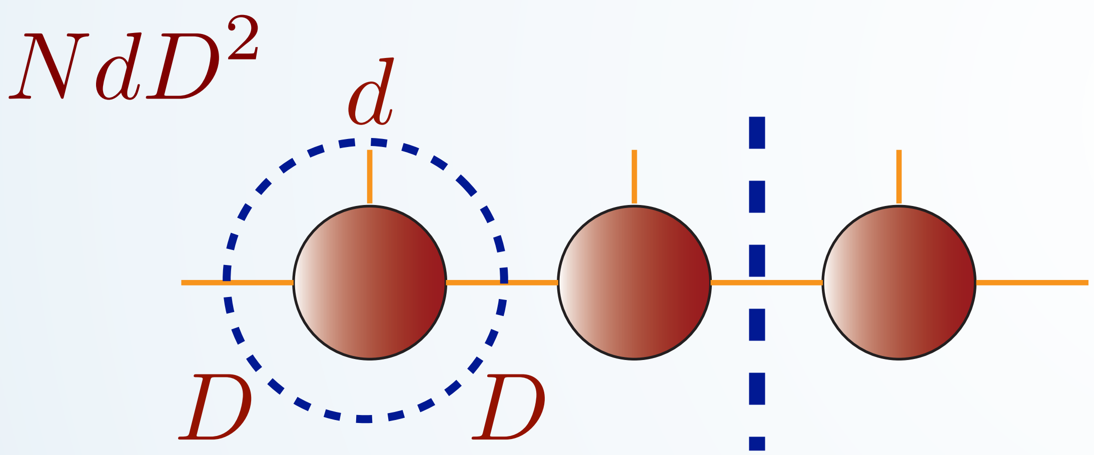


truncation as in TEBD

EVOLVING OPERATORS

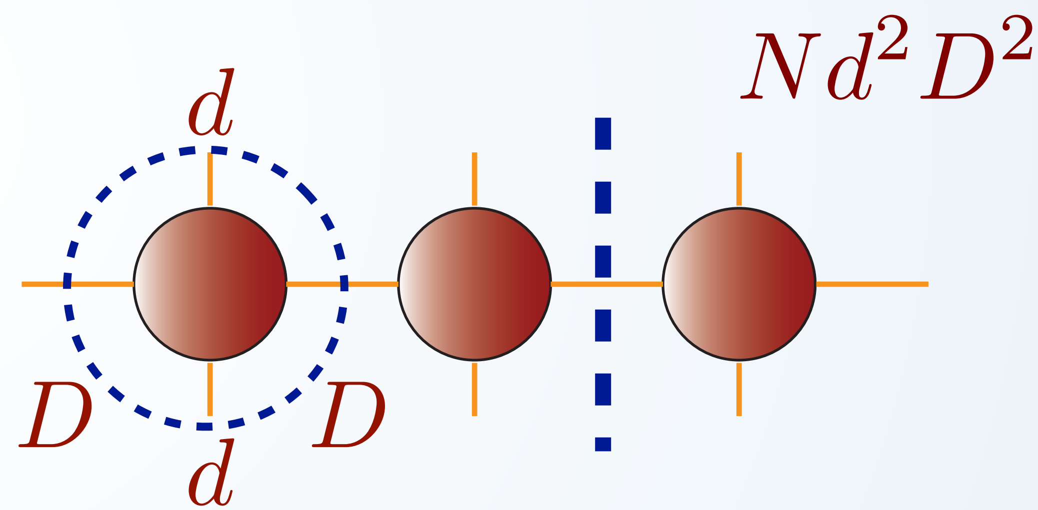
Bond dimension determines number of parameters

MPS



vs

MPO



Schmidt rank → entanglement

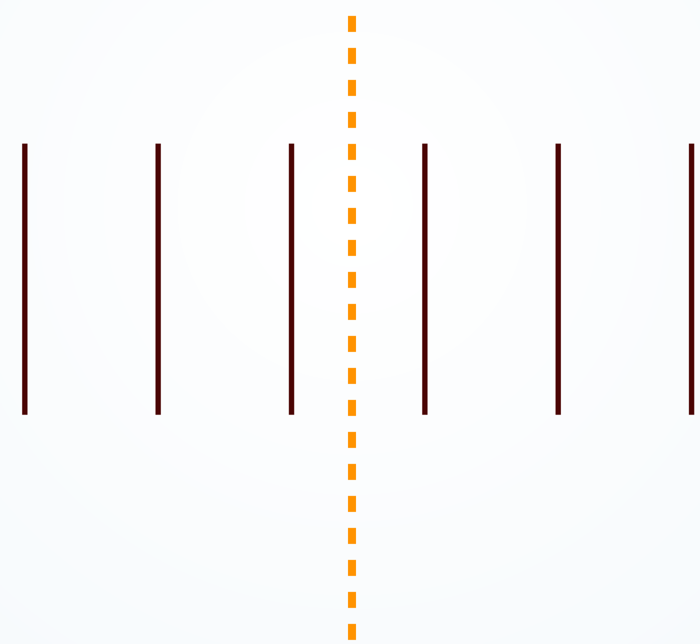
Schmidt rank in operator space → operator space entanglement entropy

EVOLVING OPERATORS

OSSE is not entanglement

example: identity

$$\rho = \frac{1}{d^N}\mathbb{1}^{\otimes N}$$



$$\rho_{N/2} = \frac{1}{d^{N/2}}\mathbb{1}^{\otimes N/2}$$

$$S(\rho_{N/2}) = \frac{N}{2}\log d$$

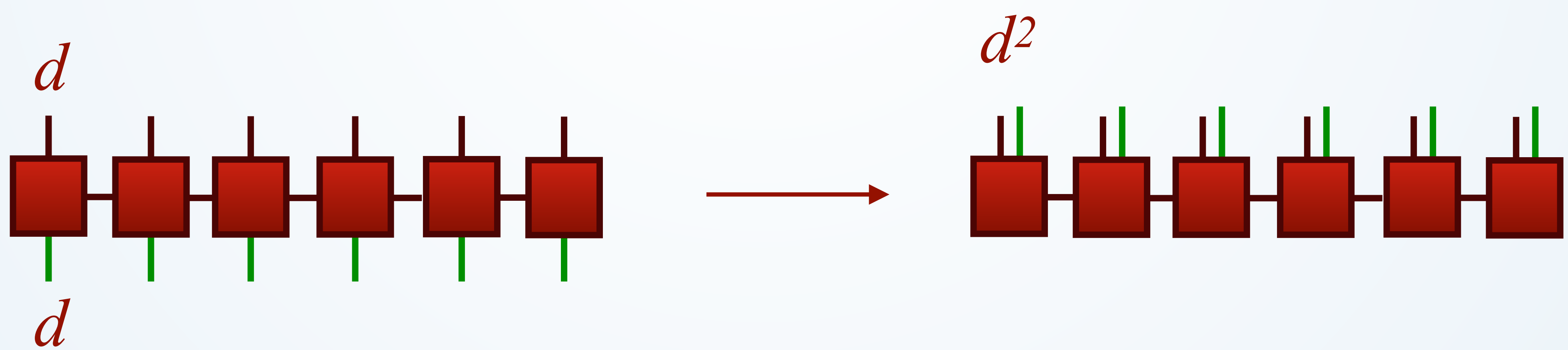
MPO with bond dimension D=1

EVOLVING OPERATORS

vectorization

in practice: map MPO to MPS

$$|i\rangle\langle j| \longrightarrow |i\ j\rangle$$



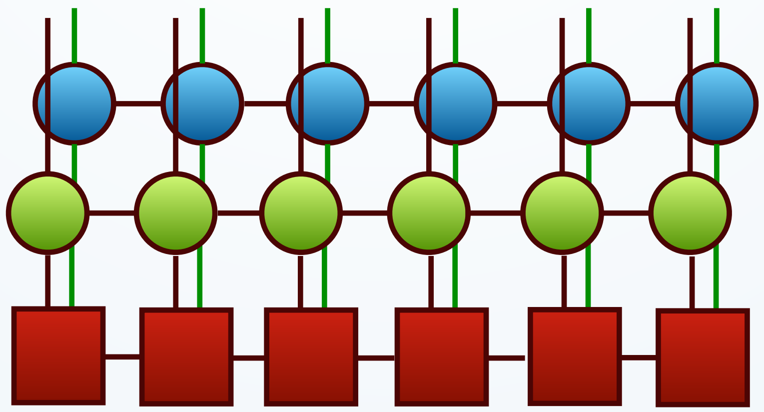
MPS with physical dimension d^2

EVOLVING OPERATORS

vectorization

$$\frac{dO}{dt} = i[H, O] \quad \rightarrow \quad \frac{d|O\rangle}{dt} = i(H \otimes \mathbb{I} - \mathbb{I} \otimes H^T)|O\rangle$$

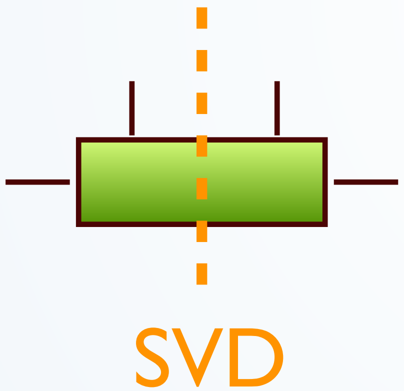
$$|O(t)\rangle = e^{iHt} \otimes e^{-iH^T t}|O(0)\rangle$$



EVOLVING OPERATORS

vectorization

truncation criterion: minimize Euclidean distance



$$\min \| |\Psi\rangle - |\Psi_D\rangle \|^2$$

$$\| |\Psi\rangle - |\Phi\rangle \|^2 < \varepsilon \quad \Rightarrow \quad |\langle\Psi|O|\Psi\rangle - \langle\Phi|O|\Phi\rangle| < 2\varepsilon \|O\|_{\mathrm{op}}$$

useful for states: bound errors in observables

EVOLVING OPERATORS

vectorization

what is this distance for vectorized operators?

$$O = \sum_{ij} O_{ij} |i\rangle\langle j| \longrightarrow |O\rangle = \sum_{ij} O_{ij} |i\, j\rangle$$

$$\| |O\rangle \|^2 = \langle O | O \rangle = \sum_{ij} O^*_{ij} O_{ij} = \sum_{ij} O^\dagger_{ji} O_{ij} = \mathrm{tr}(O^\dagger O)$$

$$= \|O\|_F^2$$

Frobenius
Hilbert-Schmidt

the relevant norm will depend on whether we approximate an operator or a state (RDM)

EVOLVING OPERATORS

vectorization

several operator norms relevant

$$\|A\|_p := \left[\sum_i \sigma_i(A)^p\right]^{1/p}$$ Schatten norms

trace norm $\|A\|_1 = \mathrm{tr}\sqrt{A^\dagger A}$ bound observable error in RDM

Frobenius norm $\|A\|_2 = \sqrt{\mathrm{tr}(A^\dagger A)}$ easiest to compute in MPO

operator norm $\|A\|_\infty = \|A\|_{\mathrm{op}}$ efficient to compute, but not to optimize

the relevant norm will depend on whether we approximate an operator or a state (RDM)

EVOLVING OPERATORS

vectorization

trace norm $\|A\|_1 = \mathrm{tr}\sqrt{A^\dagger A}$ bound observable error in RDM

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operator norm $\|A\|_\infty = \|A\|_{\mathrm{op}}$ efficient to compute, but not to optimize

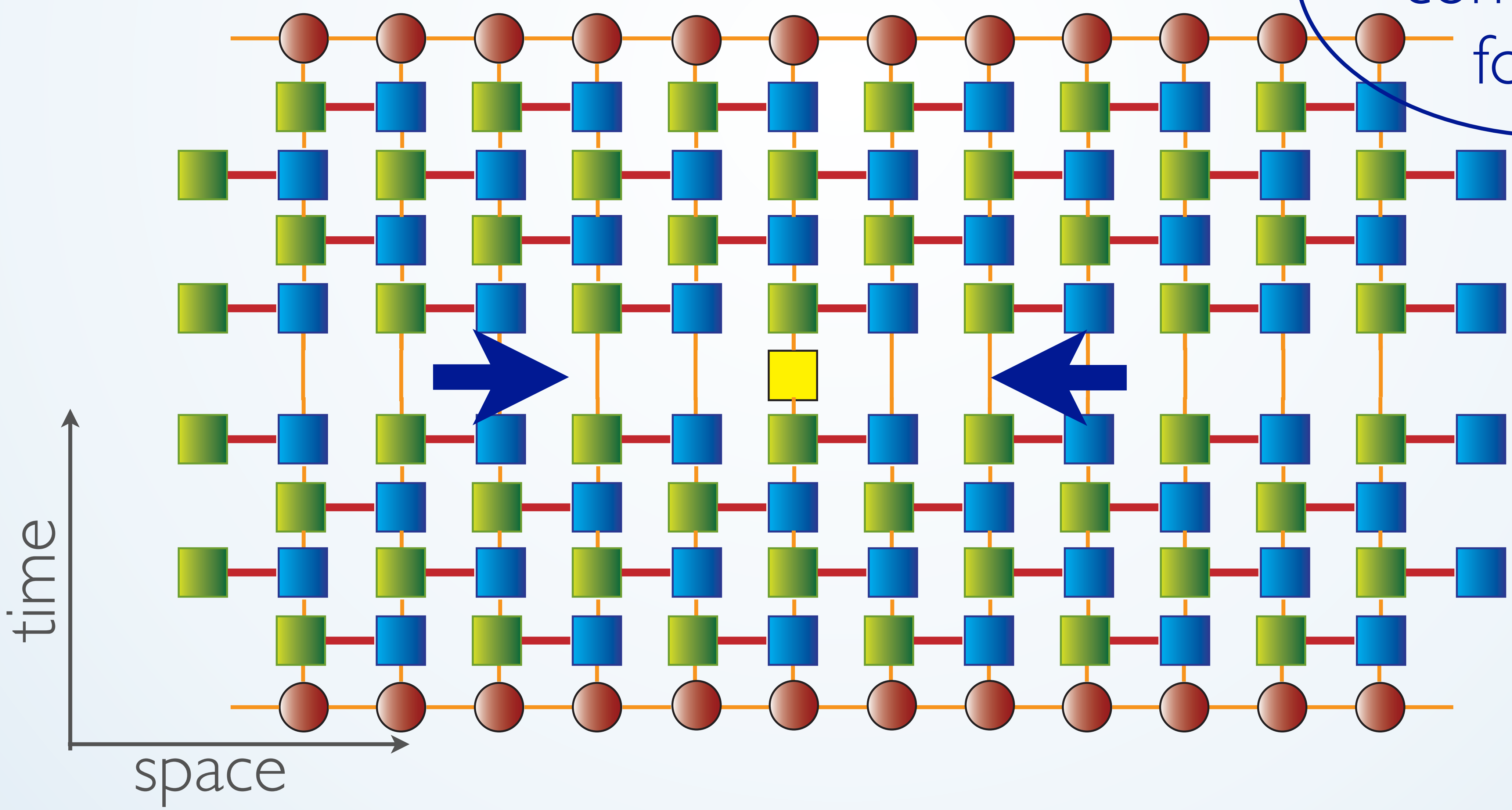
$$\frac{1}{\sqrt{\dim\mathcal{H}}}\|A\|_1 \leq \|A\|_2 \leq \sqrt{\dim\mathcal{H}}\|A\|_1$$

the relevant norm will depend on whether we approximate an operator or a state (RDM)

OBSERVABLE AS TN

different approximate contraction strategies

transverse contraction, folding



FINITE TEMPERATURE

using these tricks for
thermal equilibrium

THERMAL STATES

Gibbs ensemble as imaginary time evolution

$$\rho_\beta = \frac{e^{-\beta H}}{\mathrm{tr}(e^{-\beta H})}$$

goal: approximate as MPO

efficient!

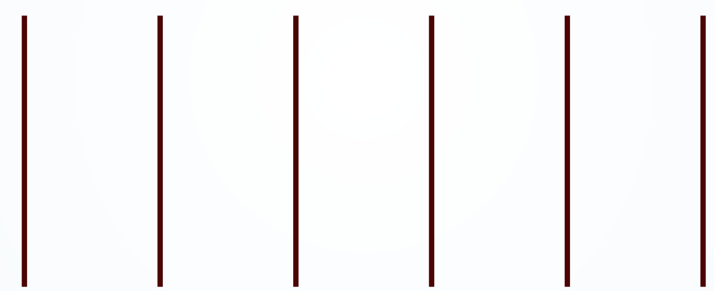
Hastings PRB 2006
Molnar et al PRB 2015

use Suzuki-Trotter expansion for exponential

$$e^{-\beta H} = e^{-\beta H}\mathbb{I} = \left(e^{-\frac{\beta}{M}H}\right)^M \mathbb{I}$$

THERMAL STATES

purification natural

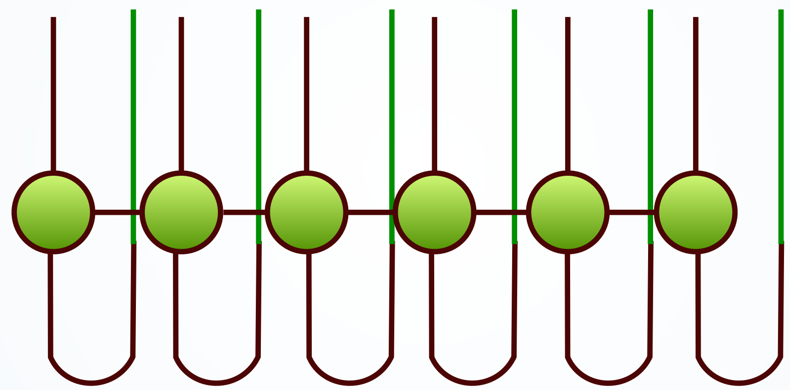


vectorize

$$e^{-\beta H} = e^{-\beta H}\mathbb{I} = \left(e^{-\frac{\beta}{M}H}\right)^{M}\mathbb{I}$$

THERMAL STATES

purification natural



vectorize

$$e^{-\beta H} = e^{-\beta H}\mathbb{I} = \left(e^{-\frac{\beta}{M}H}\right)^{M}\mathbb{I}$$

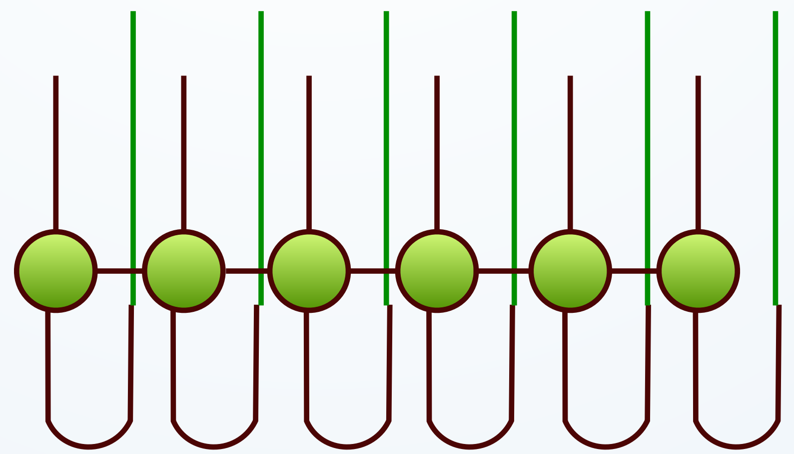
THERMAL STATES

purification ≡ thermofield double state

$$|\Psi_\beta\rangle = \sum_n e^{-\beta E_n/2} \underbrace{|E_n\rangle_S}_{\text{system}} \underbrace{|E_n\rangle_{S'}}_{\text{copy}}$$

$$\rho(\beta) \propto \mathrm{tr}_{S'}\left(|\Psi_\beta\rangle\langle\Psi_\beta|\right)$$

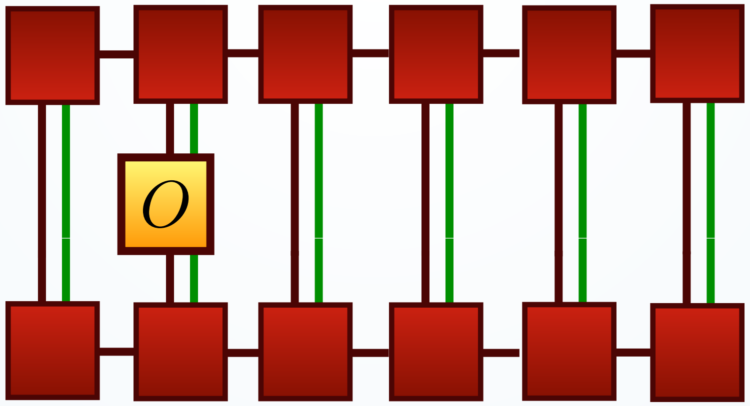
$$= e^{-\beta H_S/2} \otimes \mathbb{I}_{S'} \underbrace{\sum_n |E_n\rangle_S |E_n\rangle_{S'}}_{\text{maximally entangled state}}$$



THERMAL STATES

expectation values

$$O(\beta) = \mathrm{tr}\left(O\rho_\beta\right) = \frac{\langle\Psi_\beta|O_S|\Psi_\beta\rangle}{\langle\Psi_\beta|\Psi_\beta\rangle}$$



combining real time evolution can compute thermal response functions

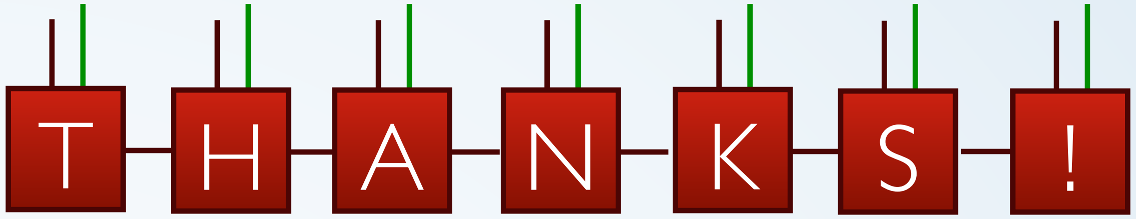
Barthel, NJP 2013

alternative method: METTS

White, PRL 2009

Binder, Barthel, PRB 2015

NOTES: TUTORIAL:



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MPQ Max Planck Institut
of Quantum Optics
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MCQST

ICCUB 27.9.2021