# TENSOR NETWORKS FOR QUANTUM MANY-BODY SYSTEMS (II)

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NTQC2024

# In this talks…

NOTES:

introducing Tensor Network States

basic numerical algorithms

unguided TUTORIAL:

# algorithms

# BASIC ALGORITHMS

two main types

**variational optimization**

used for ground states

**applying a (local) operator**

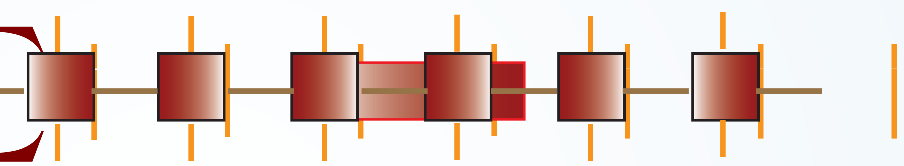
basis of most common evolution algorithms

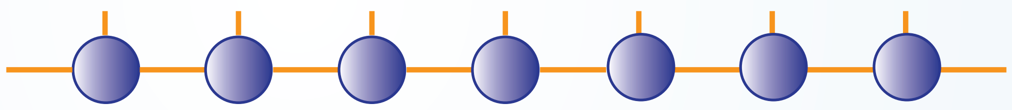
# variational optimisation

# BASIC ALGORITHMS

variational minimization of energy

*local*
Hamiltonian

$H = \sum_i$ 

$|E_0\rangle \simeq$ 

Variational principle

$$\min_{\{A\}} \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$$

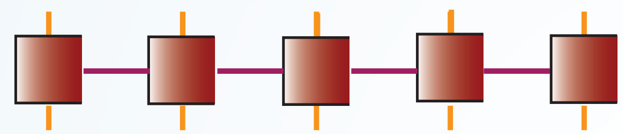
White, PRL 1992

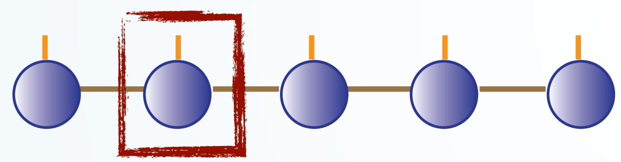
Verstraete, Porras, Cirac, PRL 2004

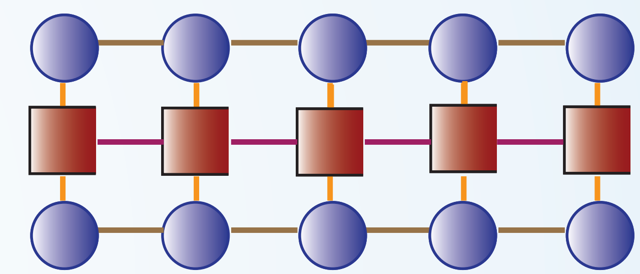
Schollwöck, RMP 2005, Ann. Phys. 2011

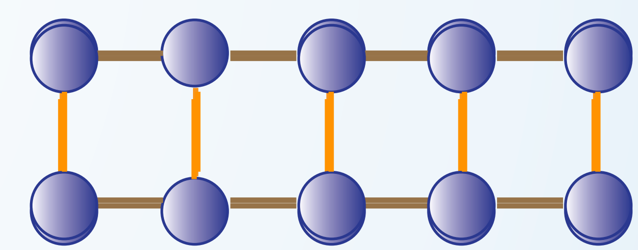
# BASIC ALGORITHMS

variational minimization of energy

$H =$ 

$|E_0\rangle \simeq$ 

$\langle\Psi|H|\Psi\rangle$ / $H_{\text{eff}}$ 

$\langle\Psi|\Psi\rangle$ / $N_{\text{eff}}$ 

Variational principle

$$\min_{\{A\}} \frac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} \longrightarrow \min_{A} \frac{\bar{A} H_{\text{eff}} A}{\bar{A} N_{\text{eff}} A}$$

sweep back and forth
over tensors

White, PRL 1992
Verstraete, Porras, Cirac, PRL 2004
Schollwöck, RMP 2005, Ann. Phys. 2011

# BASIC ALGORITHMS

variational minimization of energy

$$\min_A \frac{\bar{A} H_{\text{eff}} A}{\bar{A} N_{\text{eff}} A} \longrightarrow H_{\text{eff}} A = \lambda_{\min} N_{\text{eff}} A$$

canonical form
tensor structure
sparse matrices

$\Big\}\ O(D^3)$

**DMRG**

guaranteed convergence

PBC: higher cost $\mathbf{O}(D^5)$

also excitations

symmetries can be integrated

PEPS $\mathbf{O}(D^{10})$

# an example

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

$N = 20$ $2^N = 1048576$ $D_{\max} = 2^{N/2} = 1024$

Matlab → eigs $E_{\mathrm{GS}}/N = -1.25538985581190$

$t$=38 s

MPS

bin — -bash ▸ Emacs-x86_64-10_9 — 114×38

```
Initialized arguments: L=20, J=1, g=1, h=0, outfile=testIsing_L20_J1g1.txt, app=0, D=10
Constructed default Contractor
Initialized Contractor
Initialized random state, norm 1-1.110223025e-16i
Created the Hamiltonian
Constructed the hamil MPO
Initial value, with initial state
1.531982113+1.335737077e-16i
Starting findGroundState with initial value E=1.531982113
0       10      0.07659910564
1       10      -1.255389855
Ground state found for D=10 with eigenvalue -25.10779711 (Energy per particle=-1.255389855)  time=0.590109
Starting findGroundState with initial value E=-25.10779711
0       20      -1.255389855
Ground state found for D=20 with eigenvalue -25.10779711 (Energy per particle=-1.255389856)  time=0.74278
Starting findGroundState with initial value E=-25.10779711
0       30      -1.255389856
Ground state found for D=30 with eigenvalue -25.10779711 (Energy per particle=-1.255389856)  time=1.43884
Starting findGroundState with initial value E=-25.10779711
0       40      -1.255389856
Ground state found for D=40 with eigenvalue -25.10779711 (Energy per particle=-1.255389856)  time=2.700611
Starting findGroundState with initial value E=-25.10779711
0       50      -1.255389856
Ground state found for D=50 with eigenvalue -25.10779711 (Energy per particle=-1.255389856)  time=4.59483
Starting findGroundState with initial value E=-25.10779711
0       60      -1.255389856
Ground state found for D=60 with eigenvalue -25.10779711 (Energy per particle=-1.255389856)  time=6.448116
Starting findGroundState with initial value E=-25.10779711
0       70      -1.255389856
```

# an example

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

$N=20$ $2^N = 1048576$ $D_{\max} = 2^{N/2} = 1024$

$N=200$ $2^N \sim 10^{60}$ $D_{\max} = 2^{N/2} \sim 10^{30}$

MPS

bin — -bash ▸ Emacs-x86_64-10_9 — 112×31

```
Initialized arguments: L=200, J=1, g=1, h=0, outfile=testIsing_L200_J1g1.txt, app=0, D=10
Constructed default Contractor
Initialized Contractor
Initialized random state, norm 1+8.326672685e-17i
Created the Hamiltonian
Constructed the hamil MPO
Initial value, with initial state
10.37197956+7.21644966e-16i
Starting findGroundState with initial value E=10.37197956
0       10      0.05185989779
1       10      -1.271418419
Ground state found for D=10 with eigenvalue -254.2849239 (Energy per particle=-1.271424619)  time=8.0116
Starting findGroundState with initial value E=-254.2849239
0       20      -1.271424619
Ground state found for D=20 with eigenvalue -254.2851697 (Energy per particle=-1.271425849)  time=16.437139
Starting findGroundState with initial value E=-254.2851697
0       30      -1.271425849
Ground state found for D=30 with eigenvalue -254.2851813 (Energy per particle=-1.271425906)  time=42.901364
Starting findGroundState with initial value E=-254.2851813
0       40      -1.271425906
Ground state found for D=40 with eigenvalue -254.2851816 (Energy per particle=-1.271425908)  time=102.71914
Starting findGroundState with initial value E=-254.2851816
0       50      -1.271425908
Ground state found for D=50 with eigenvalue -254.2851816 (Energy per particle=-1.271425908)  time=197.829282
Starting findGroundState with initial value E=-254.2851816
0       60      -1.271425908
Ground state found for D=60 with eigenvalue -254.2851816 (Energy per particle=-1.271425908)  time=298.47571
Starting findGroundState with initial value E=-254.2851816
0       70      -1.271425908
```

# applying a (local) operator

# BASIC ALGORITHMS

approximate action of local operators

local truncation

TEBD

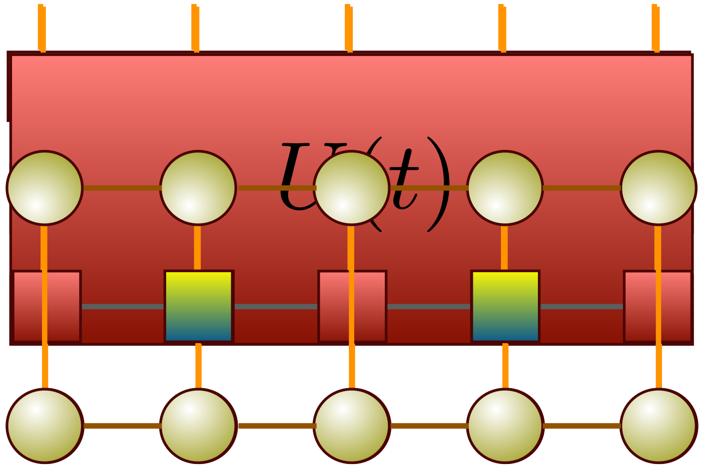
variational truncation

basis of most common evolution algorithms

disclaimer: also other algorithms exist

# basic time evolution algorithms

**time evolved state approximated by MPS**




TEBD, t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

initial MPS

discrete time

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

Suzuki-Trotter expansion

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

truncate bond dimension

iterate

compute observables

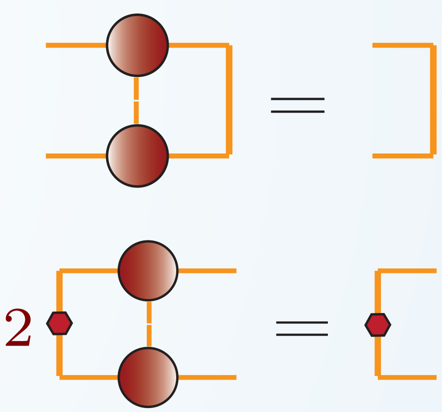
# local truncation: TEBD

photo: Alejandro Piñero Amerio @ Unsplash

# BASIC ALGORITHMS

## local truncation: TEBD

recall canonical form

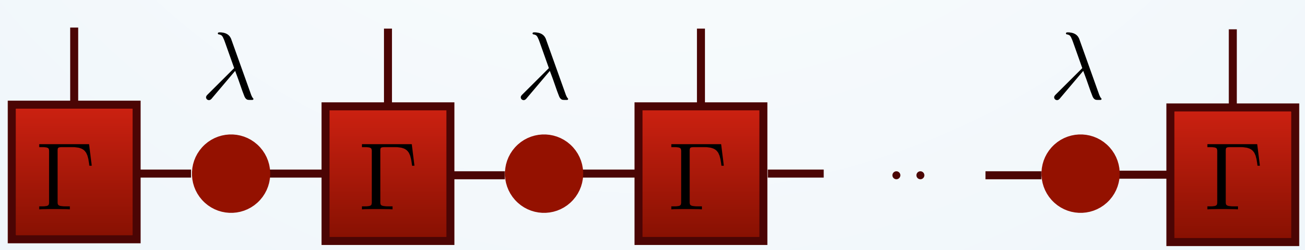


can be made explicit

Schmidt values

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

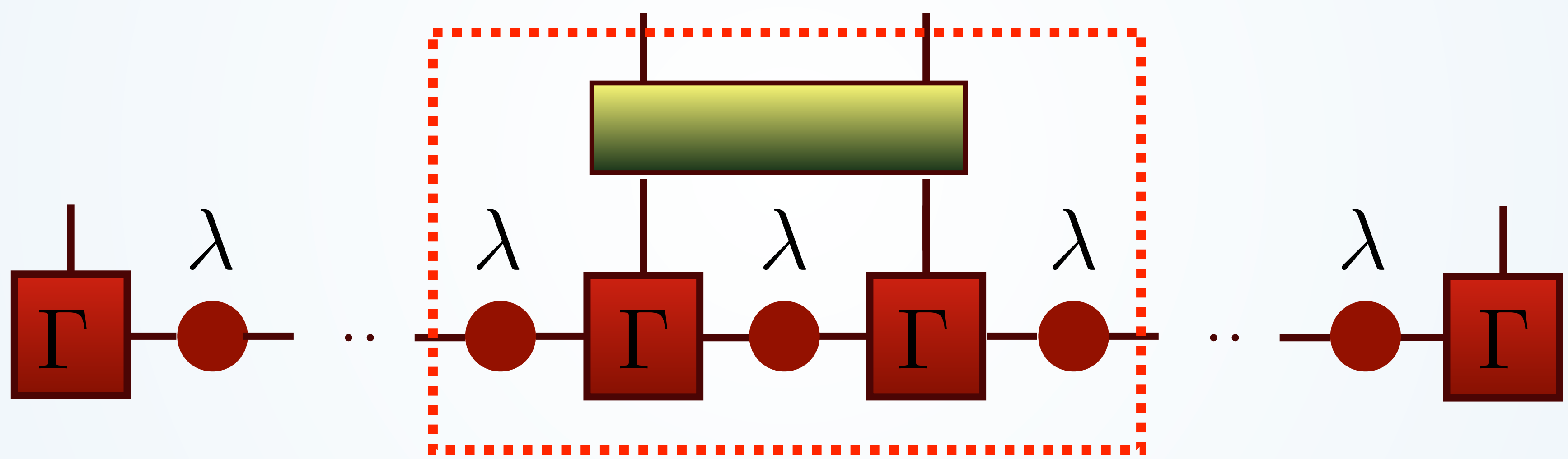
$$A^{[k]} = \Gamma^{[k]} \lambda^{[k]}$$




Vidal, PRL 2003, 2004

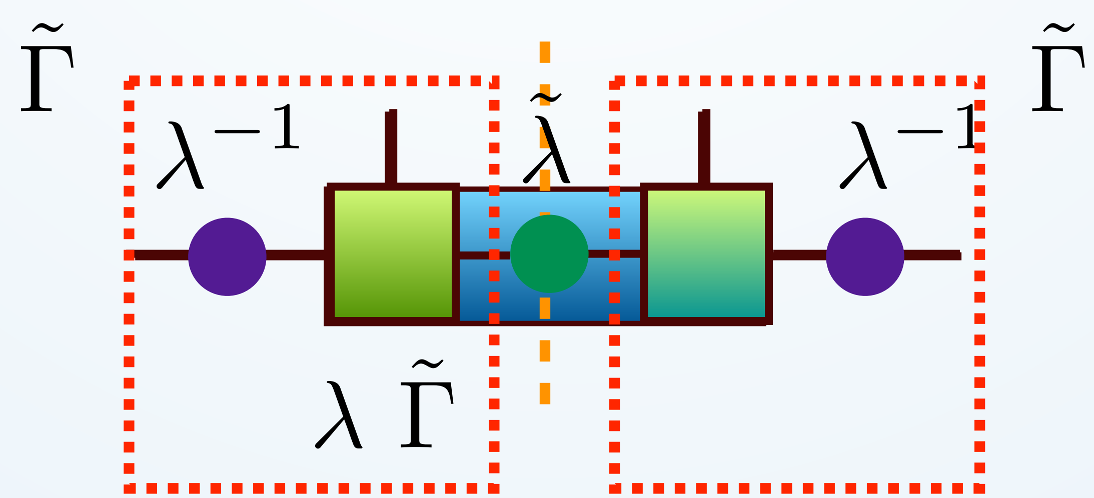
# BASIC ALGORITHMS

## local truncation: TEBD




**unitary gate**
**⇒canonical form preserved**

up to truncation




**also possible in the TD limit**

canonical form lost

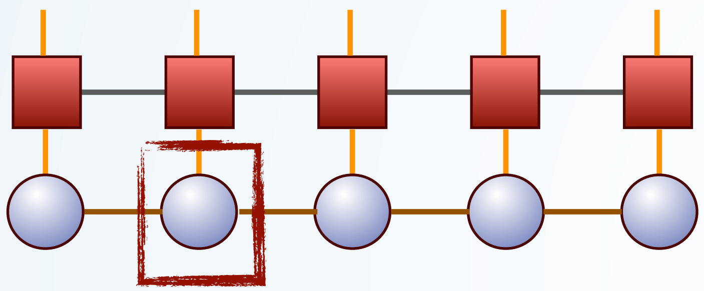
Vidal, PRL 2003, 2004

# global truncation:
# t-MPS, t-DMRG

# BASIC ALGORITHMS

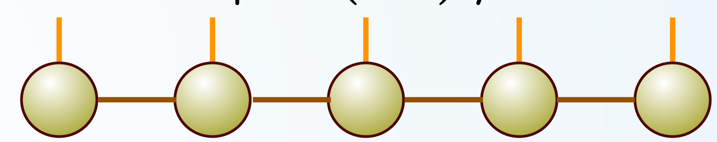
## global truncation

$|\Phi_0\rangle$



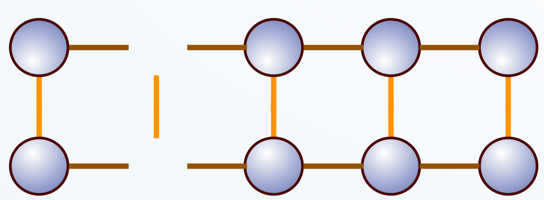
$\approx$

$|\Psi(A)\rangle$

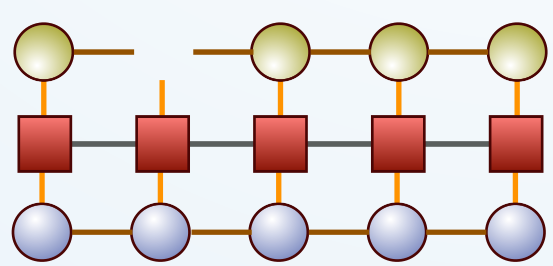


$$\min_{\{A\}} \| |\Psi\rangle - O|\Phi_0\rangle \|^2 \longrightarrow \min_A (\bar{A} N_{\text{eff}} A - \bar{A} M - \bar{M} A + \text{const})$$

$N_{\text{eff}}$



$M$



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

# BASIC ALGORITHMS

imaginary time evolution ⇒ ground state

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

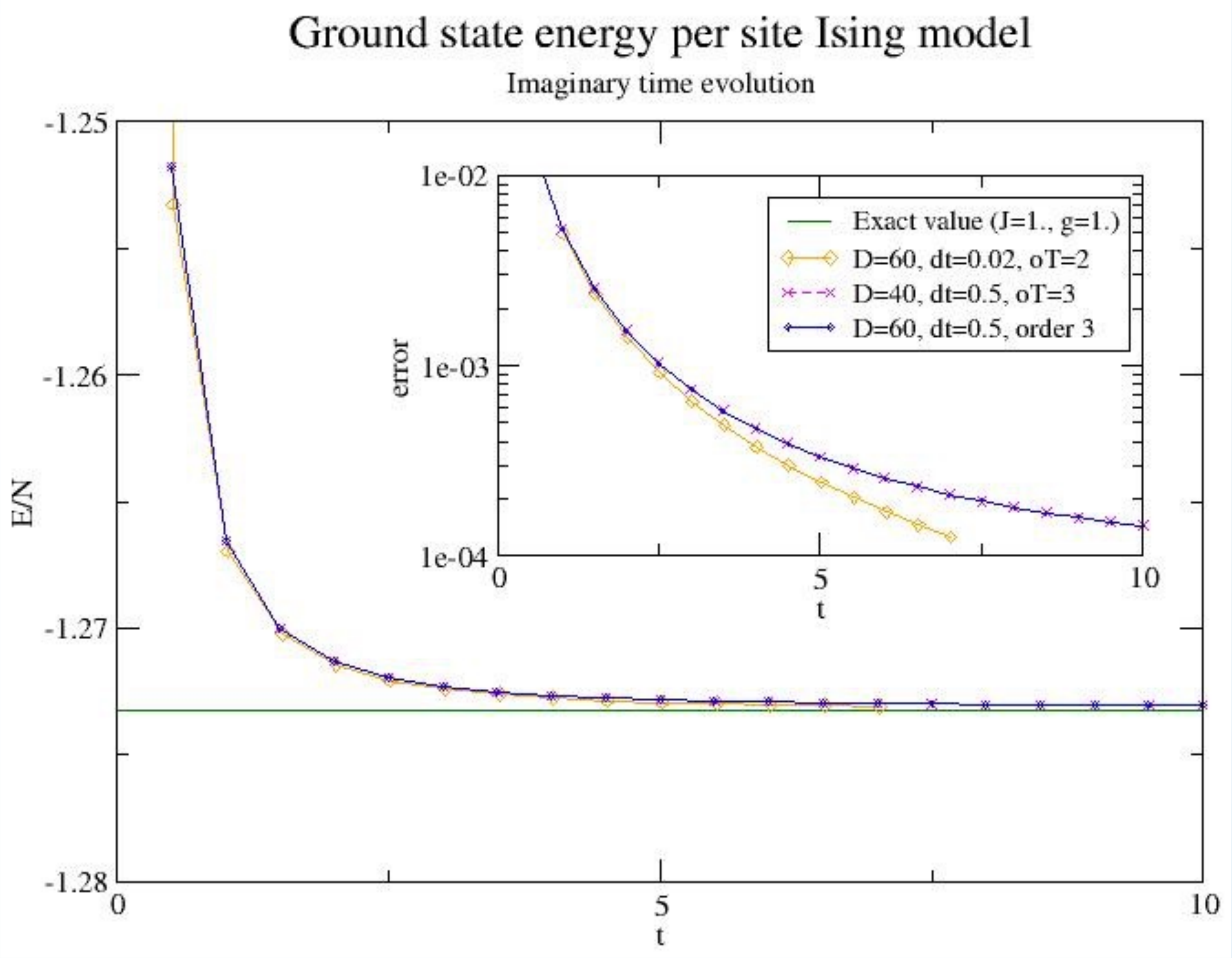
$$|\Phi_0\rangle = \sum c_n |E_n\rangle$$

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

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

# BASIC ALGORITHMS

imaginary time evolution ⇒ ground state



# BASIC ALGORITHMS

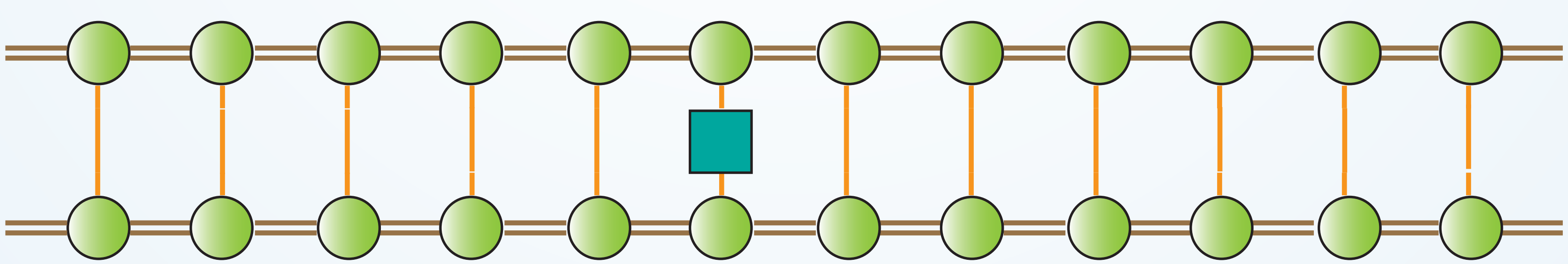
simulate time evolution

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

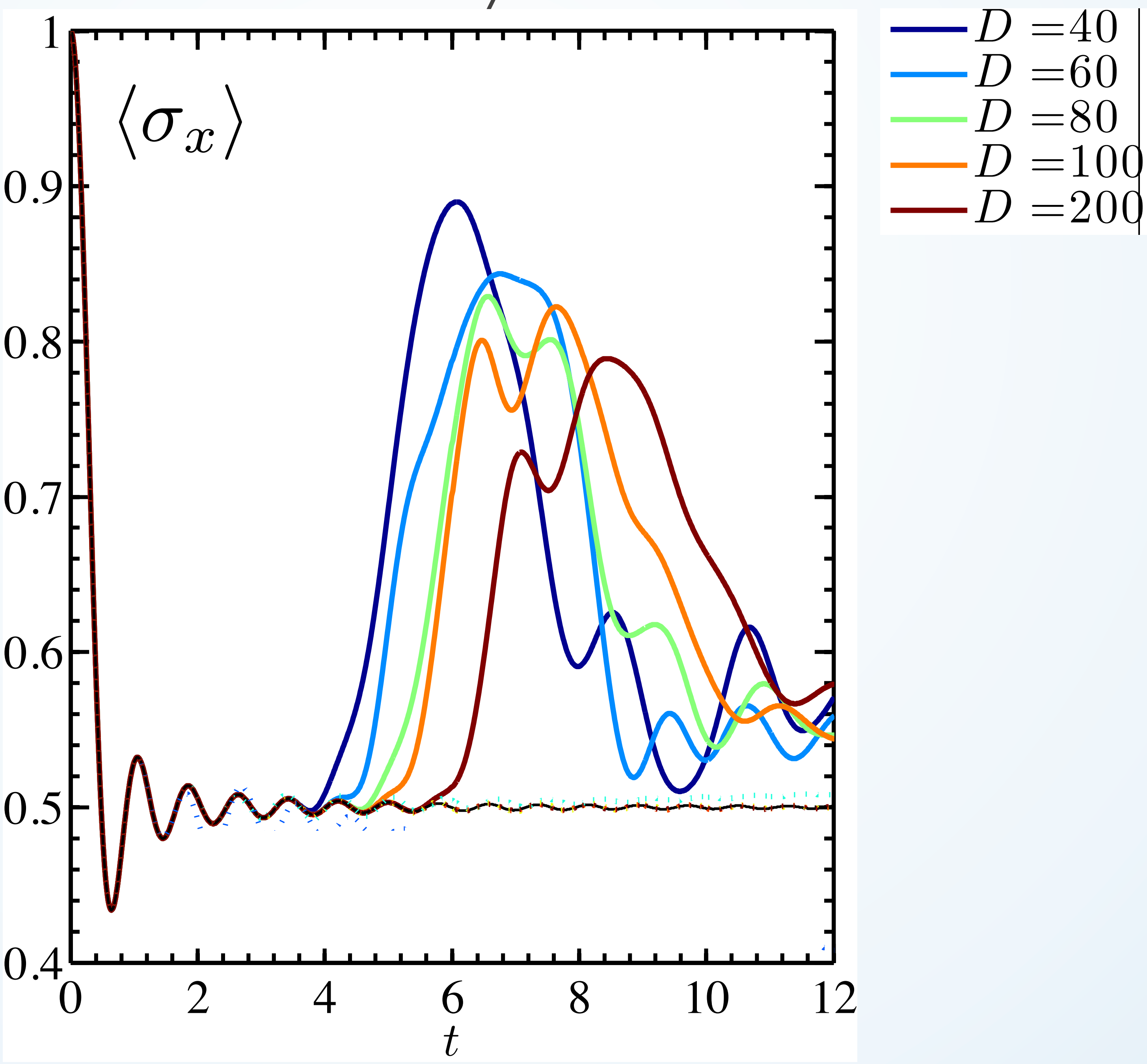


compute
observables

TEBD
t-DMRG

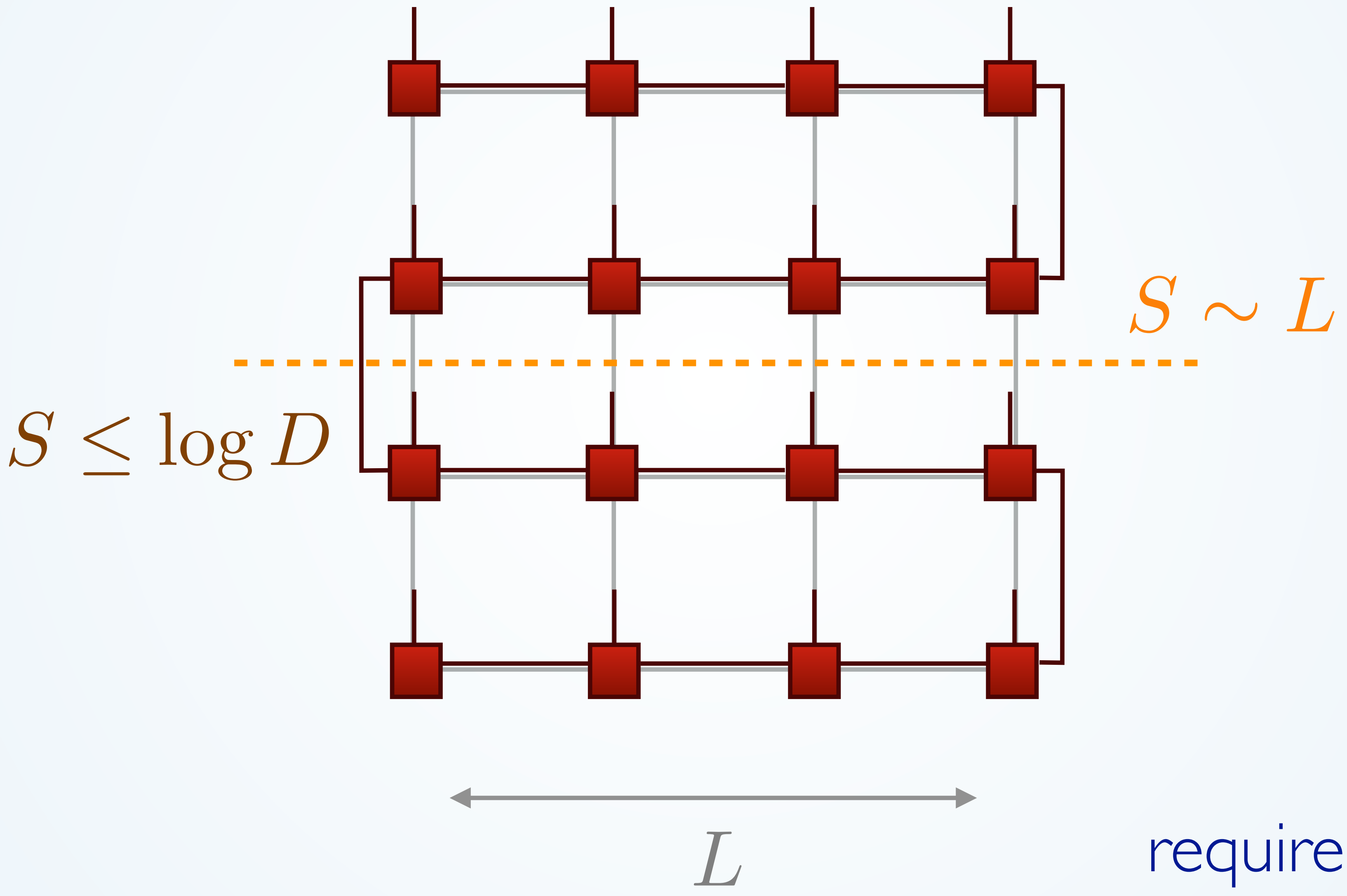
# BASIC ALGORITHMS

real time dynamics



# higher dimensions

MPS complete family

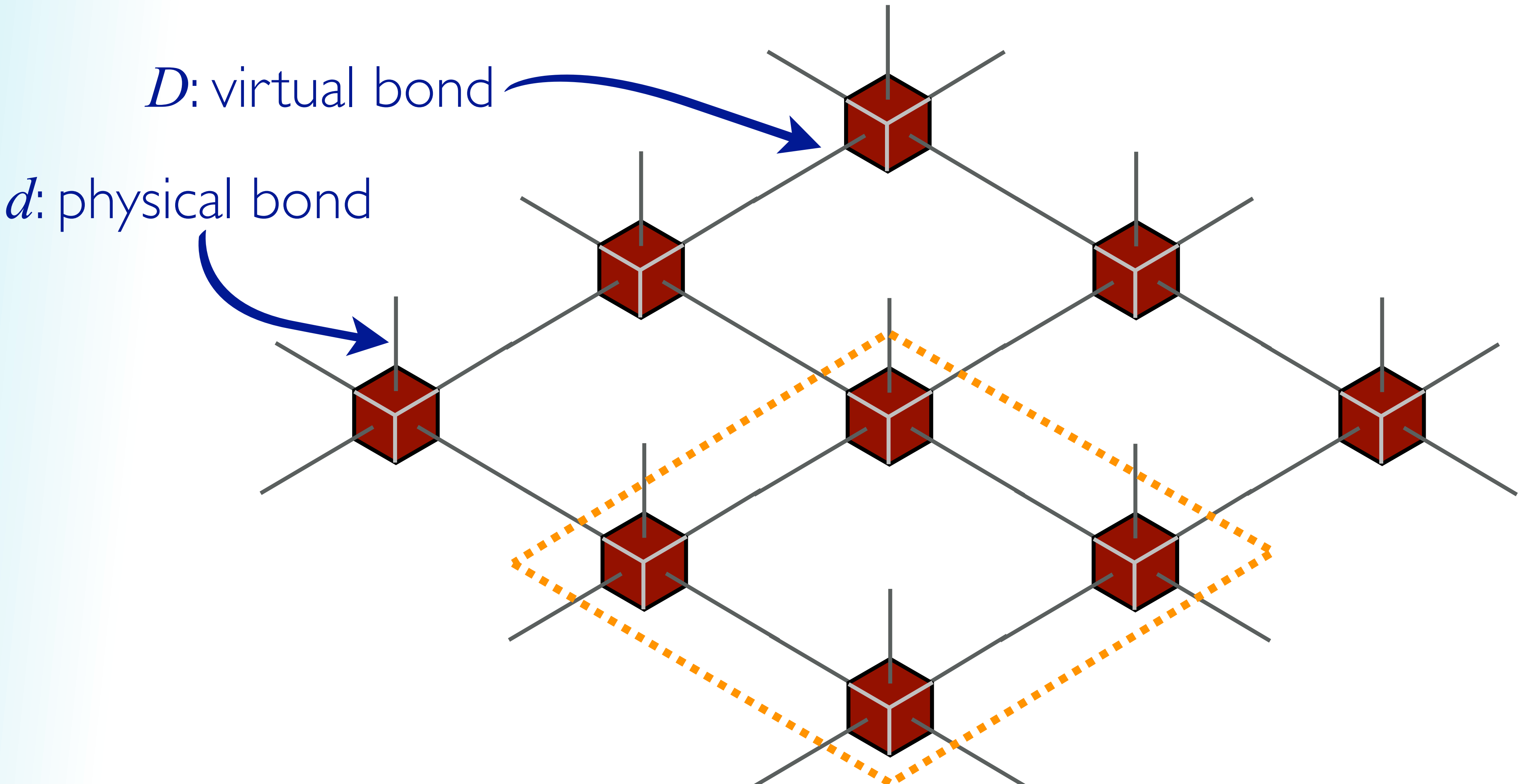



requires exponentially
large bond dimension

# PEPS

natural MPS generalization

Projected Entangled Pairs

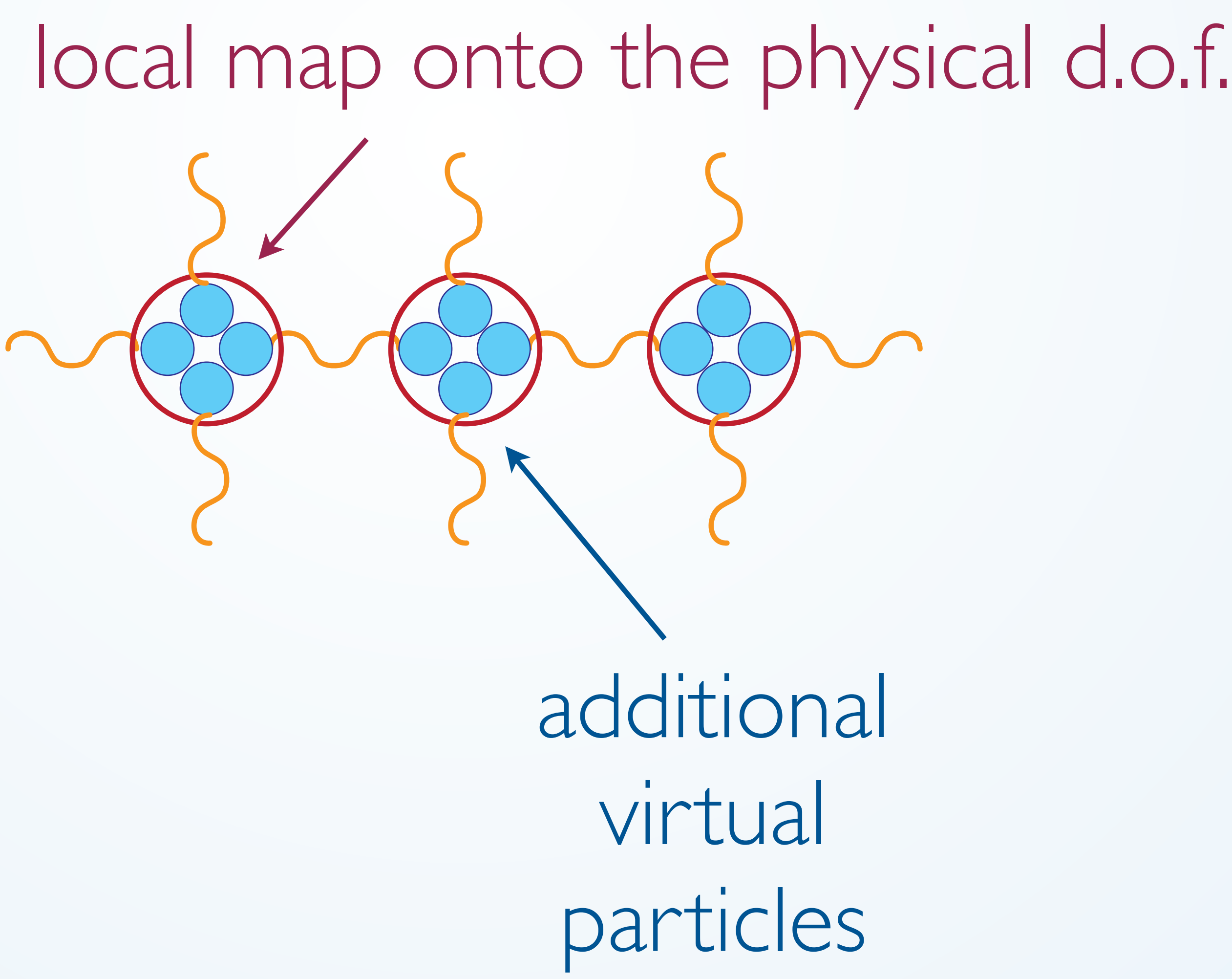



entropy bounded by the number of bonds cut

# PEPS

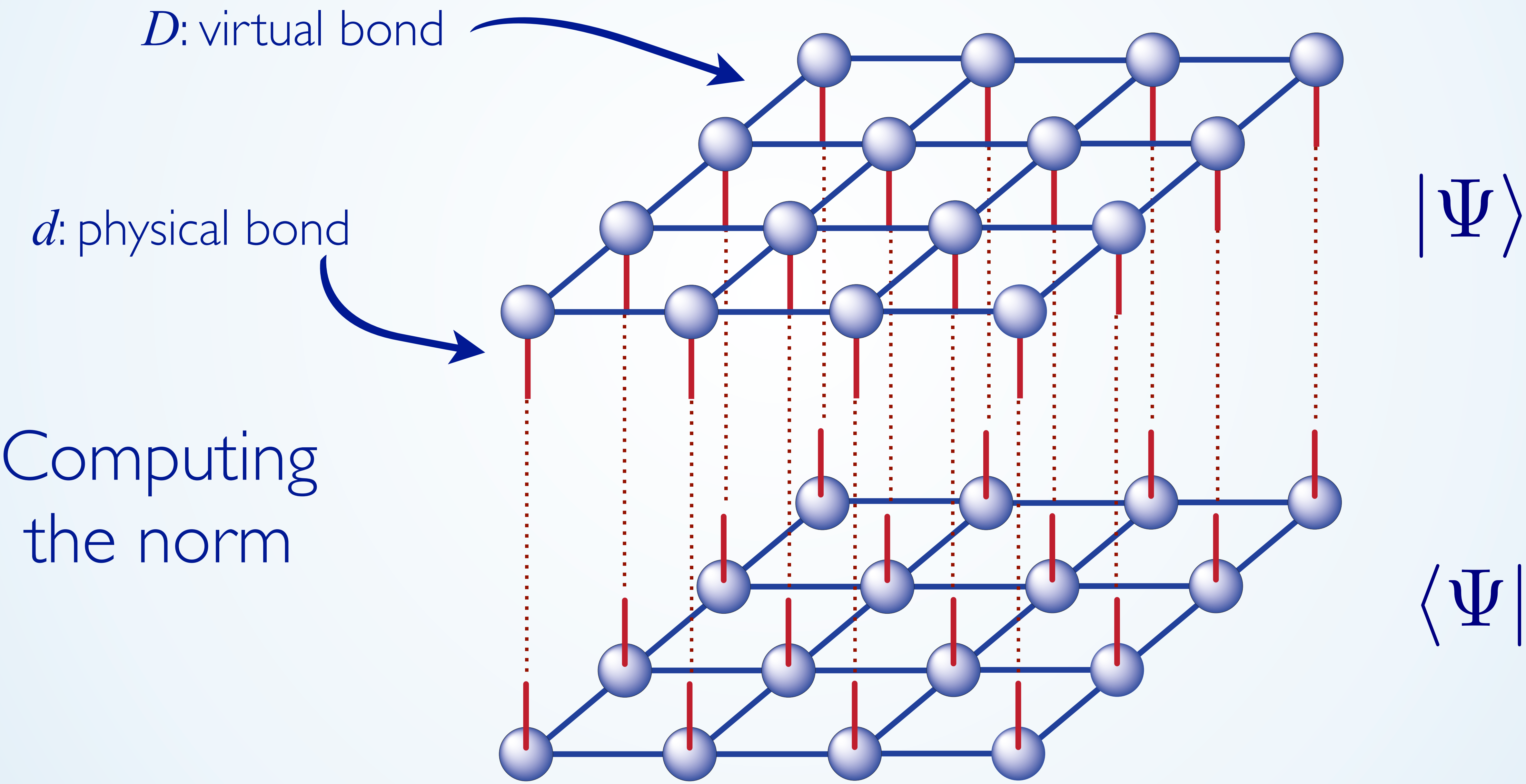
Projected Entangled Pairs States

generalize MPS construction to any lattice



# PEPS

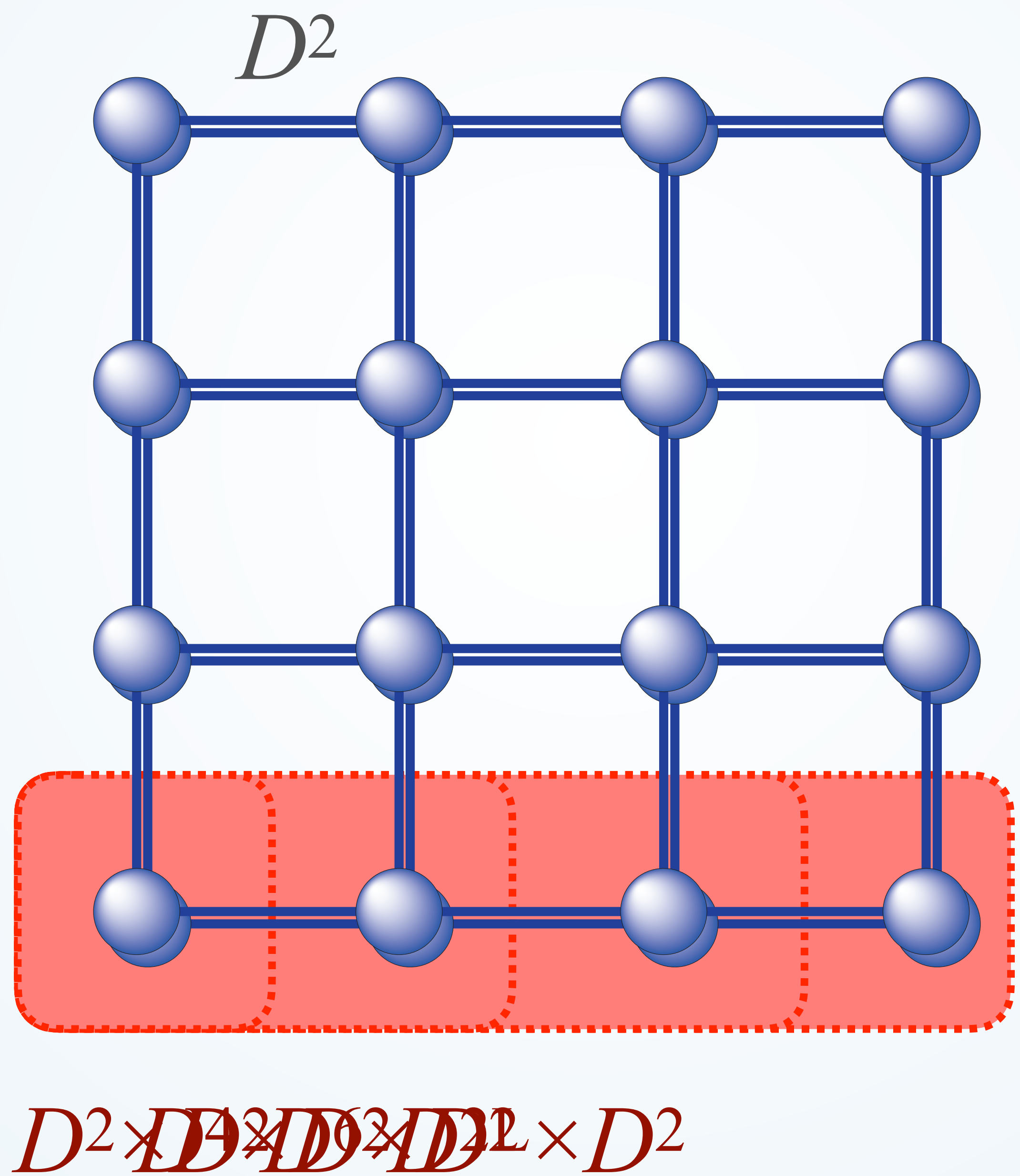
Projected Entangled Pairs States




Computing the norm

# PEPS

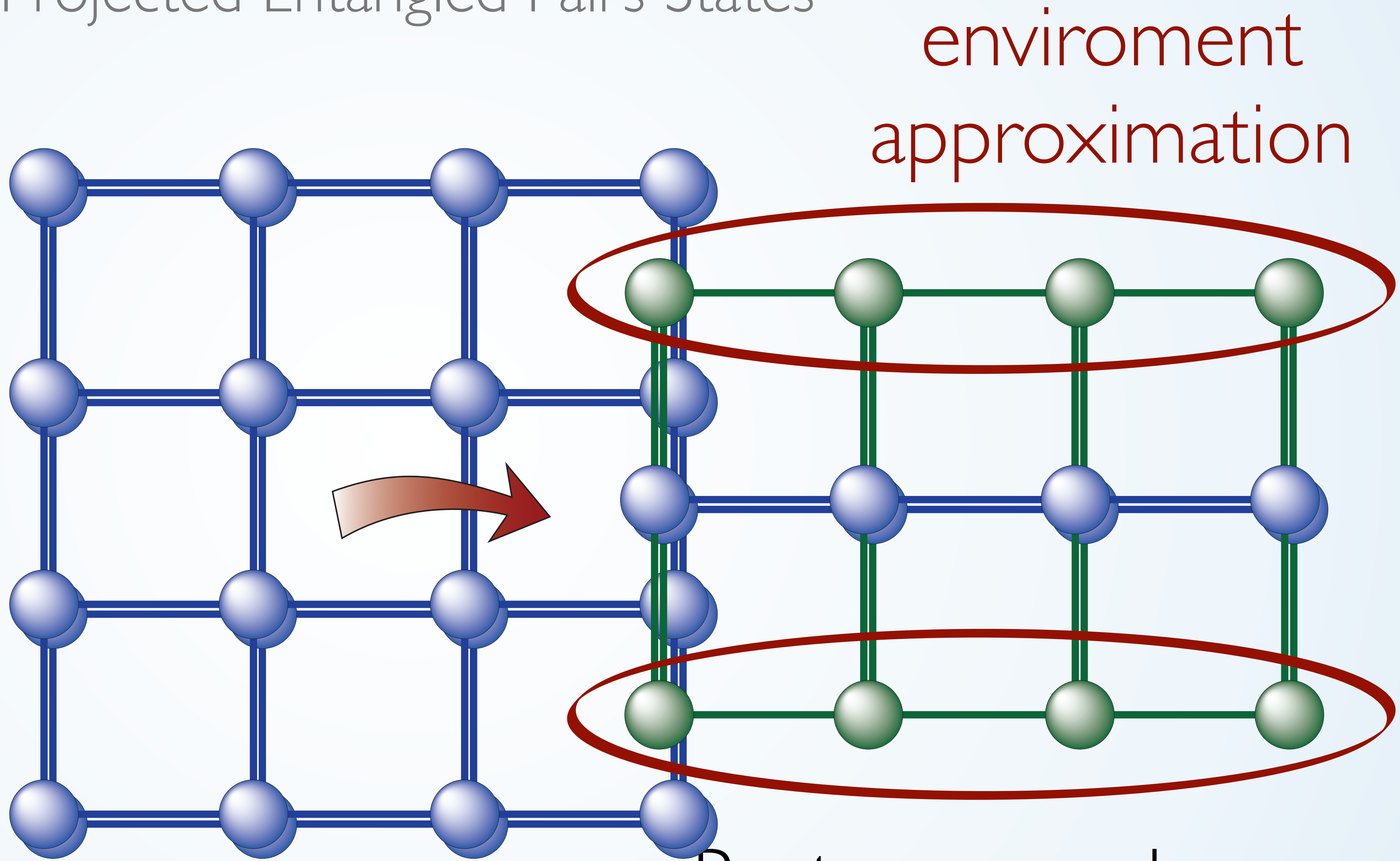
Projected Entangled Pairs States




contracting
#P-complete

# PEPS

Projected Entangled Pairs States



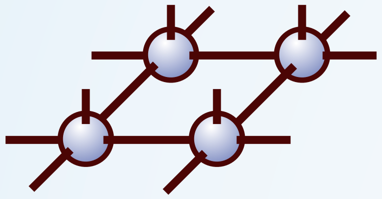

Needed for expectation values and tensor updates

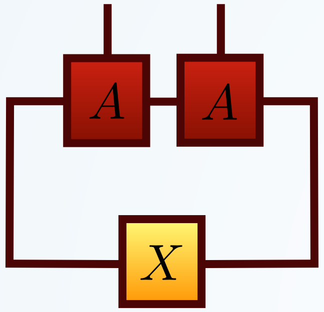
Best we can do: approximate (e.g. via MPO-MPS contractions)

# PEPS

Projected Entangled Pairs States

## local parent Hamiltonian





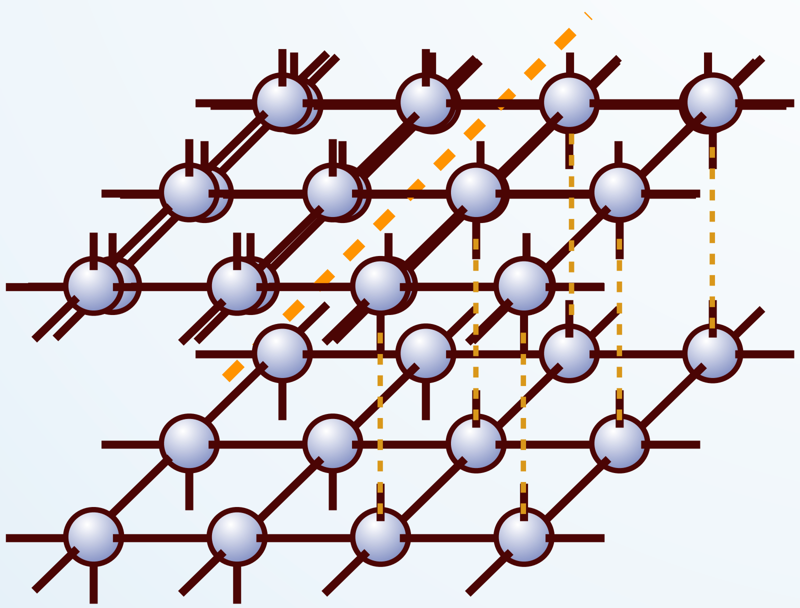

$$H = \sum_{i=1}^{N-1} (1 - \Pi_{S_2})$$

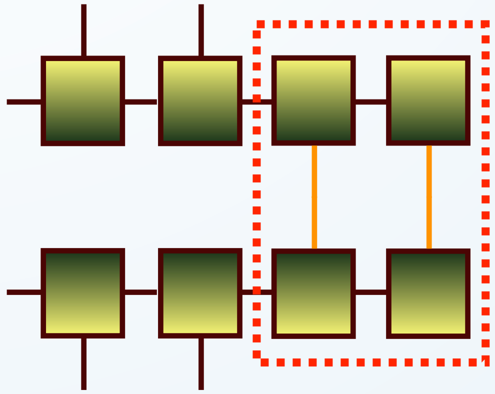
local, frustration-free

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

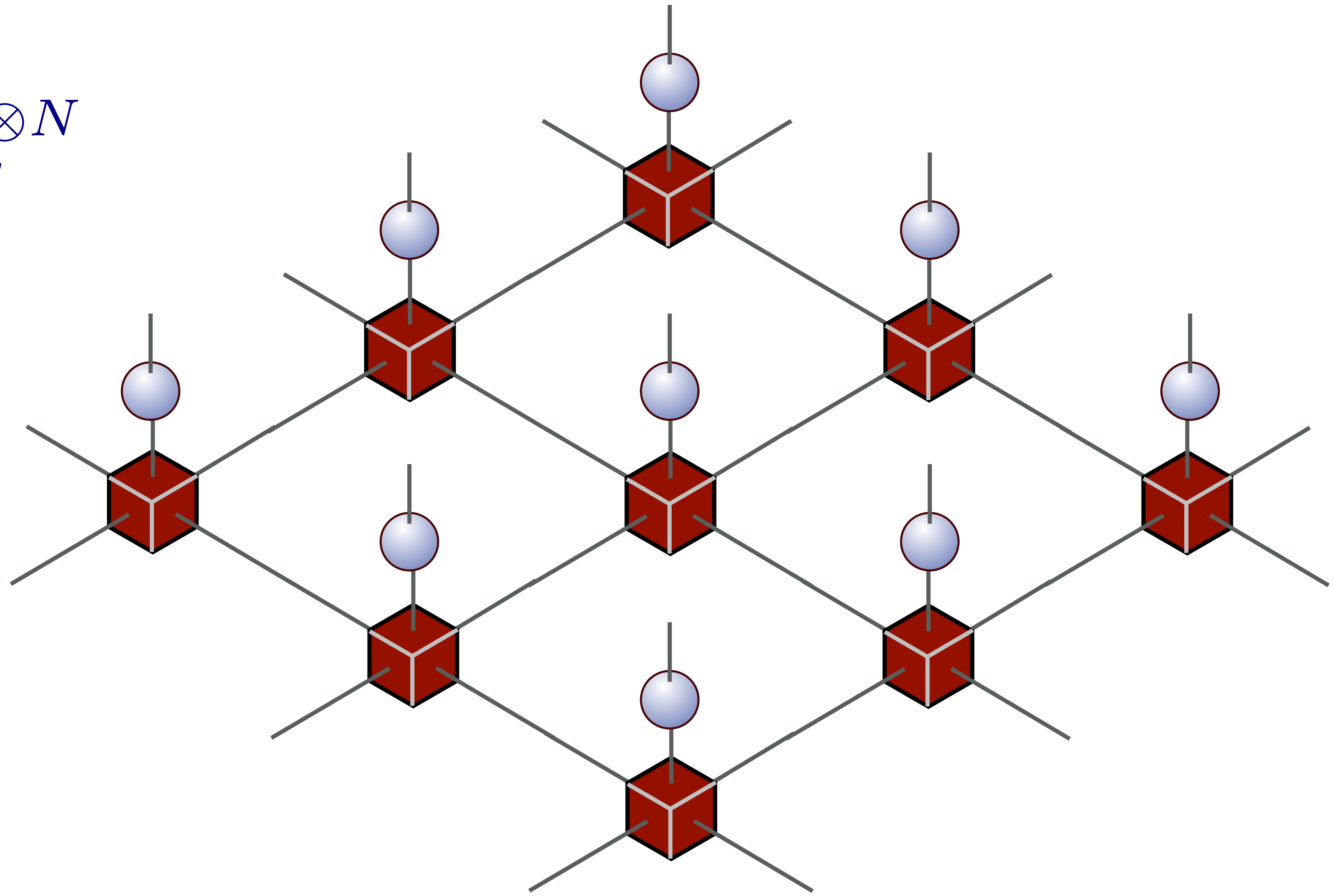
efficient approximation of thermal states

Hastings PRB 2006
Molnar et al PRB 2015

# TNS play well with symmetries

# state invariant under global symmetry

$U_g^{\otimes N}$



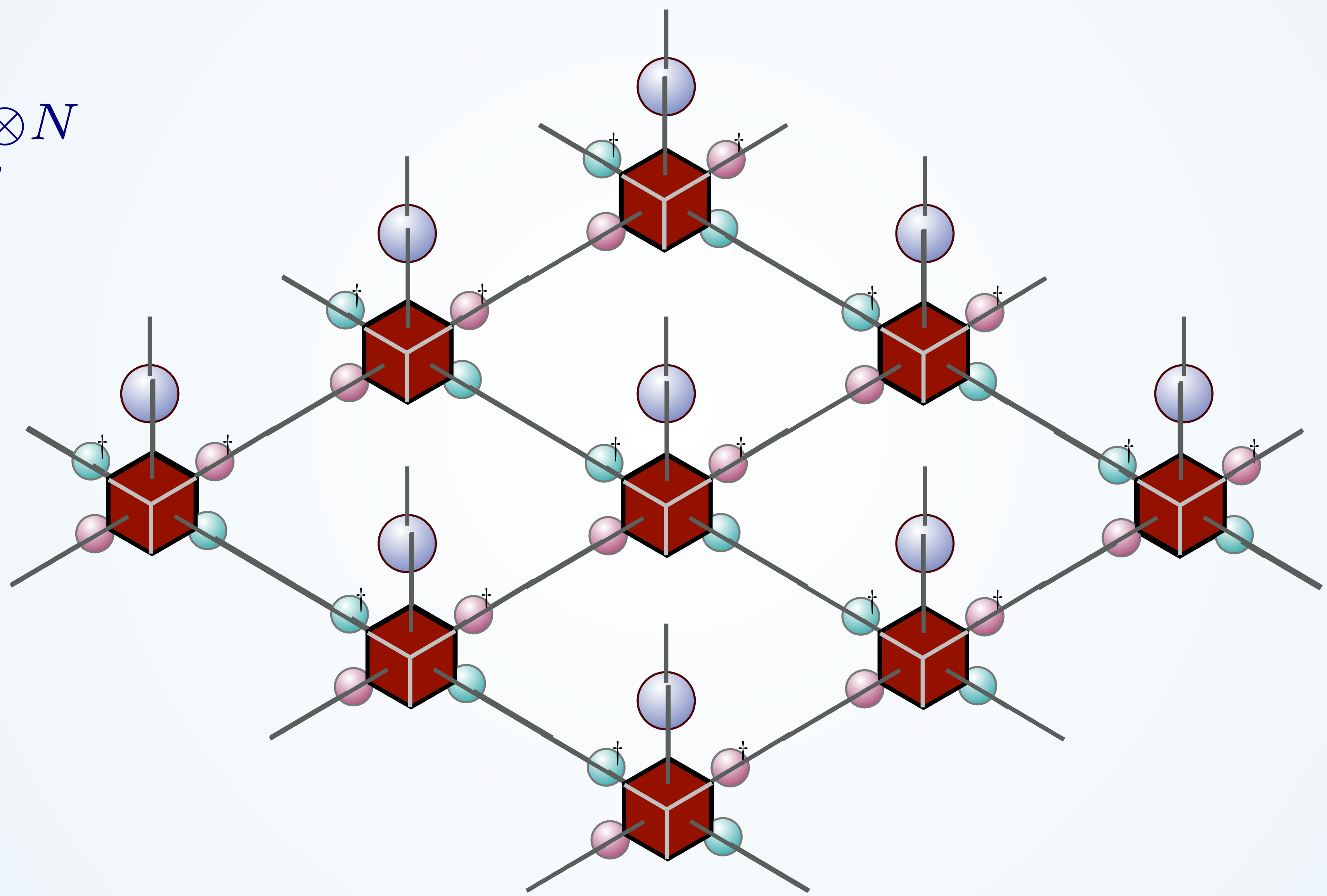
state invariant under global symmetry

constructed with invariant tensors


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

# SYMMETRIC PEPS

$U_g^{\otimes N}$



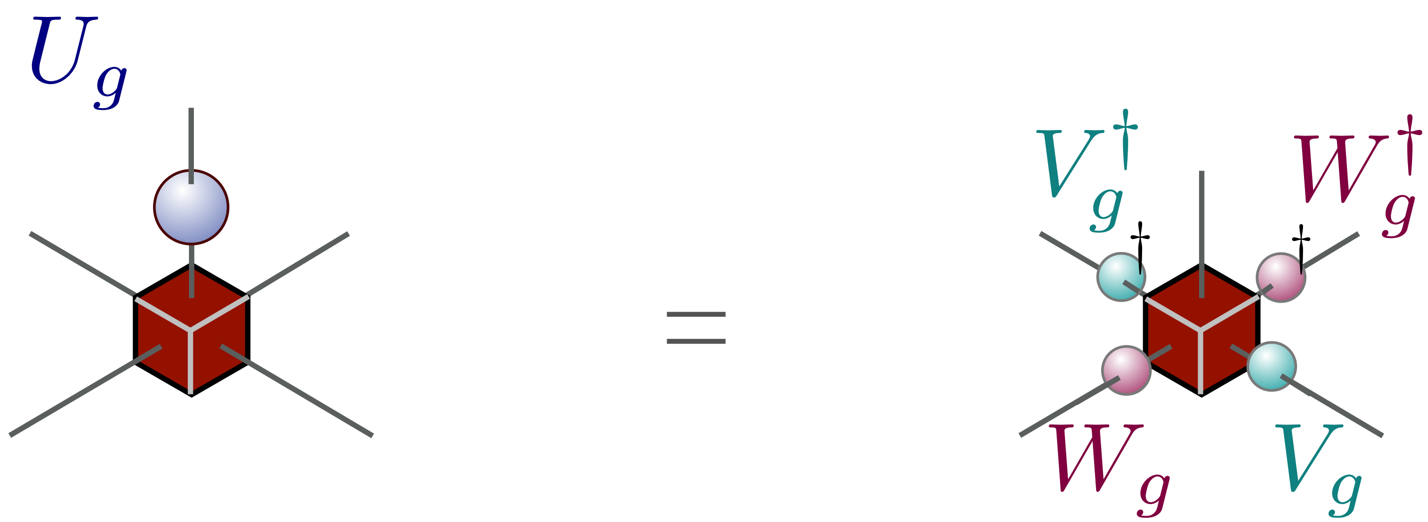
Pérez-García et al., PRL 2008
Sanz et al., PRA 2009
Schuch et al., Ann. Phys. 2010
Singh et al., NJP 2007, PRA 2010

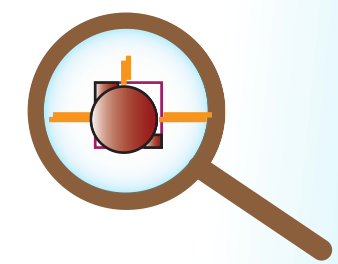
state invariant under global symmetry

constructed with invariant tensors

for MPS & PEPS

state (globally) invariant ⇔



structure
of
tensors

also gauge symmetries

Tagliacozzo et al PRX 2014
Haegeman et al PRX 2014
Zohar et al Ann Phys 2015

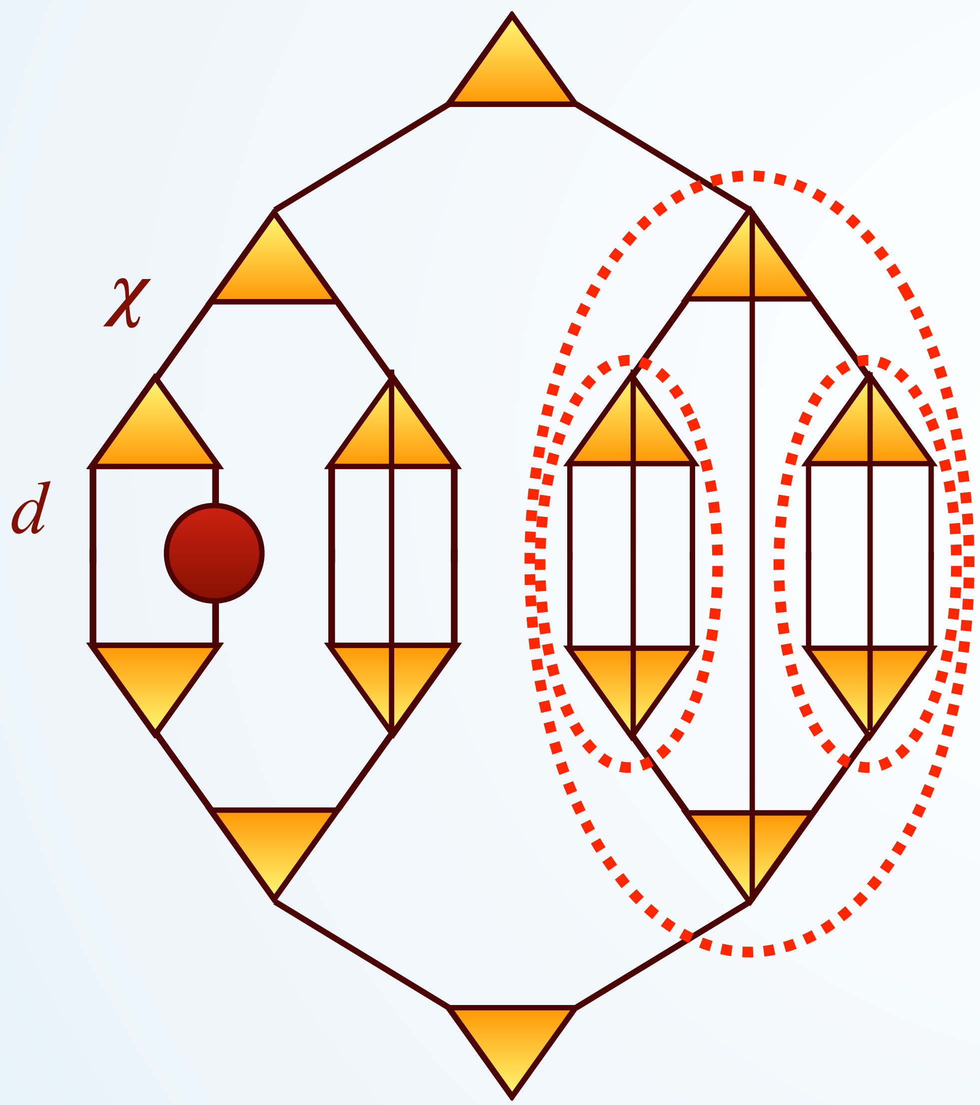
Pérez-García et al., PRL 2008
Sanz et al., PRA 2009
Schuch et al., Ann. Phys. 2010
Singh et al., NJP 2007, PRA 2010

# OTHER TNS

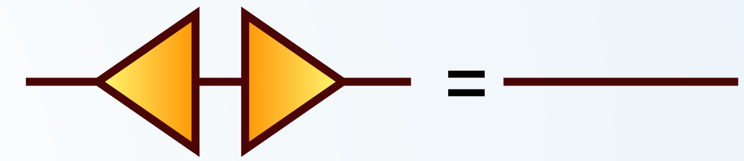
not fulfilling area law

# TTN

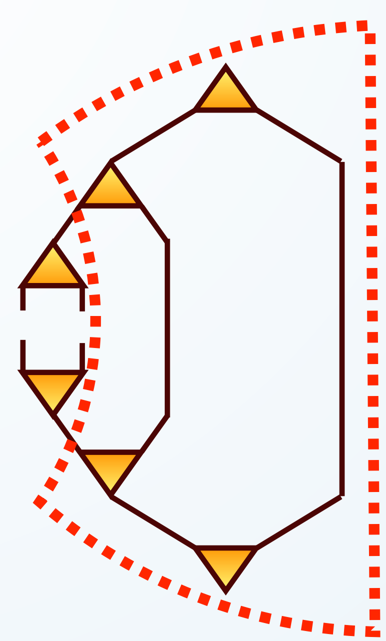
## Tree Tensor States




## efficient contraction

isometries 


## reduced density matrix

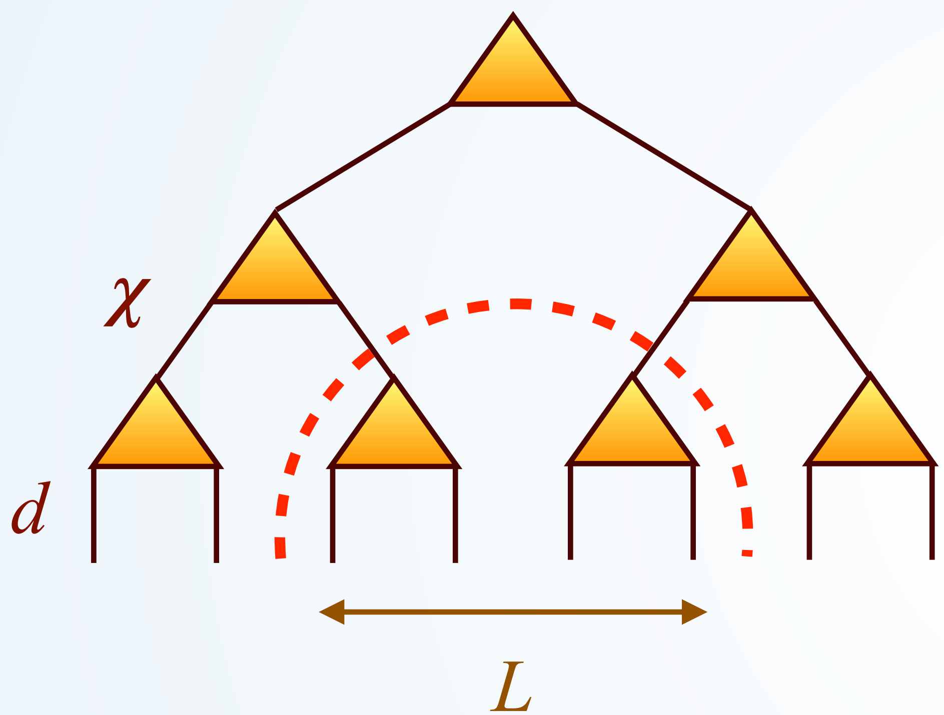


the rank of
this matrix
determines
the max
entanglement

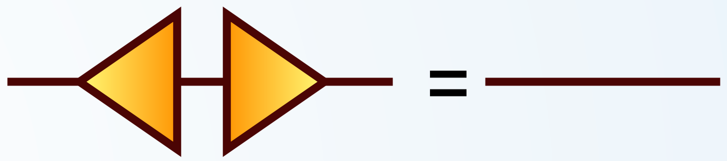
Shi et al PRA (2006)
Tagliacozzo et al PRB80 (2009)
Silvi et al PRA81 (2010)

# TTN

## Tree Tensor States




efficient contraction

isometries 

can be $\mathbf{log}\ L$

homogeneous case: average correlations decay as power law

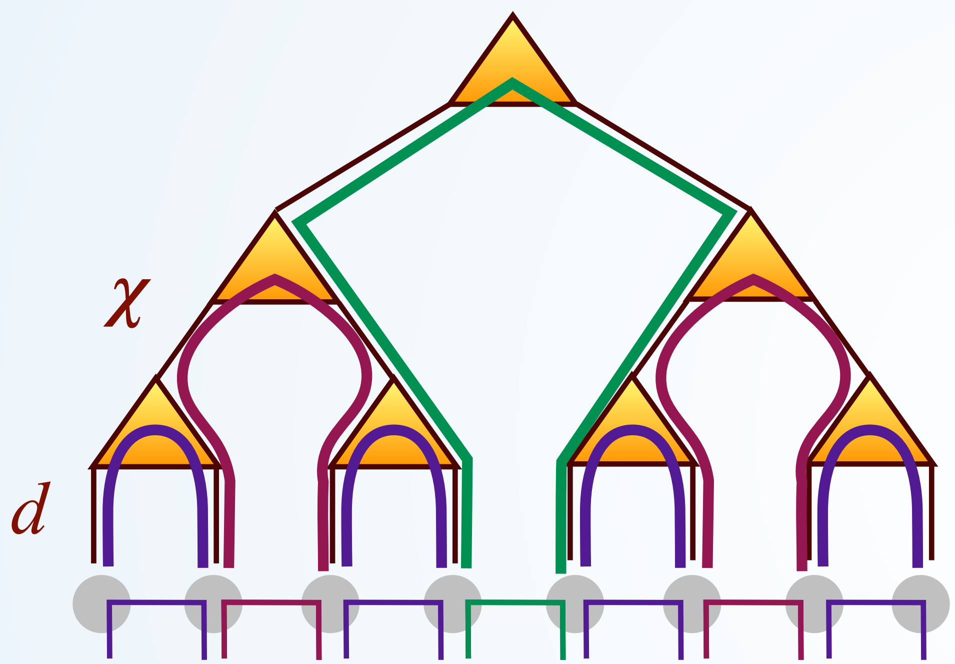
works also in two dimensions, or PBC

because no loops ⇒ canonical form

Shi et al PRA74 (2006)
Tagliacozzo et al PRB80 (2009)
Silvi et al PRA81 (2010)

# MERA

Multiscale Entanglement Renormalization Ansatz




tree as real space renormalization

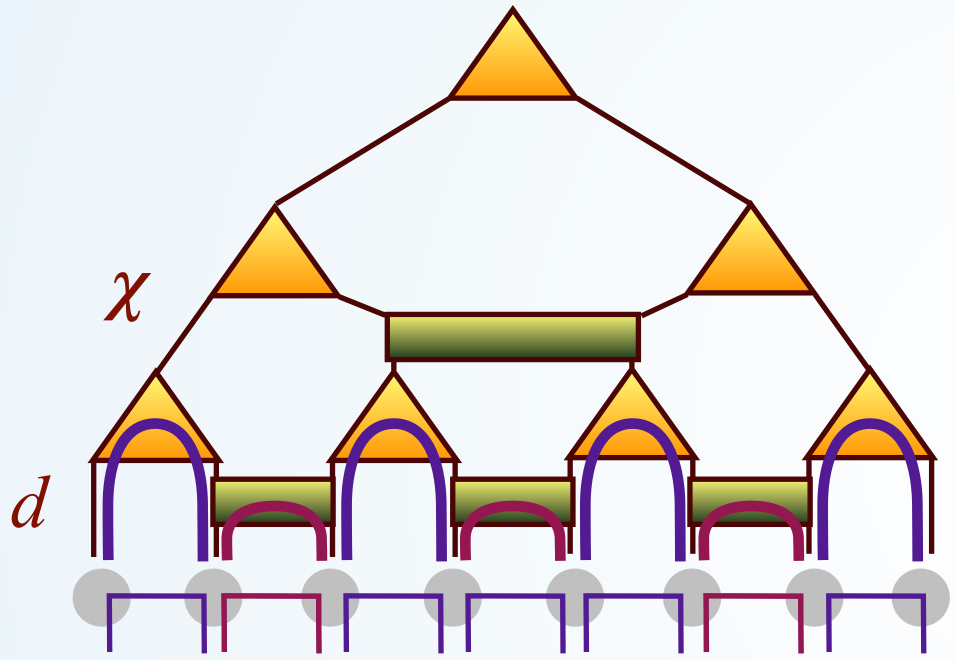
cannot get rid of short range correlations

state with short-range correlations

Vidal PRL99 (2007)

# MERA

Multiscale Entanglement Renormalization Ansatz



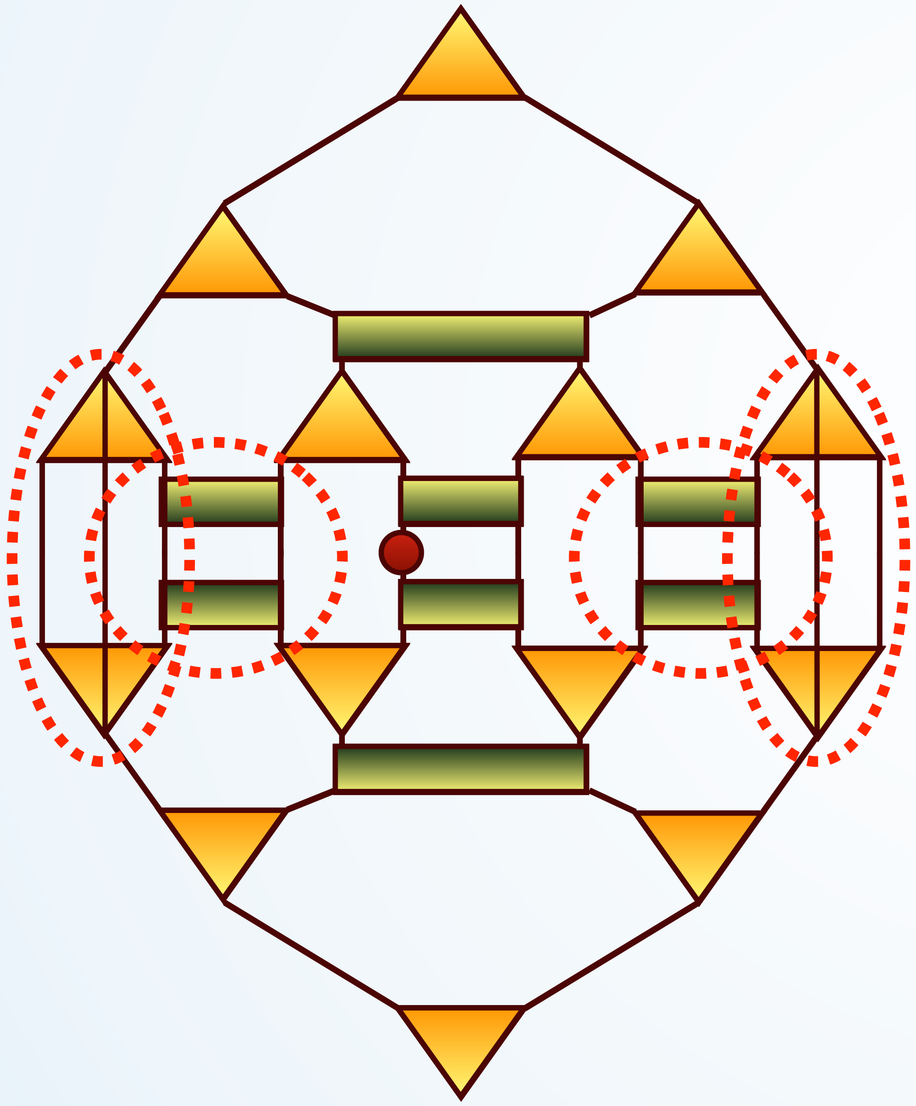

state with short-range correlations

disentanglers

MERA = Q circuit to prepare the state

# MERA

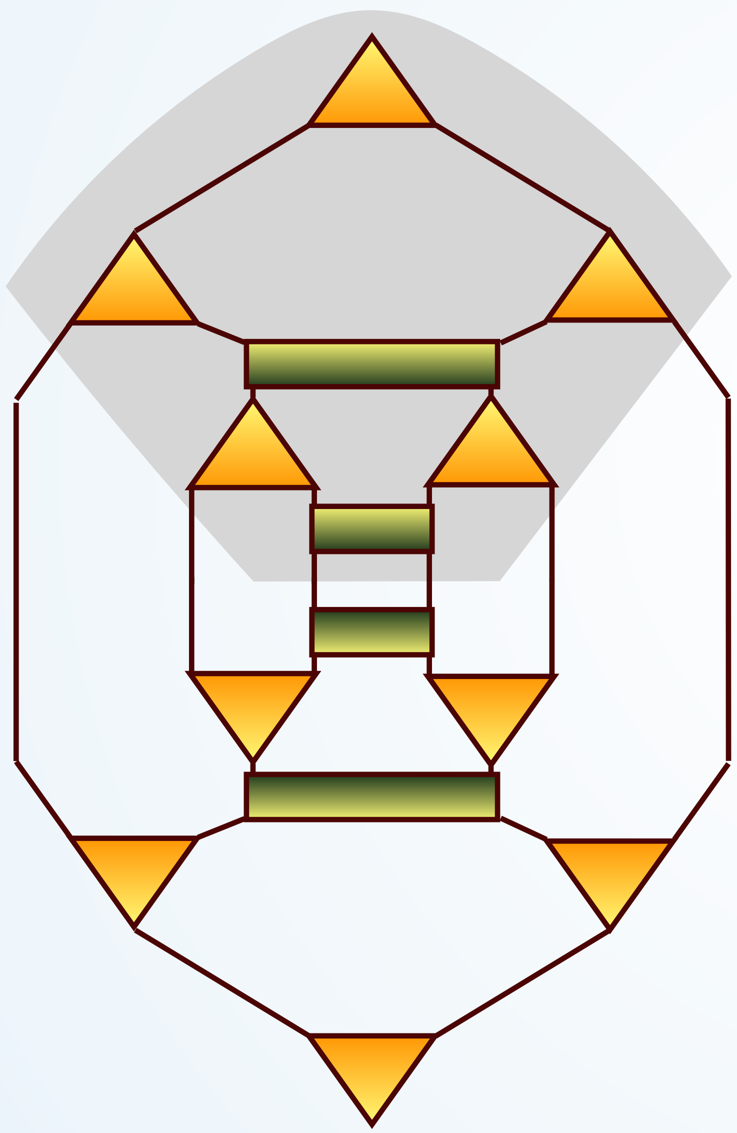
Multiscale Entanglement Renormalization Ansatz



efficient contraction

# MERA

Multiscale Entanglement Renormalization Ansatz



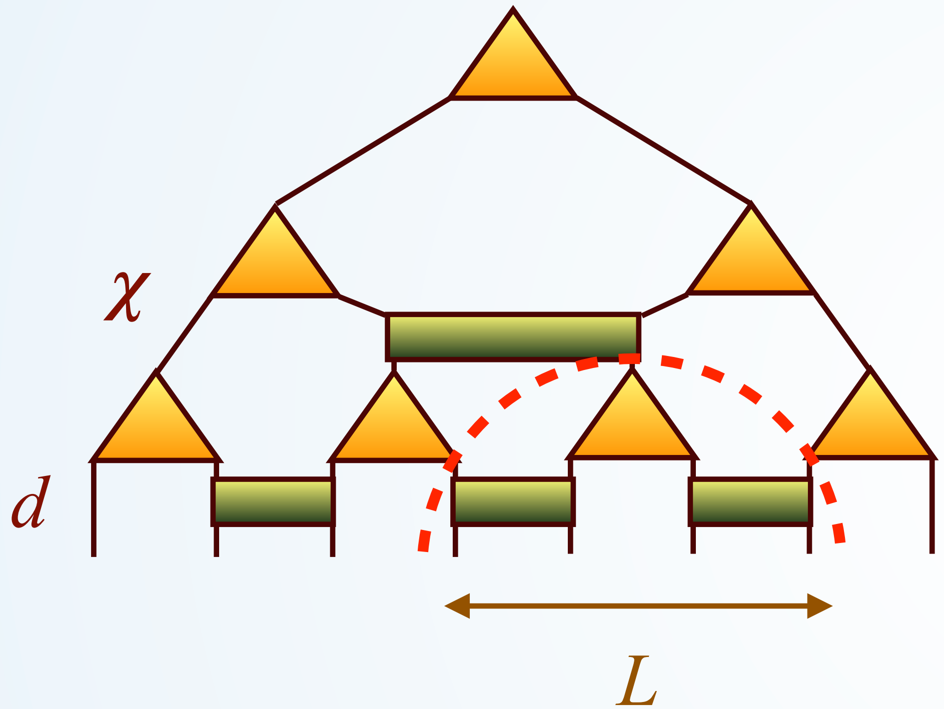
efficient contraction

causal cone

bounded width
$\log L$ height

# MERA

Multiscale Entanglement Renormalization Ansatz




efficient contraction

causal cone

bounded width
$\log L$ height

$$S(L) \leq \log\chi \log L$$

logarithmic violation of area law
can describe critical systems

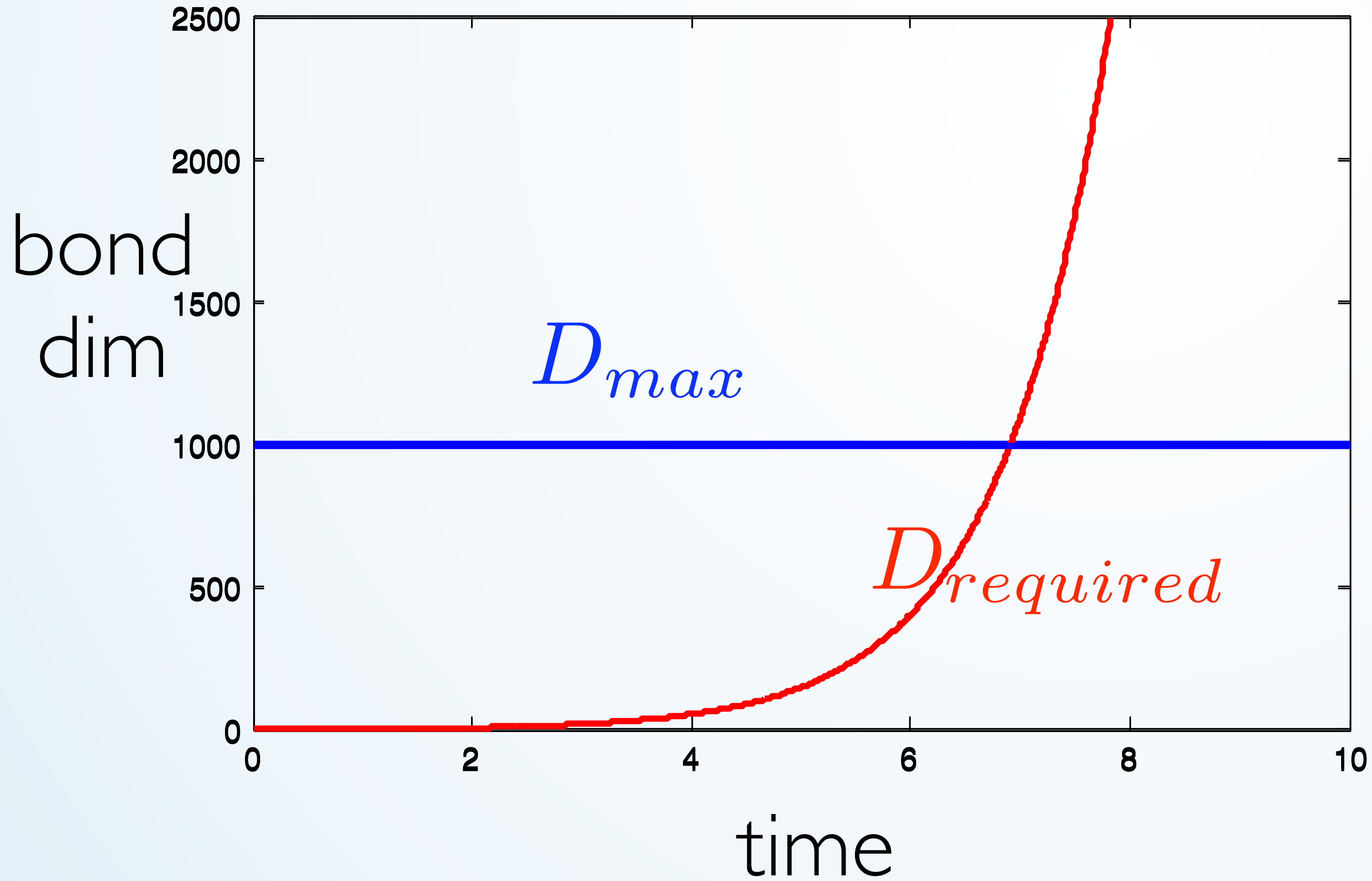
in 2D MERA are a subset of PEPS

# 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

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

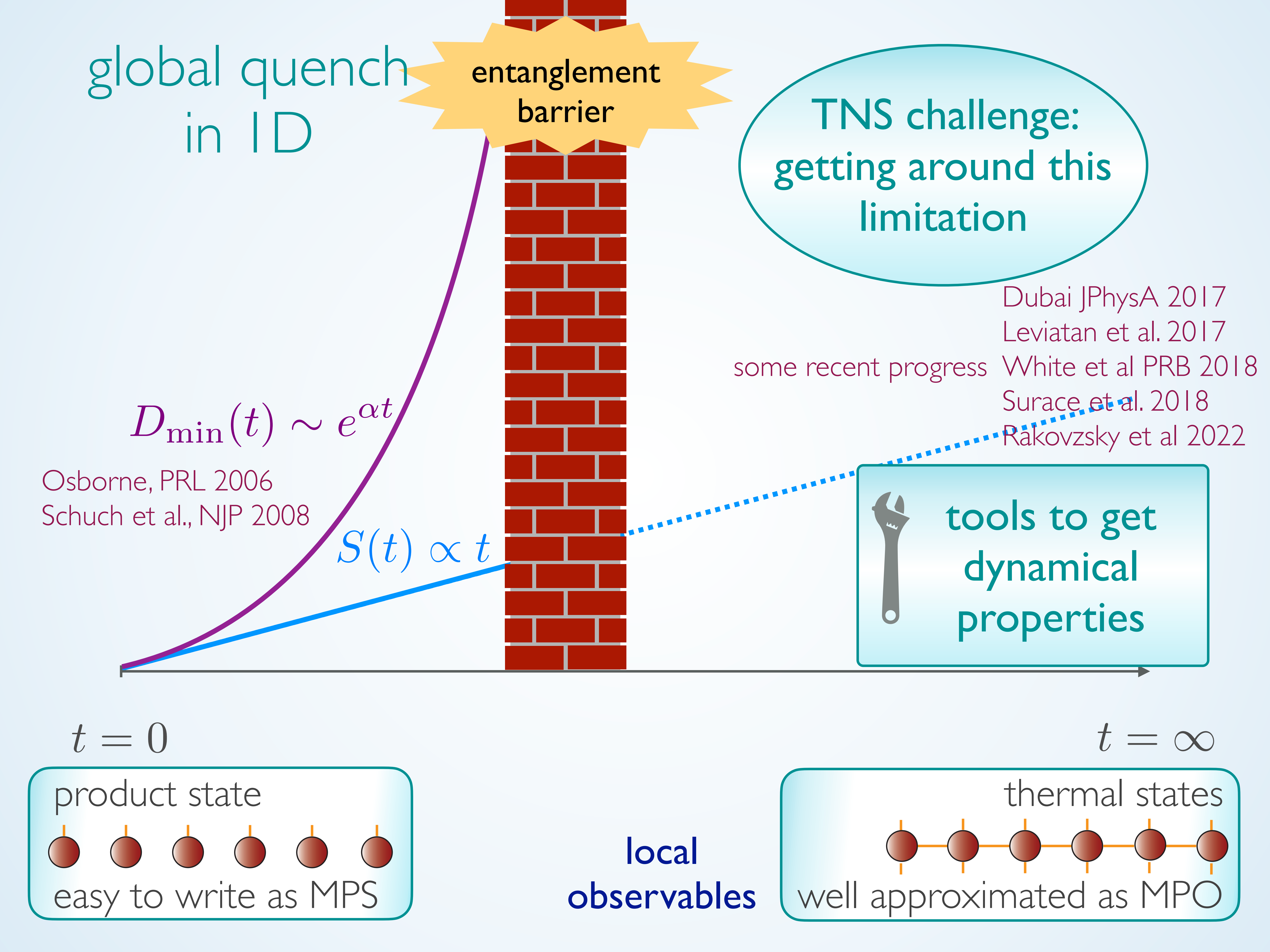
limits the simulation of out of equilibrium many physical situations (in closed and open quantum systems) can be successfully studied!

short times, adiabatic, low energy can work well

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

entanglement growth in non-equilibrium scenarios limits the applicability of MPS

fundamental questions: thermalization, ETH…



global quench
in 1D
entanglement
barrier
TNS challenge:
getting around this
limitation
$D_{\min}(t) \sim e^{\alpha t}$
Osborne, PRL 2006
Schuch et al., NJP 2008
$S(t) \propto t$
some recent progress
Dubai JPhysA 2017
Leviatan et al. 2017
White et al PRB 2018
Surace et al. 2018
Rakovzsky et al 2022
tools to get
dynamical
properties
$t = 0$
$t = \infty$
product state
easy to write as MPS
local
observables
thermal states
well approximated as MPO

# to conclude…

TNS: quantum inspired methods to describe quantum many-body systems

NOTES&REFS:

PhD? postdoc?

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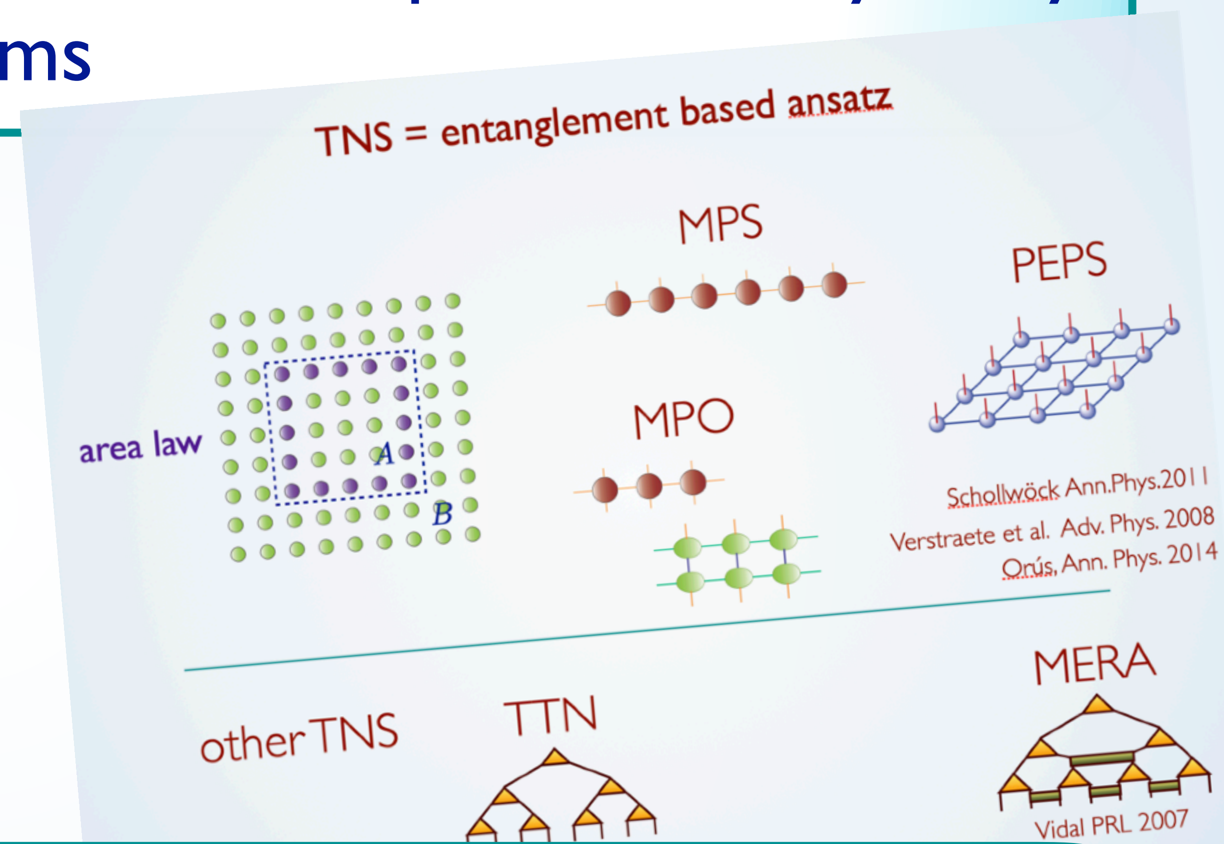


efficient algorithms to find ground states, thermal states

simulating time evolution/arbitrary quantum circuits requires truncation ⇒ limited!

alternatives for local properties?

yet… Pan & Zhang, PRL128, 030501(2022)
Tindall et al. arXiv:2306.14887

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T-NiSQ

Tensor Networks in Simulation of Quantum Matter

# T H A N K S !

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MCQST

Renormalization and tensor product states in spin chains and lattices, J. I. Cirac, F. Verstraete, J. Phys. A: Math. Theor. 42, 504004 (2009), arXiv:0910.1130

The density-matrix renormalization group in the age of matrix product states
Ulrich Schollwöck, Annals of Physics 326, 96 (2011), arXiv:1008.3477

Matrix Product States, Projected Entangled Pair States, and variational renormalization group methods for quantum spin systems, F. Verstraete, J.I. Cirac, V. Murg, Adv. Phys. 57,143 (2008), arXiv:0907.2796

A Practical Introduction to Tensor Networks: Matrix Product States and Projected Entangled Pair States, Roman Orús, Annals of Physics 349 (2014) 117, arXiv:1306.2164

Hand-waving and Interpretive Dance: An Introductory Course on Tensor Networks, Jacob C. Bridgeman, Christopher T. Chubb, J. Phys. A: Math. Theor. 50 223001 (2017), arXiv:1603.03039

The Tensor Networks Anthology: Simulation techniques for many-body quantum lattice systems, P. Silvi et al, SciPost Phys. Lect. Notes 8 (2019), arXiv:1710.03733

Tensor Network Algorithms: a Route Map, MCB, Annu. Rev. Condens. Matter Phys. 2023 14:1, arXiv:2205.10345

TUTORIAL:

NOTES