

TENSOR NETWORKS FOR QUANTUM MANY-BODY SYSTEMS

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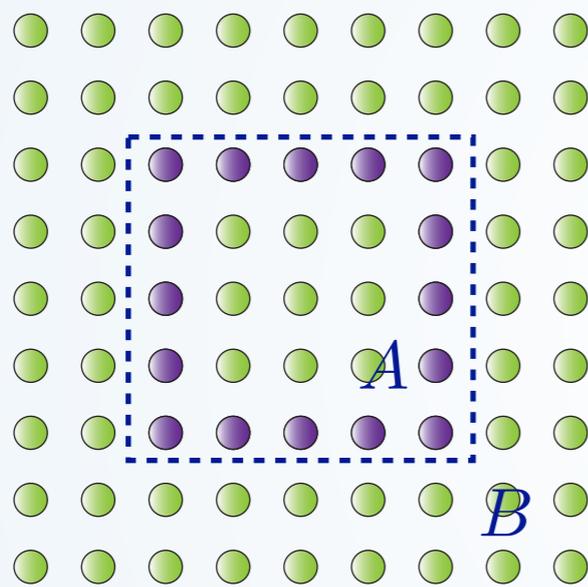


CIRM March 2022

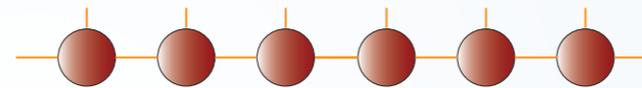
In first session...

TNS = entanglement based ansatz

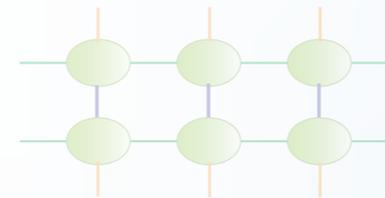
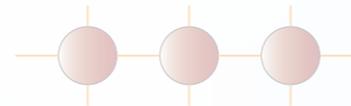
area law



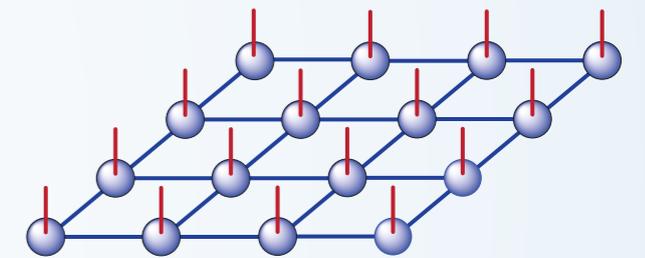
MPS



MPO



PEPS



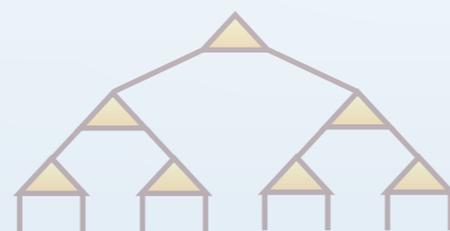
Schollwöck Ann.Phys.2011

Verstraete et al. Adv. Phys. 2008

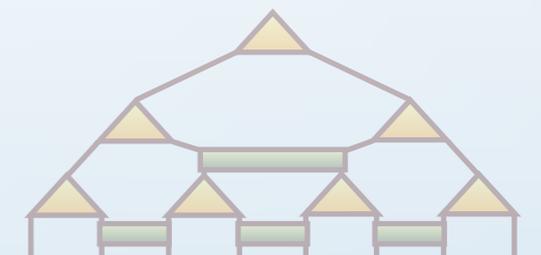
Orús, Ann. Phys. 2014

other TNS

TTN



MERA



MPS PROPERTIES

Matrix Product States

RECAP

good approximation of ground states

Verstraete, Cirac, PRB 2006

Hastings, J. Stat. Phys 2007

gapped finite range Hamiltonian \Rightarrow
area law (ground state)

Cramer, Eisert, Plenio, RMP 2009

efficient calculation of expectation values

exponentially decaying correlations

can be prepared efficiently

PEPS PROPERTIES

Projected Entangled Pairs States

RECAP

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

In this session...

other TNS

basic algorithms

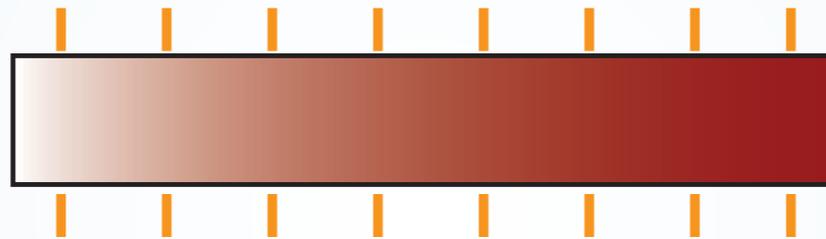
MPO

Matrix Product Operators

MPO

Matrix Product Operator

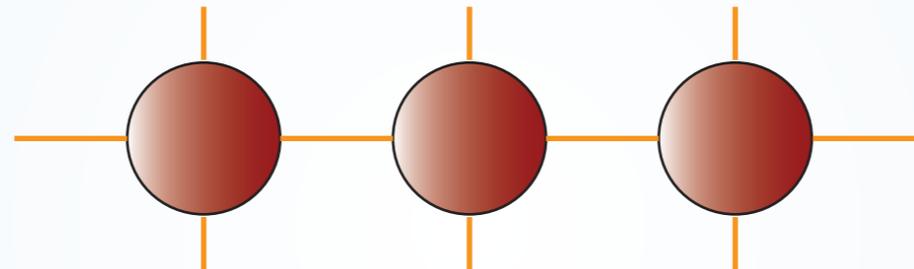
Same kind of ansatz for operators



MPO

Matrix Product Operator

Same kind of ansatz for operators



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

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	...

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

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

MPO

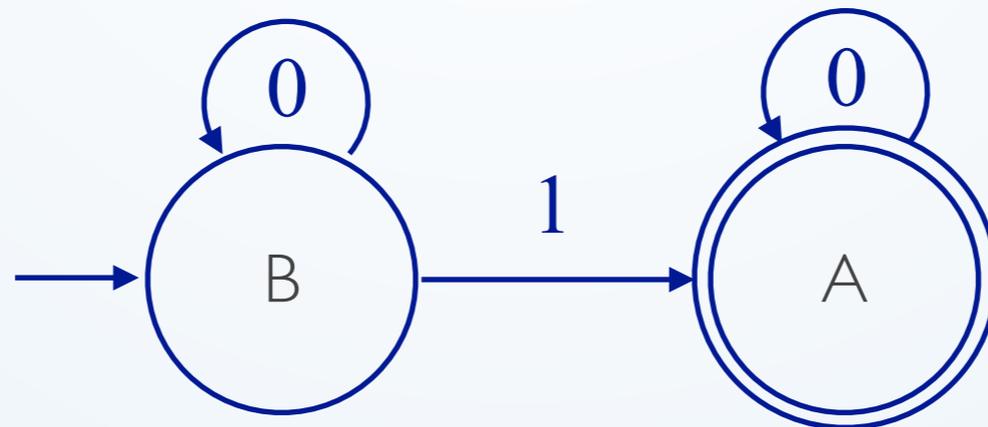
local Hamiltonians are simple MPOs

finite state automata \longrightarrow recognize regular expressions

FSA = computational model

\mathcal{S} states $S_0, S_f \in \mathcal{S}$ B: before 1
 Σ input alphabet 0, 1 A: after 1
 $\mathcal{S} \times \Sigma \rightarrow \mathcal{S}$ transitions

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

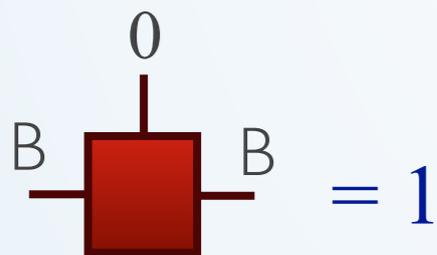
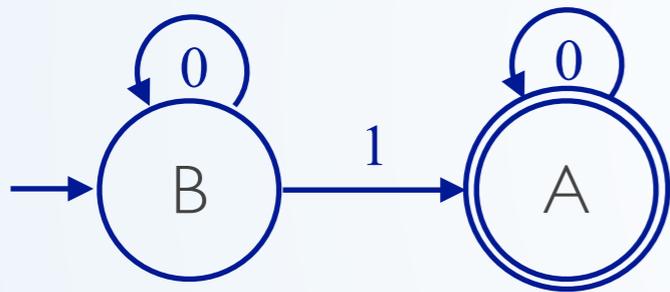


MPO

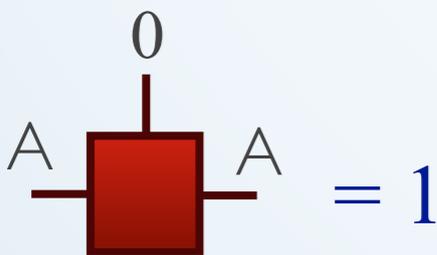
Matrix Product Operator

local Hamiltonians are simple MPOs

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



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



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

boundaries

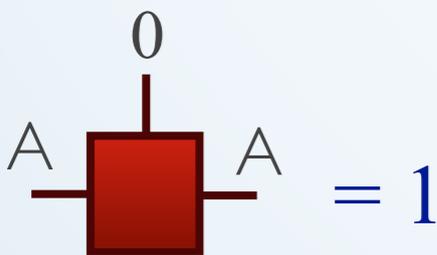
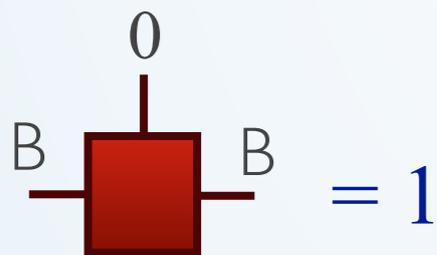
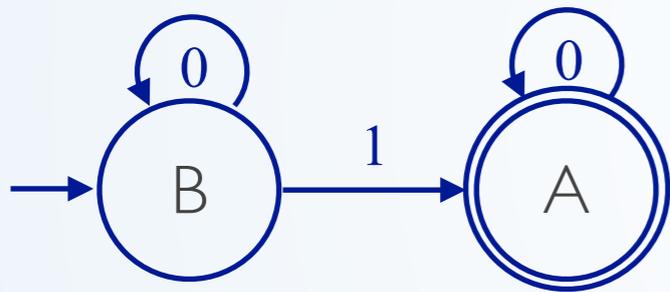
M_L, M_R

MPO

Matrix Product Operator

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translate to MPS/MPO \longrightarrow input symbols = physical indices
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$$M^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

B A

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

boundaries

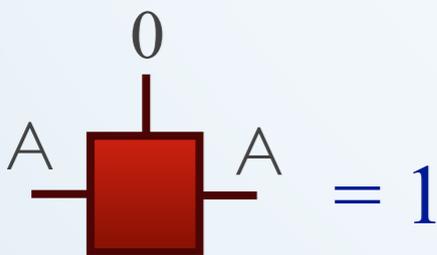
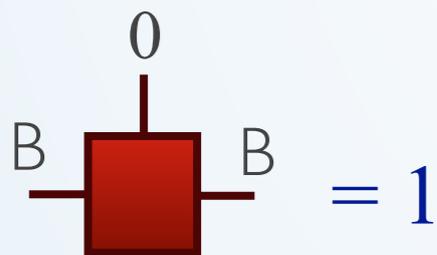
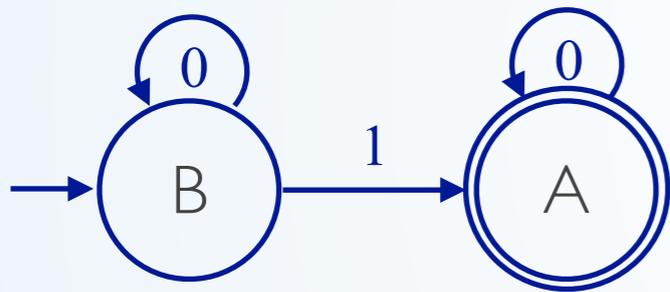
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$$M^0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(Arrows labeled B and A point to the first and second columns of the matrix, respectively.)

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

boundaries

M_L, M_R

MPO

Matrix Product Operator

local Hamiltonians are simple MPOs

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

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

expressed as operator(vector) valued matrix

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

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

$$\sum_i \sigma_x^{[i]}$$

MPO for Ising Hamiltonian

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

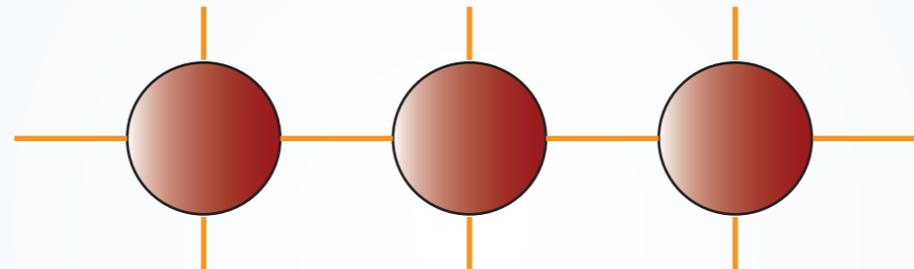
$$\sum_{\{i_k\}} M_L^{i_1} M^{i_2} \dots M^{i_{N-1}} M_R^{i_N} |i_1 \dots i_N\rangle \quad i_k = \mathbb{1}, \sigma_x, \sigma_z$$

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

MPO

Matrix Product Operator

an ansatz for density matrices



need some
properties

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

can we impose them *locally*?

$$\rho = \rho^\dagger$$

$$\text{tr} \rho = 1$$

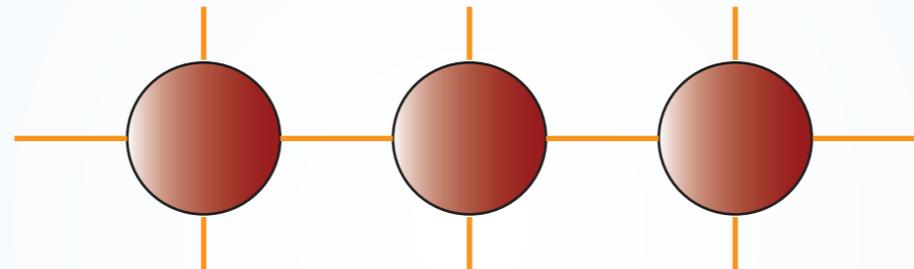
$$\rho \geq 0$$

not all MPO satisfy them!

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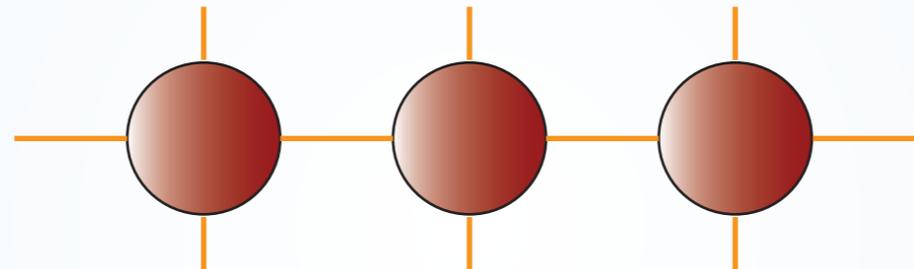
$$\rho \geq 0$$

A diagram showing the adjoint of an MPO tensor. On the left is a brown circular MPO tensor with four orange lines. This is followed by an equals sign, then a brown circular MPO tensor with four orange lines enclosed in large parentheses, with an asterisk superscript to the right of the parentheses. This represents the adjoint operation on the tensor.

MPO

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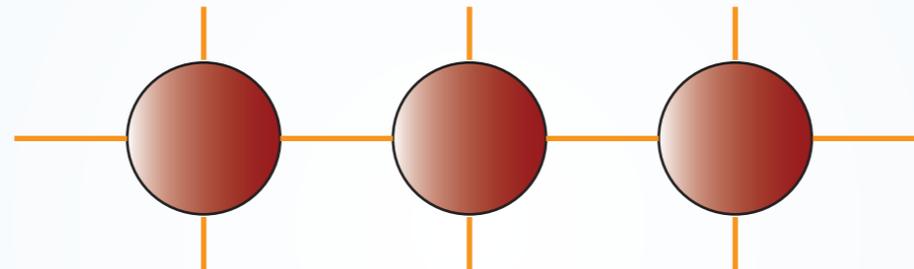
$$\text{tr} \rho = 1$$

$$\rho \geq 0$$

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Matrix Product Operator

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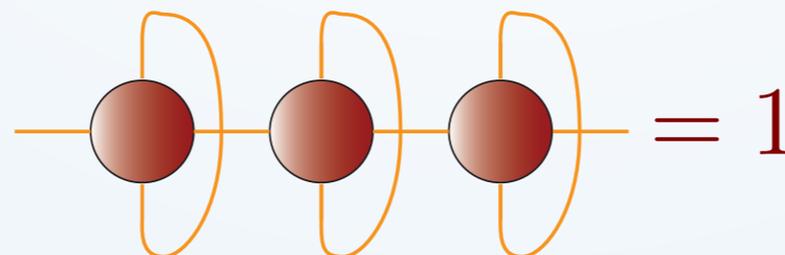
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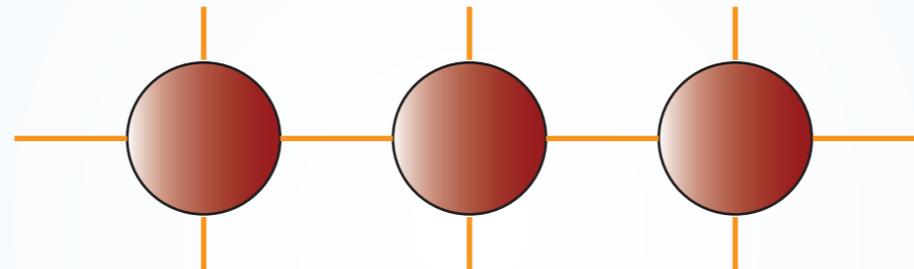
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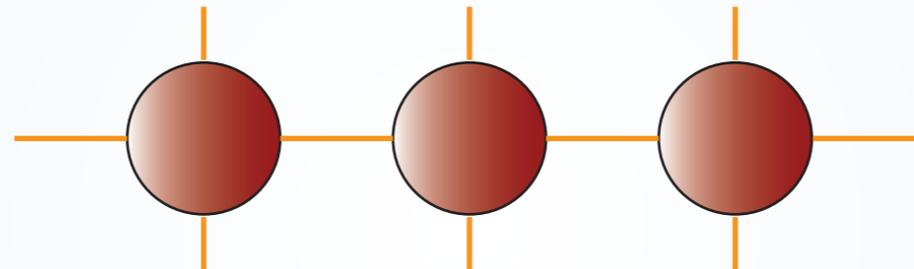
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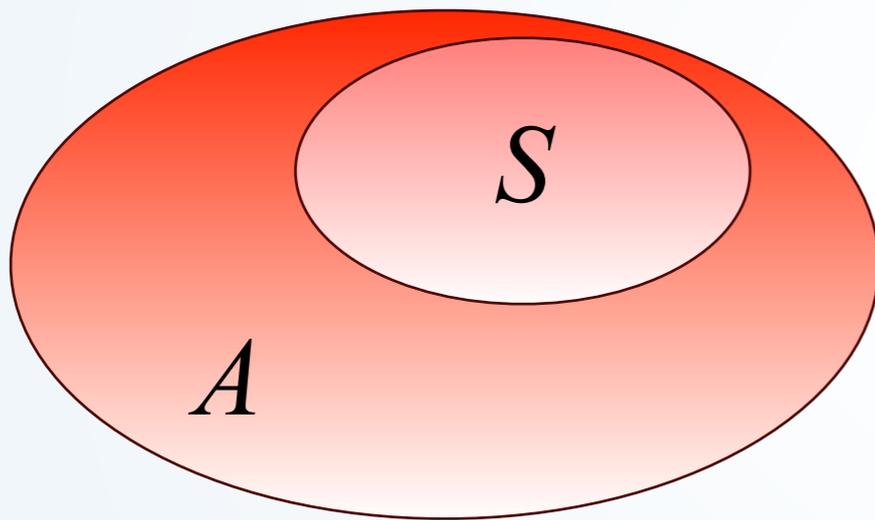
✗ $\rho \geq 0$

there is a way

MPO

Matrix Product Operator

purification



$$\rho_S = \sum_i \lambda_i |\varphi_i\rangle\langle\varphi_i| \quad \begin{array}{l} 0 \leq \lambda_i \leq 1 \\ \sum_i \lambda_i = 1 \end{array}$$

ancillary system A

$$d_A \leq d_S$$

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

orthogonal

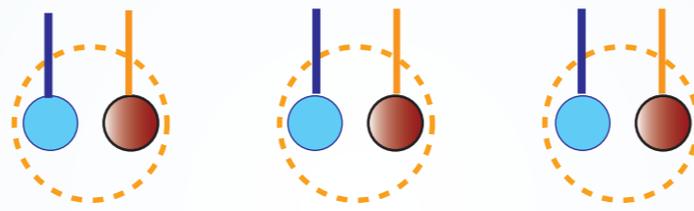
$$\rho_S = \text{tr}_A (|\Psi\rangle_{SA}\langle\Psi|_{SA})$$

unitary freedom on ancilla

MPO

Matrix Product Operator

purification



need some
properties

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

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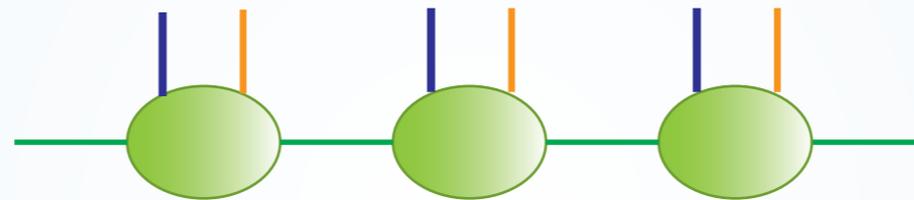
$\rho \geq 0$

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

MPO

Matrix Product Operator

purification



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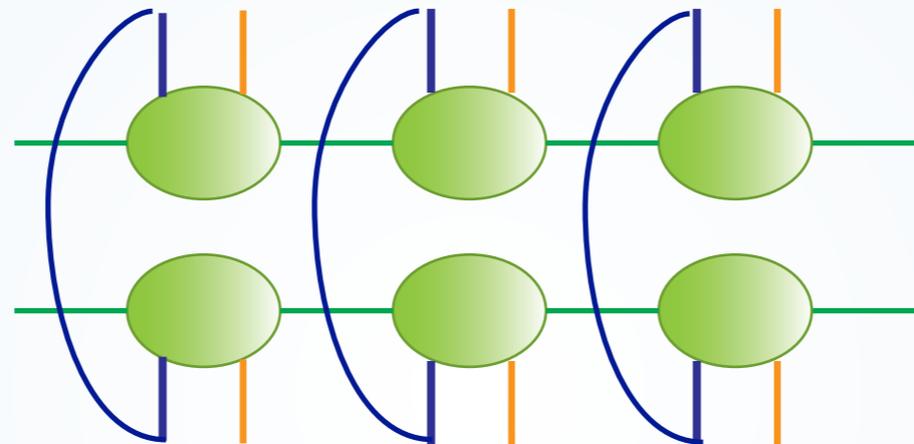
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purification



need some properties

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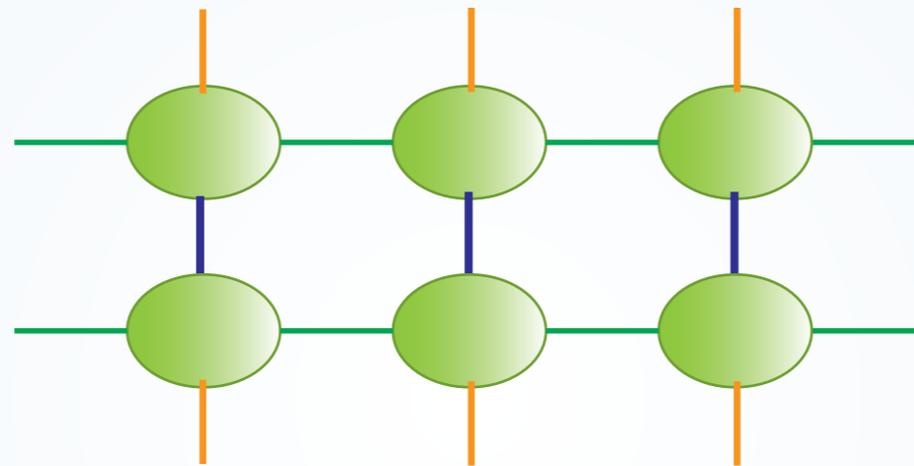
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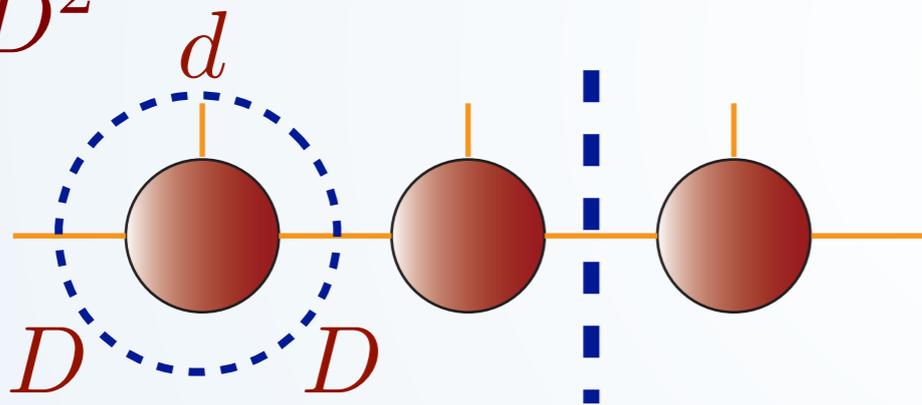
$$\rho_S = \text{tr}_A |\Psi_{SA}\rangle \langle \Psi_{SA}|$$

MPO

Matrix Product Operator

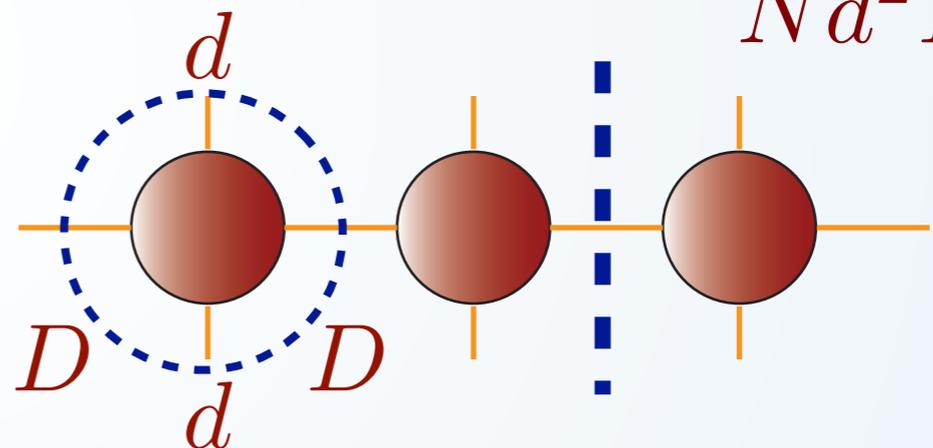
Bond dimension determines
number of parameters

$$NdD^2$$



VS

$$Nd^2D^2$$



Schmidt rank \rightarrow
entanglement

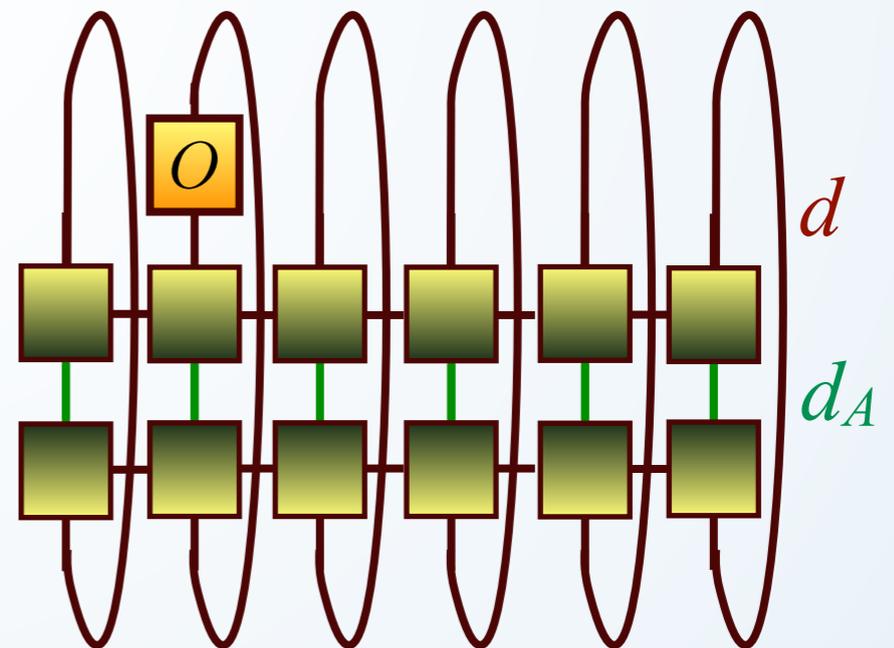
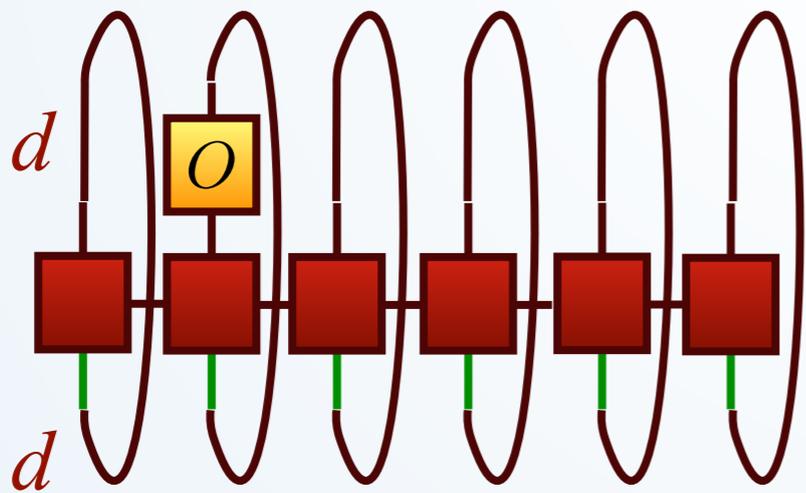
Schmidt rank in operator space
 \rightarrow operator space entanglement
entropy

MPO

Matrix Product Operator

expectation values

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

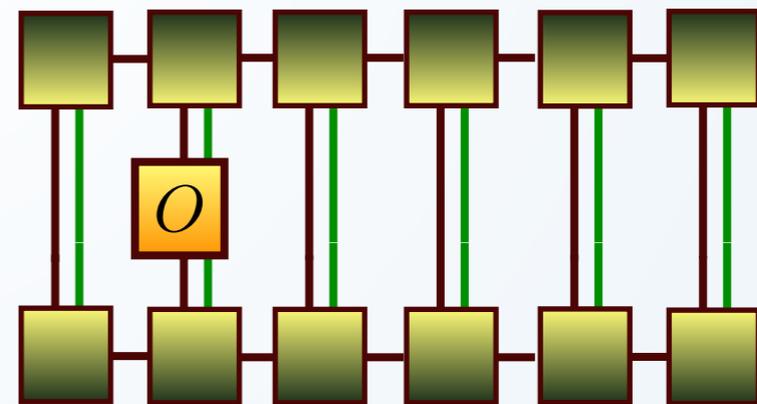
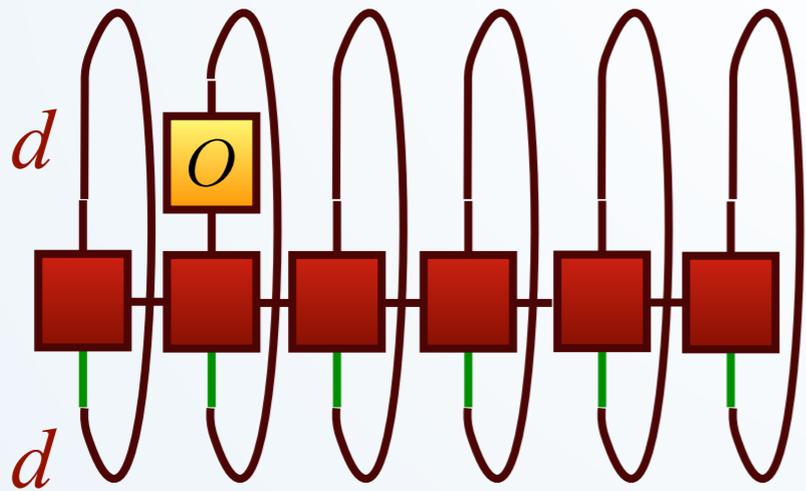


MPO

Matrix Product Operator

expectation values

$$\begin{aligned}\langle O \rangle_{\rho} &= \text{tr}(O \rho) = \text{tr}_S [O \text{tr}_A (|\Psi\rangle\langle\Psi|)] = \text{tr}(O |\Psi\rangle\langle\Psi|) \\ &= \langle \Psi | O | \Psi \rangle\end{aligned}$$

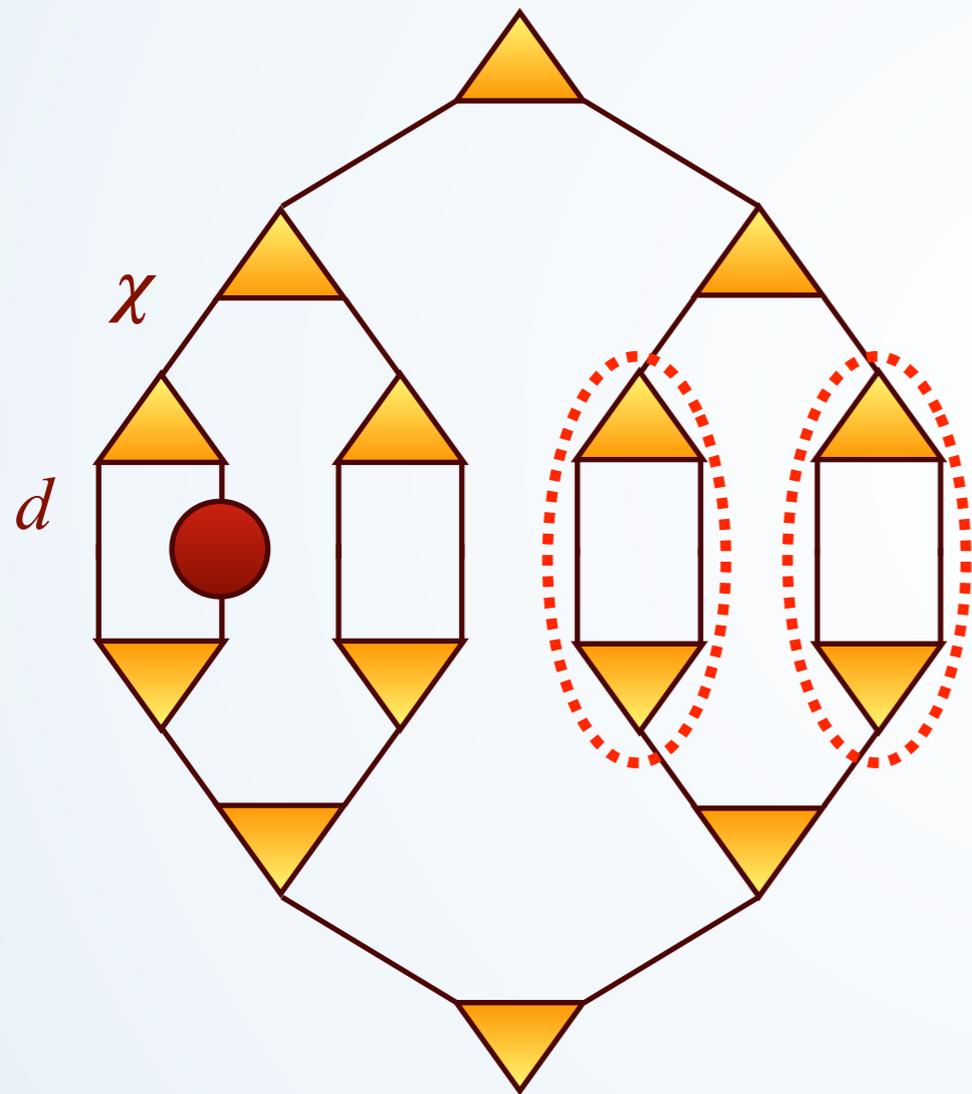


OTHER TNS

not fulfilling area law

TTN

Tree Tensor States

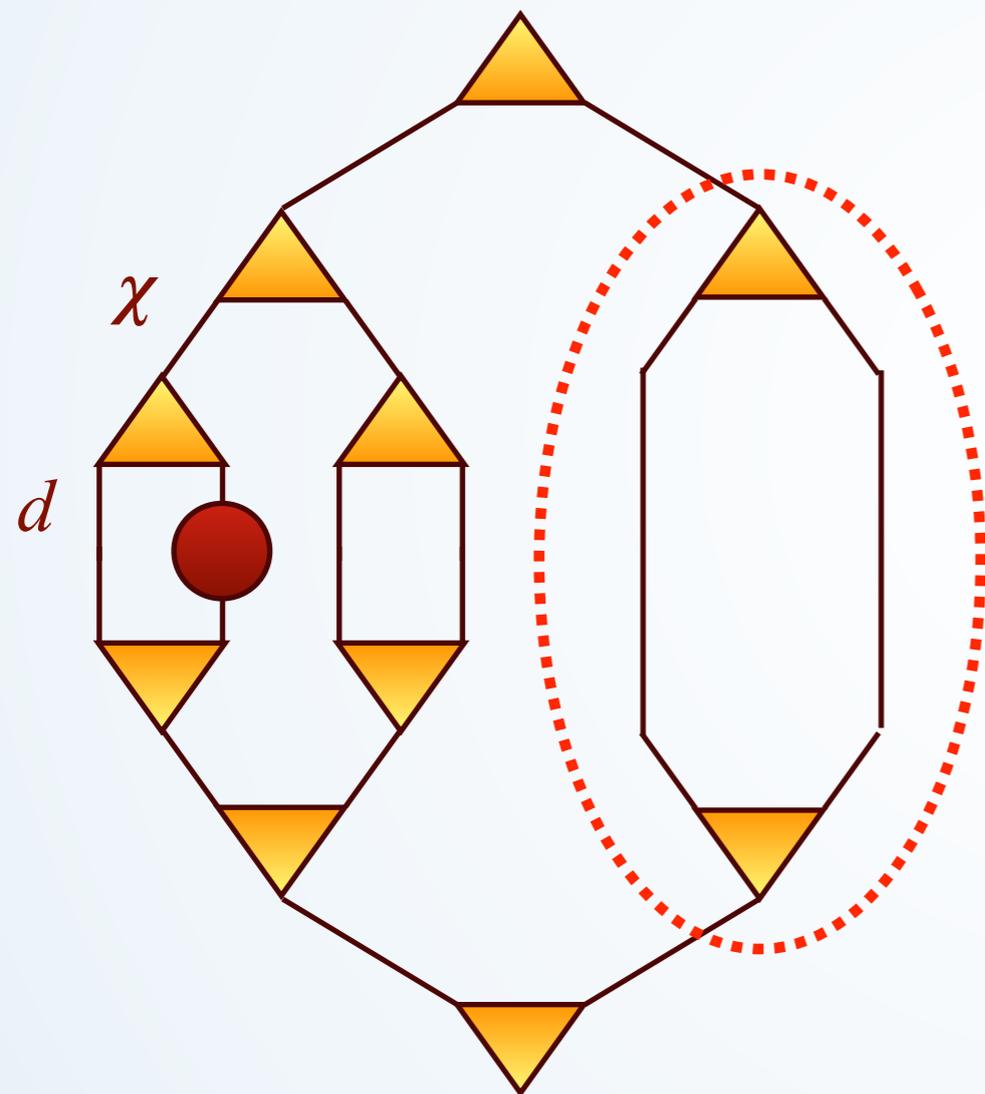


efficient contraction

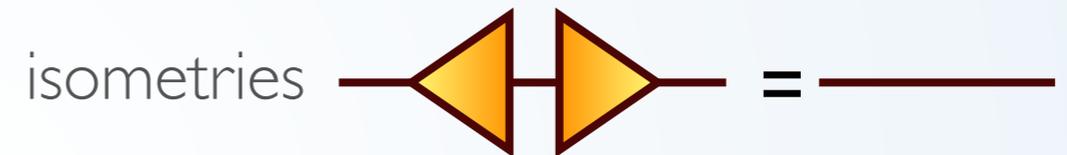


TTN

Tree Tensor States

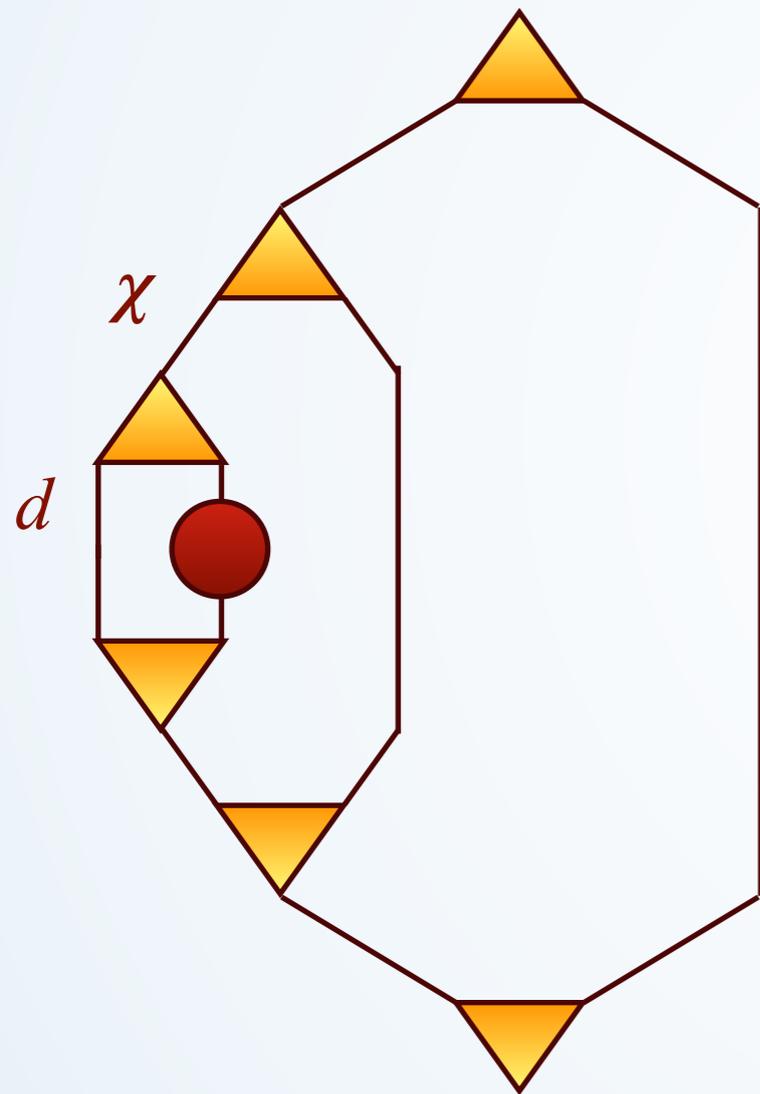


efficient contraction



TTN

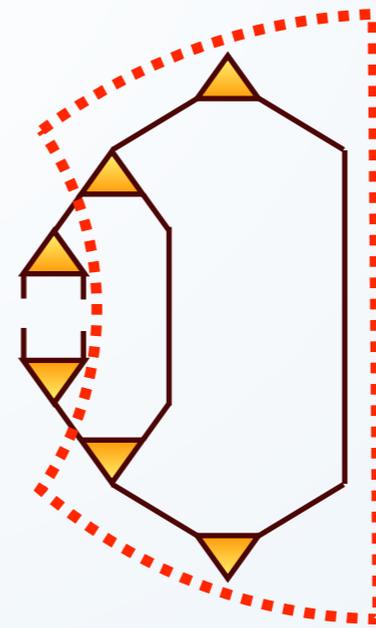
Tree Tensor States



efficient contraction



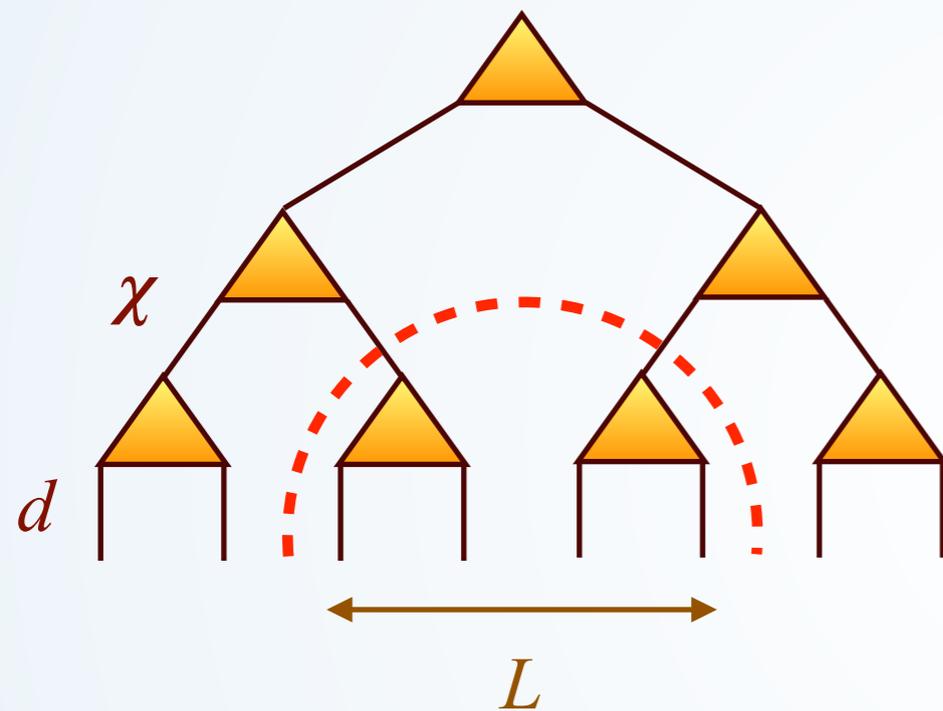
reduced density matrix



the rank of
this matrix
determines
the max
entanglement

TTN

Tree Tensor States



efficient contraction



can be $\log L$

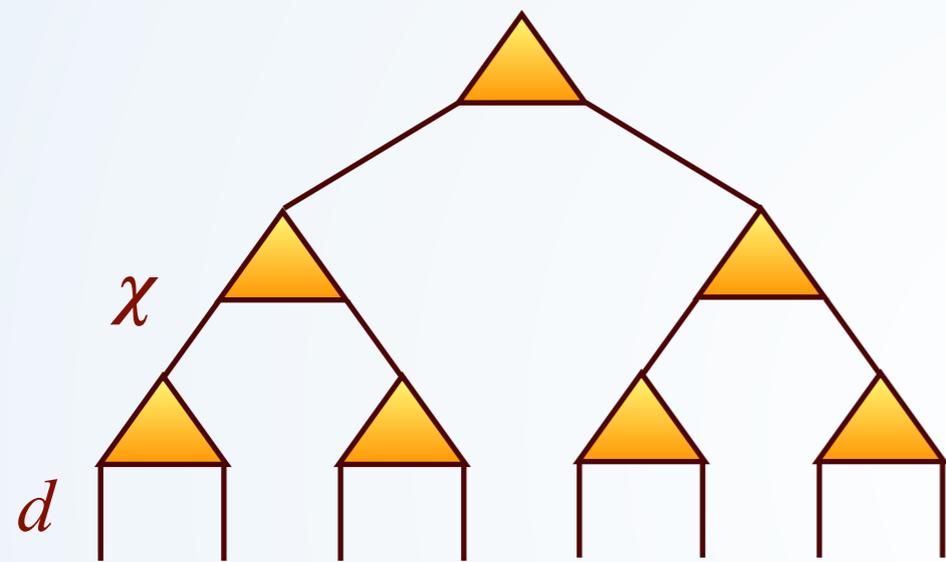
homogeneous case: average correlations decay as power law

works also in two dimensions, or PBC

because no loops \Rightarrow canonical form

MERA

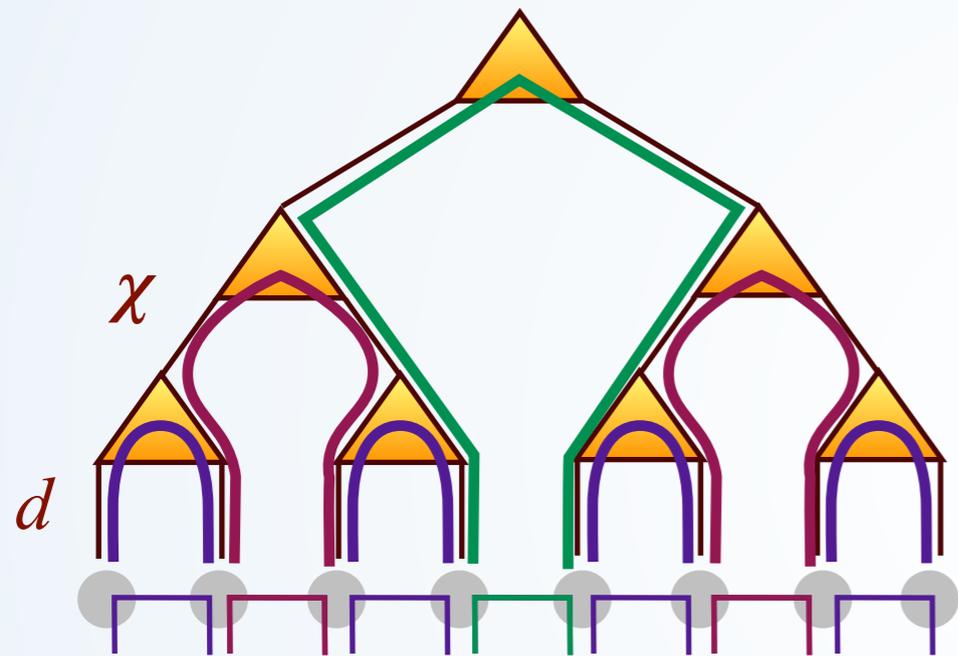
Multiscale Entanglement Renormalization Ansatz



tree as real space renormalization

MERA

Multiscale Entanglement Renormalization Ansatz



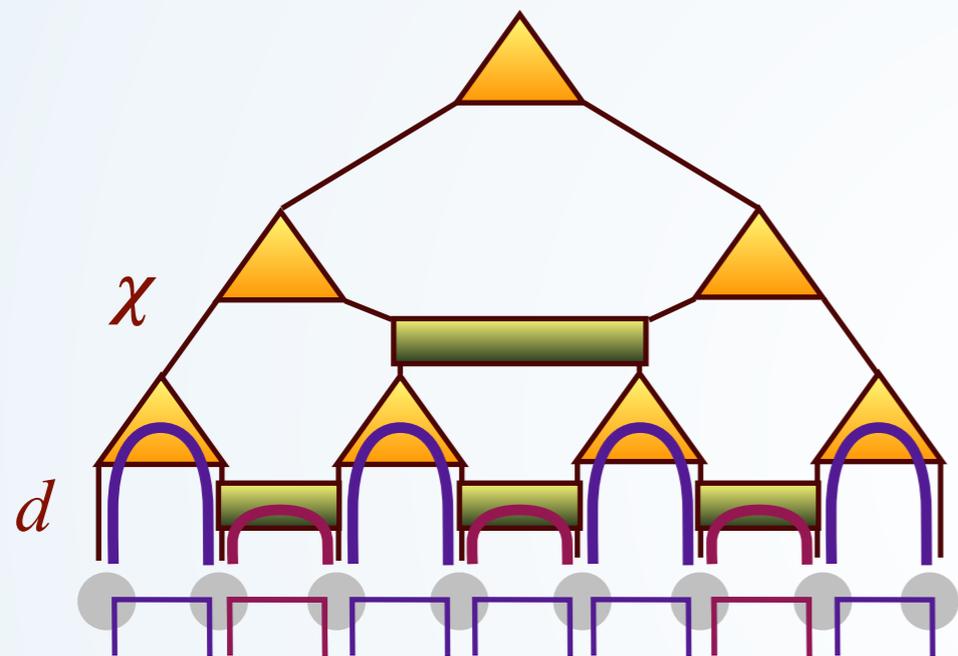
tree as real space renormalization

cannot get rid of short range correlations

state with short-range correlations

MERA

Multiscale Entanglement Renormalization Ansatz



state with
short-range
correlations

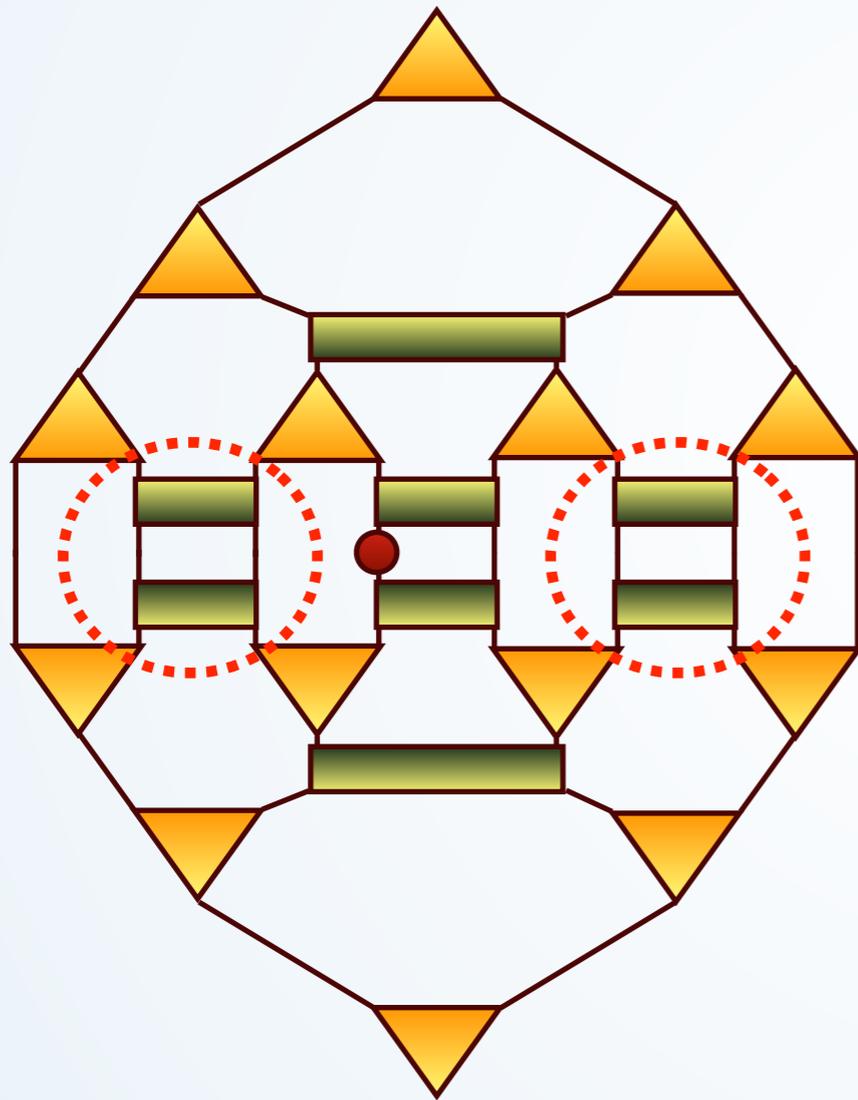
disentanglers

MERA = Q circuit to
prepare the state

MERA

Multiscale Entanglement Renormalization Ansatz

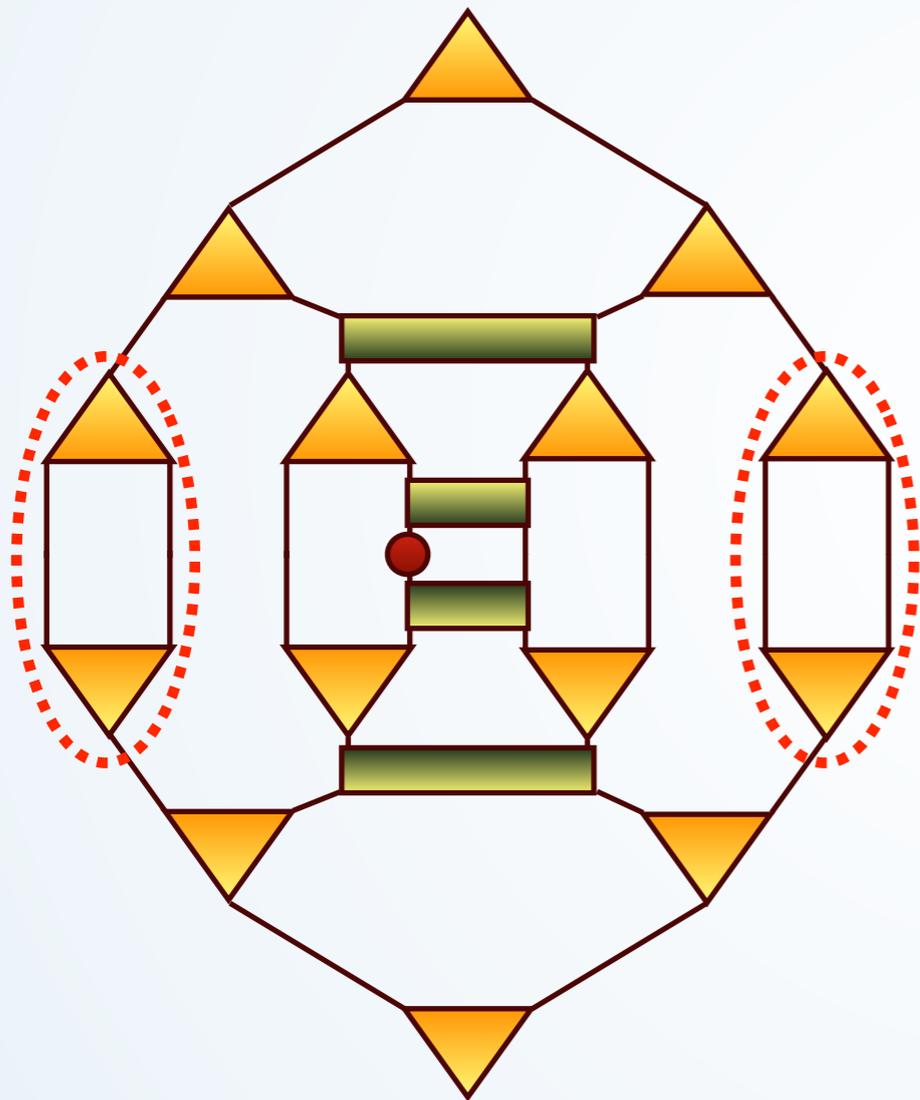
efficient contraction



MERA

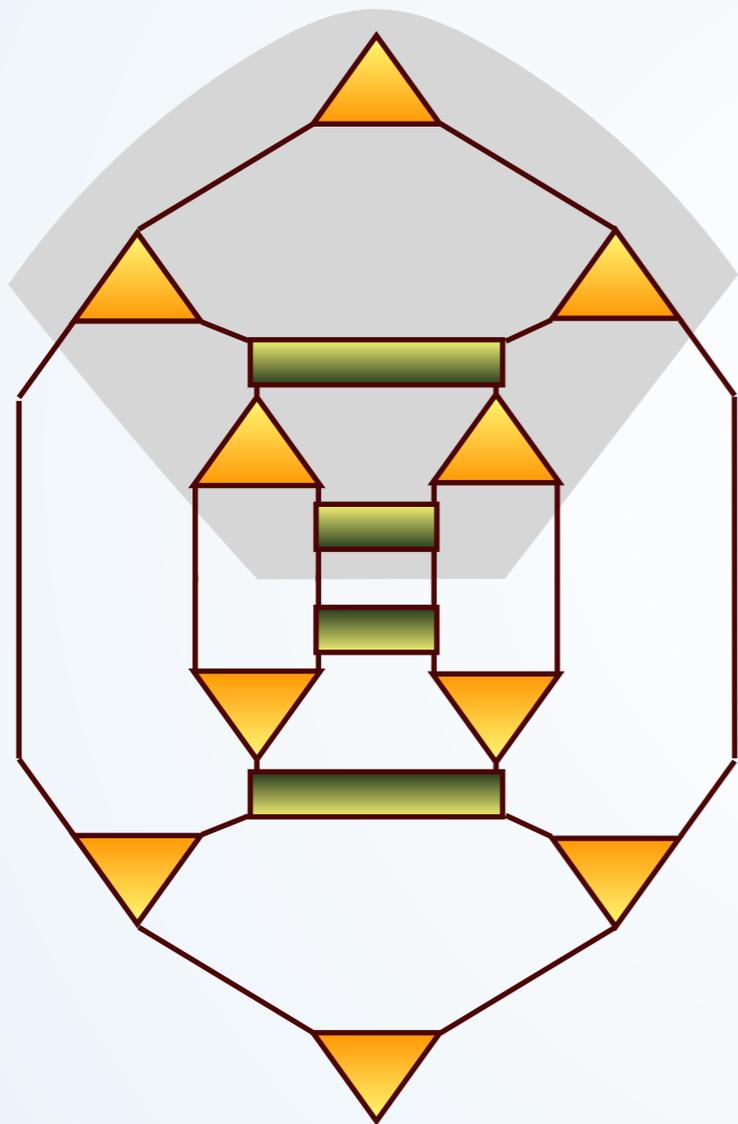
Multiscale Entanglement Renormalization Ansatz

efficient contraction



MERA

Multiscale Entanglement Renormalization Ansatz



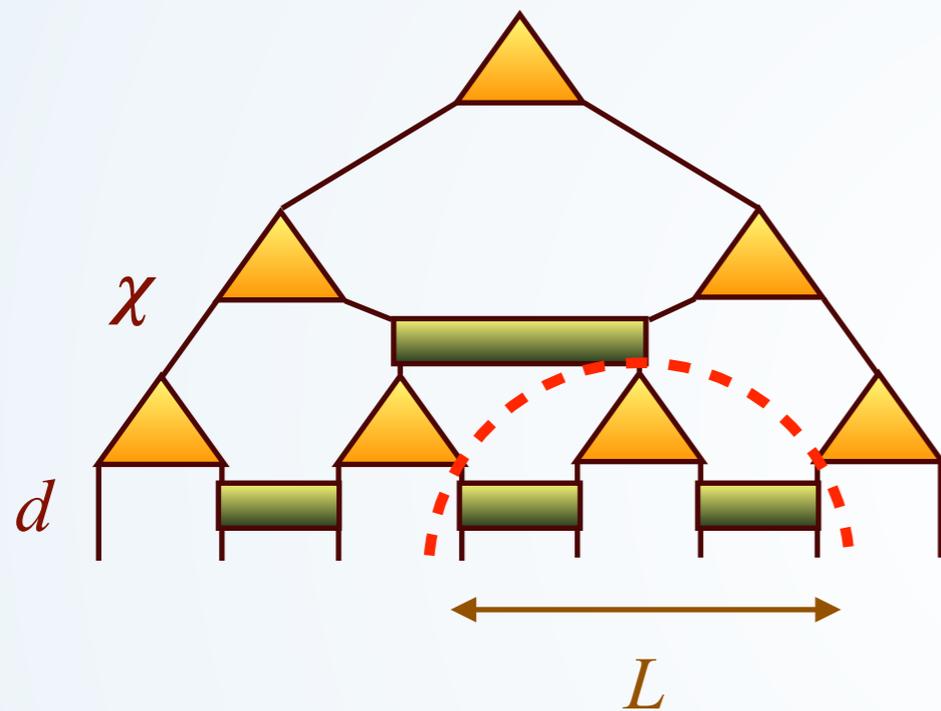
efficient contraction

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

WHAT CAN WE DO WITH TNS?

The TNS toolbox

The background image shows a workshop or toolbox. On the left, a wooden toolbox is open, revealing various tools inside. On the right, a wall is covered with hanging tools, including several screwdrivers with different handles, a pair of pliers, and other hand tools. The lighting is dramatic, with strong shadows and highlights, giving it a professional and industrial feel.

BASIC ALGORITHMS

two main types

variational optimization

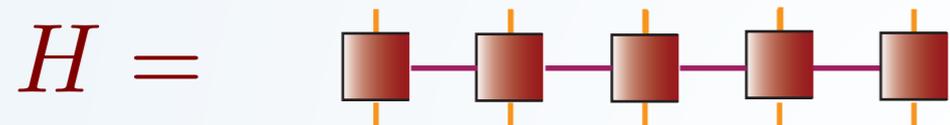
used for ground states

applying a (local) operator

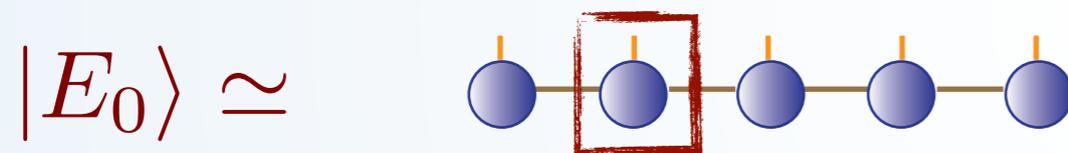
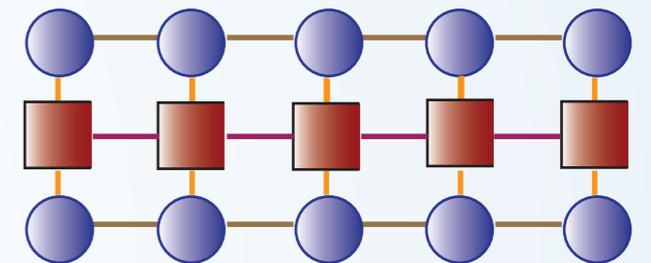
basis of most common
evolution algorithms

BASIC ALGORITHMS

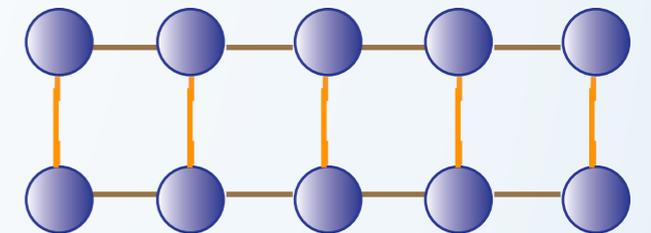
variational minimization of energy



$$\langle \Psi | H | \Psi \rangle$$



$$\langle \Psi | \Psi \rangle$$



Variational principle

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

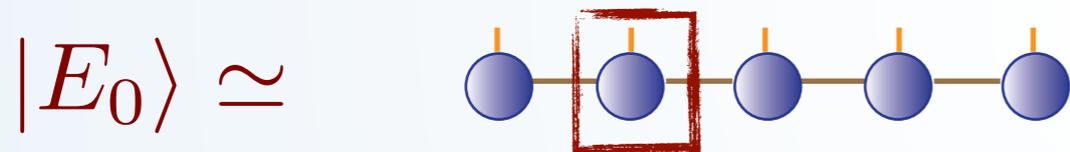
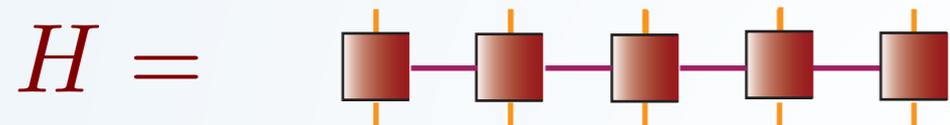
White, PRL 1992

Verstraete, Porras, Cirac, PRL 2004

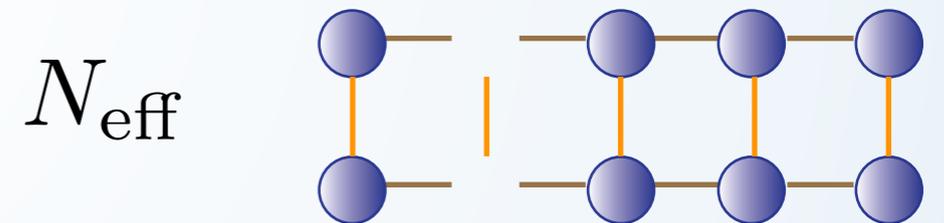
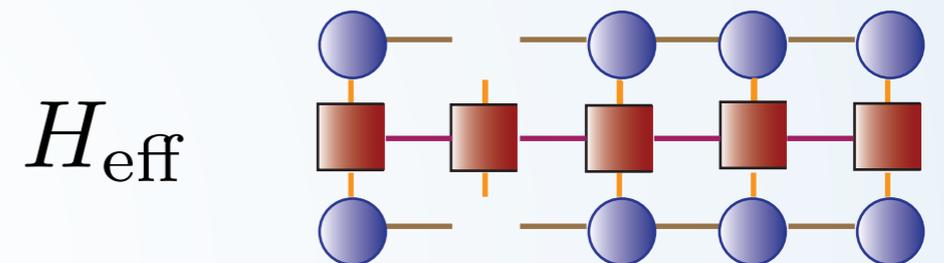
Schollwöck, RMP 2005, Ann. Phys. 2011

BASIC ALGORITHMS

variational minimization of energy



Variational principle



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

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

} $O(D^3)$

DMRG

guaranteed convergence

PBC: higher cost $O(D^5)$

also excitations

symmetries can be integrated

PEPS $O(D^{10})$

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 \rightarrow eigs $E_{GS}/N = -1.255389855581190$
 $t=38$ s

MPS

```
bin - bash Emacs-x86_64-10_9 - 114x38
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
Ground state found for D=70 with eigenvalue -25.10779711 (Energy per particle=-1.255389856) time=8.444515
```

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 — 112x31
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
```

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

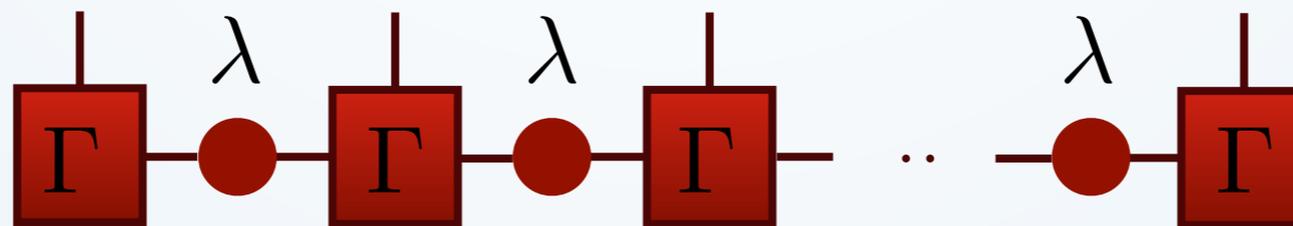
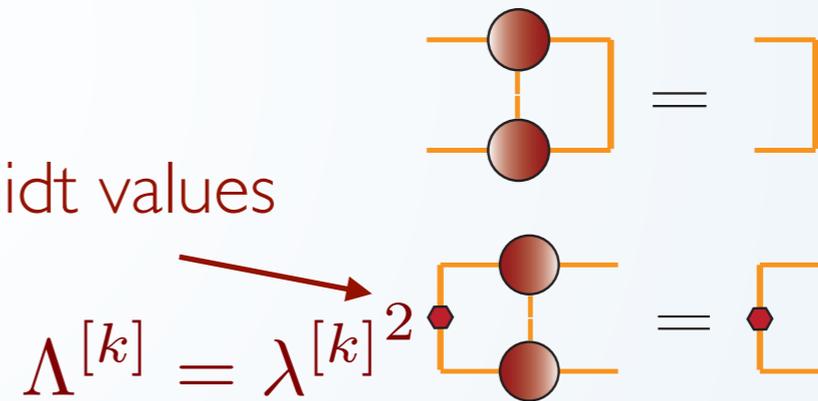


recall canonical form

can be made explicit

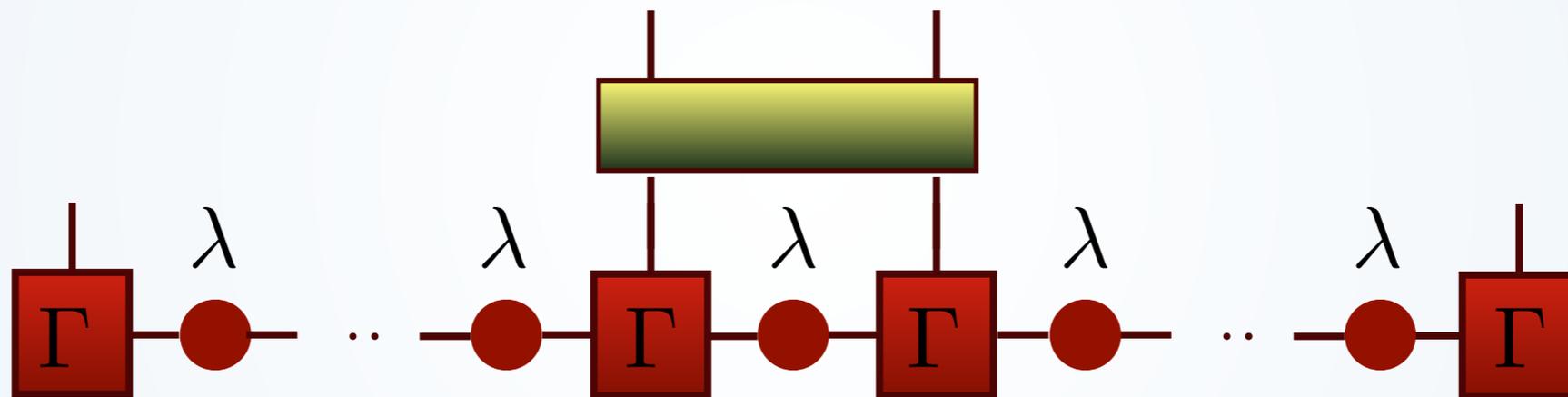
$$A^{[k]} = \Gamma^{[k]} \lambda^{[k]}$$

Schmidt values



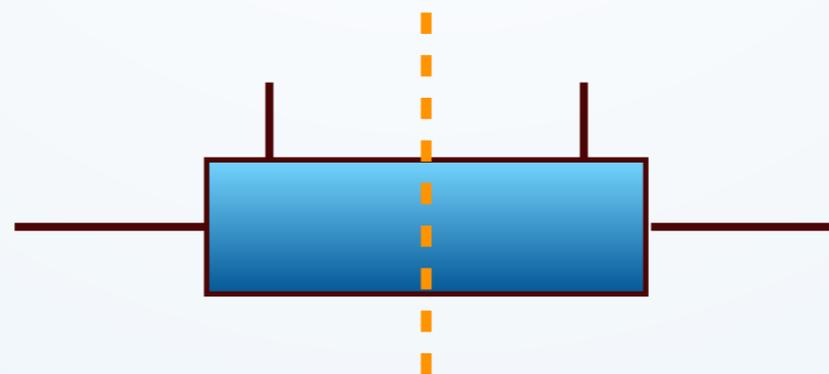
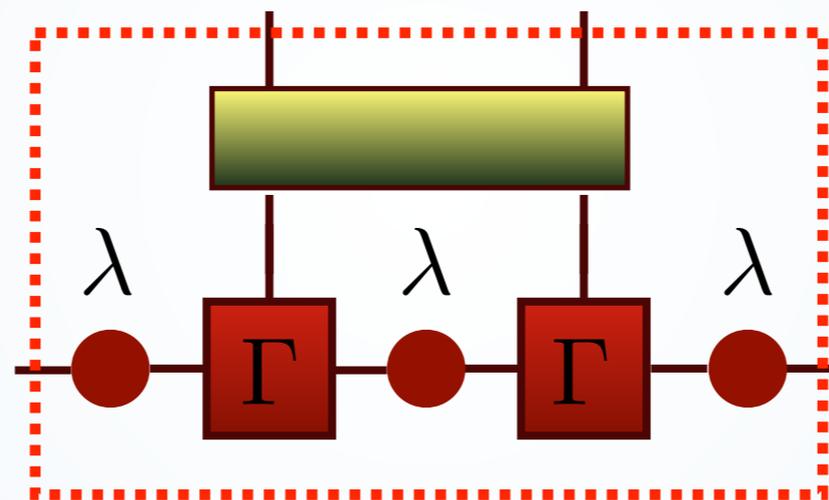
BASIC ALGORITHMS

local truncation:TEBD



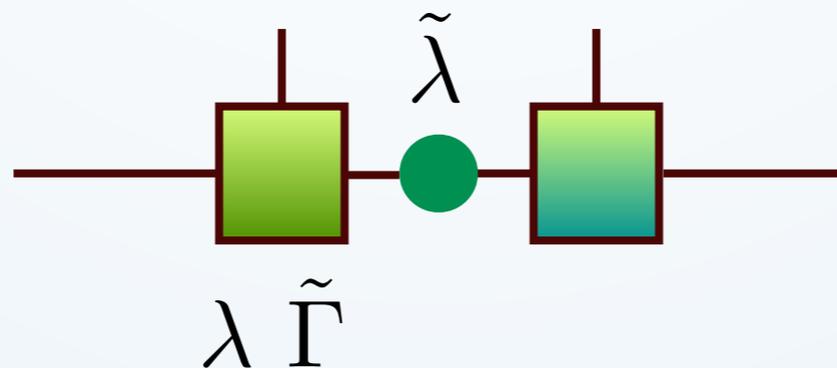
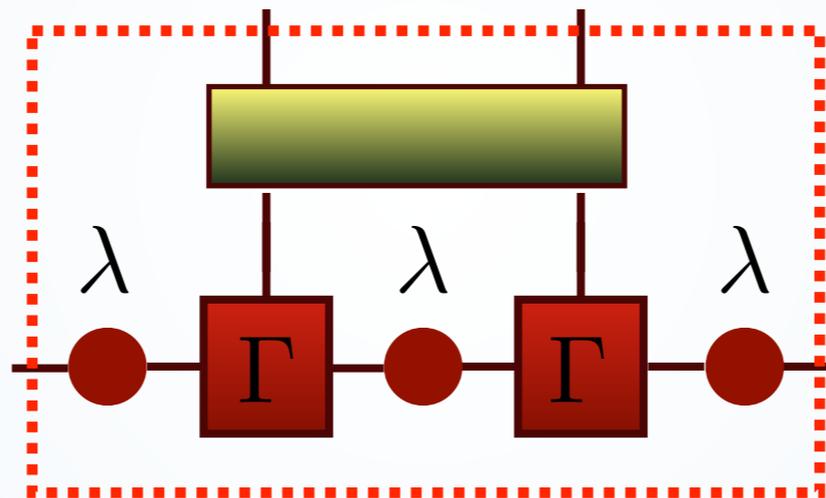
BASIC ALGORITHMS

local truncation:TEBD



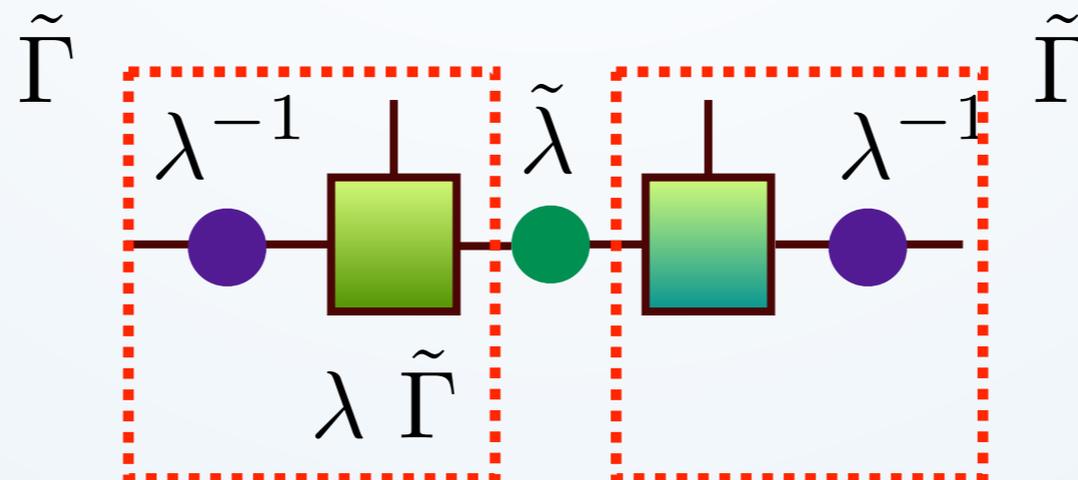
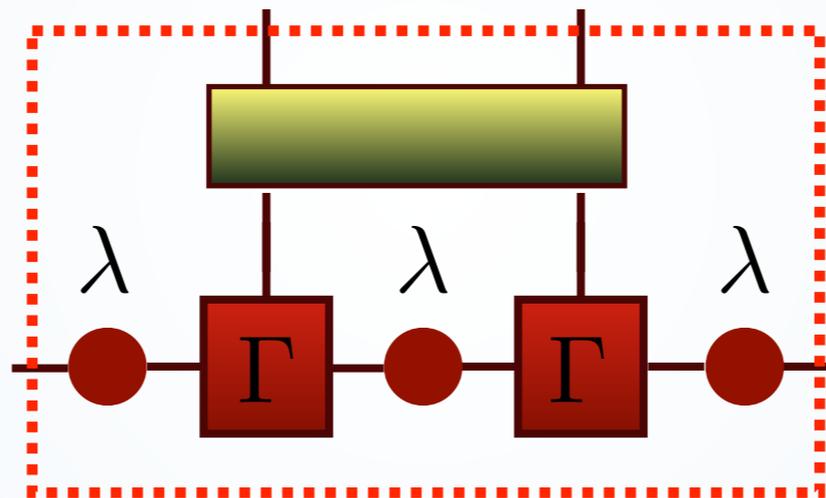
BASIC ALGORITHMS

local truncation:TEBD



BASIC ALGORITHMS

local truncation:TEBD



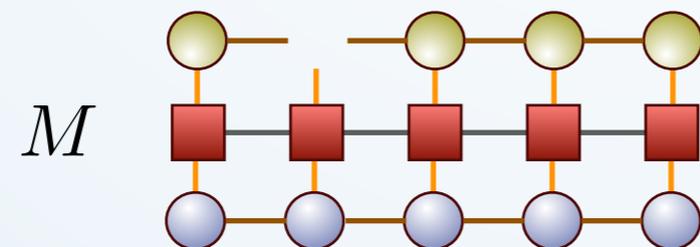
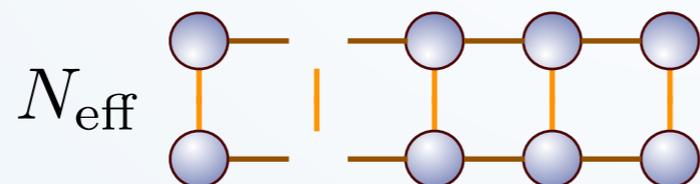
also possible in
the TD limit

BASIC ALGORITHMS

global truncation



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



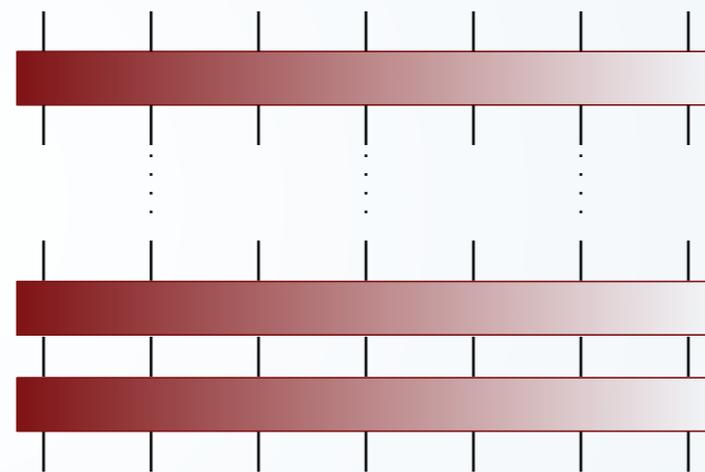
$$N_{\text{eff}}A = M$$

TIME EVOLUTION WITH MPS

BASIC ALGORITHMS

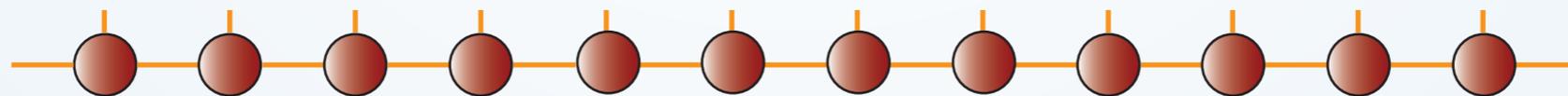
simulate time evolution

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



initial MPS

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



TEBD
t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

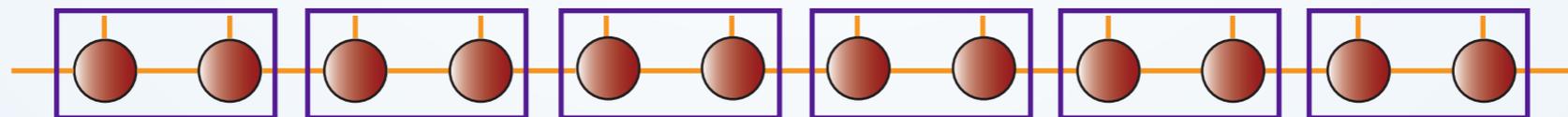
simulate time evolution

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

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

apply evolution step

Suzuki-Trotter expansion



TEBD
t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

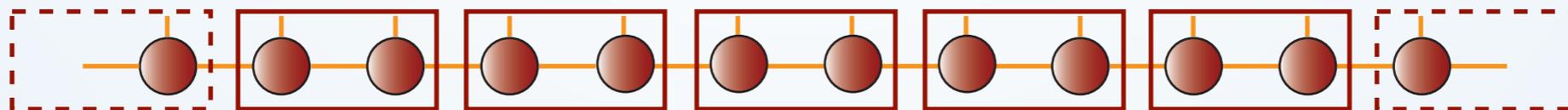
simulate time evolution

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

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

apply evolution step

Suzuki-Trotter expansion



TEBD
t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

simulate time evolution

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

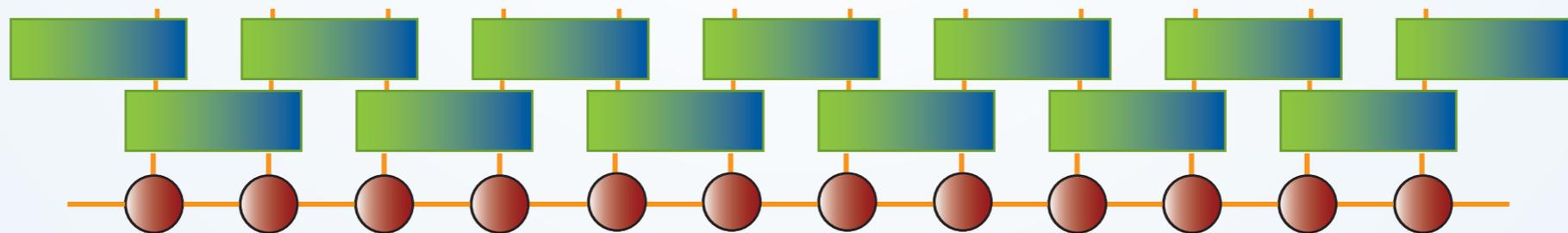
apply evolution step

$$H = H_e + H_o$$

Suzuki-Trotter expansion

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

as local terms!



TEBD
t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

simulate time evolution

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

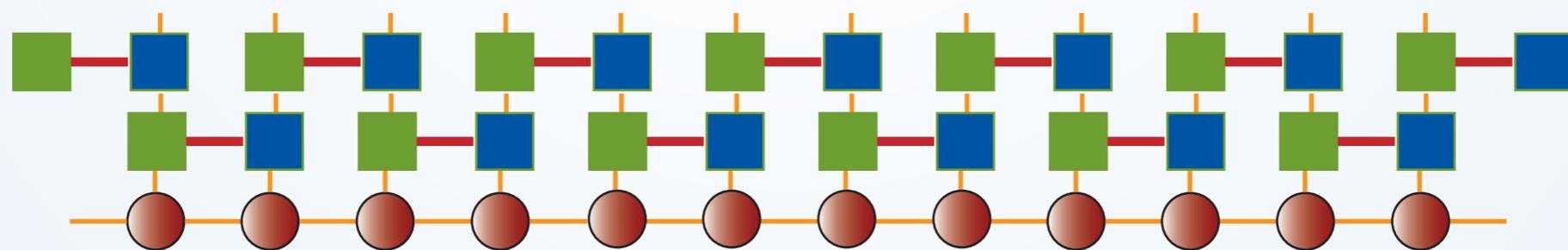
apply evolution step

$$H = H_e + H_o$$

Suzuki-Trotter expansion

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

as local terms!



MPOs

TEBD
t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

basic time evolution algorithms

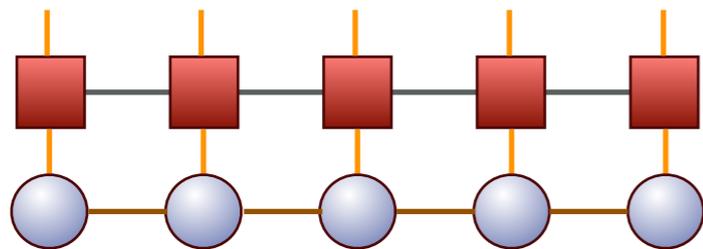
initial MPS

discrete time

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

Suzuki-Trotter expansion

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



TEBD, t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

basic time evolution algorithms

initial MPS

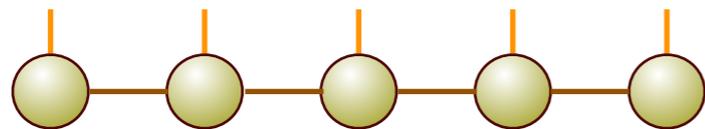
discrete time

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

Suzuki-Trotter expansion

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

truncate bond dimension



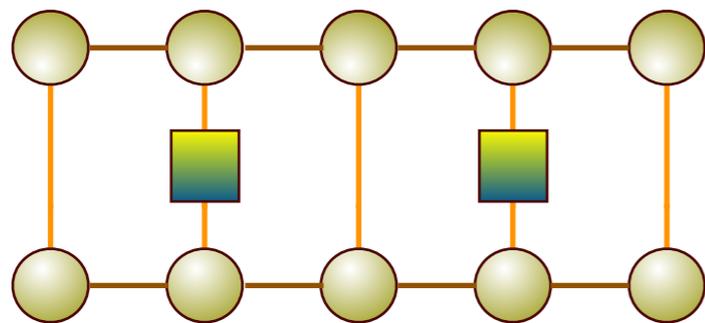
TEBD, t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

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

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

Suzuki-Trotter expansion

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

truncate bond dimension

iterate

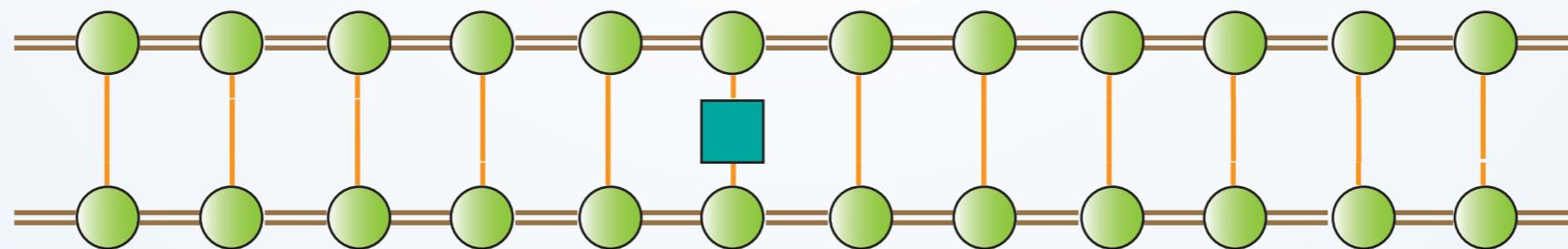
compute observables

BASIC ALGORITHMS

simulate time evolution

works for real and imaginary time

imaginary time for ground states,
thermal equilibrium



compute
observables

TEBD
t-DMRG

Vidal, PRL 2003, 2004

Verstraete, García-Ripoll, Cirac, PRL 2004

BASIC ALGORITHMS

imaginary time evolution \Rightarrow ground state

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

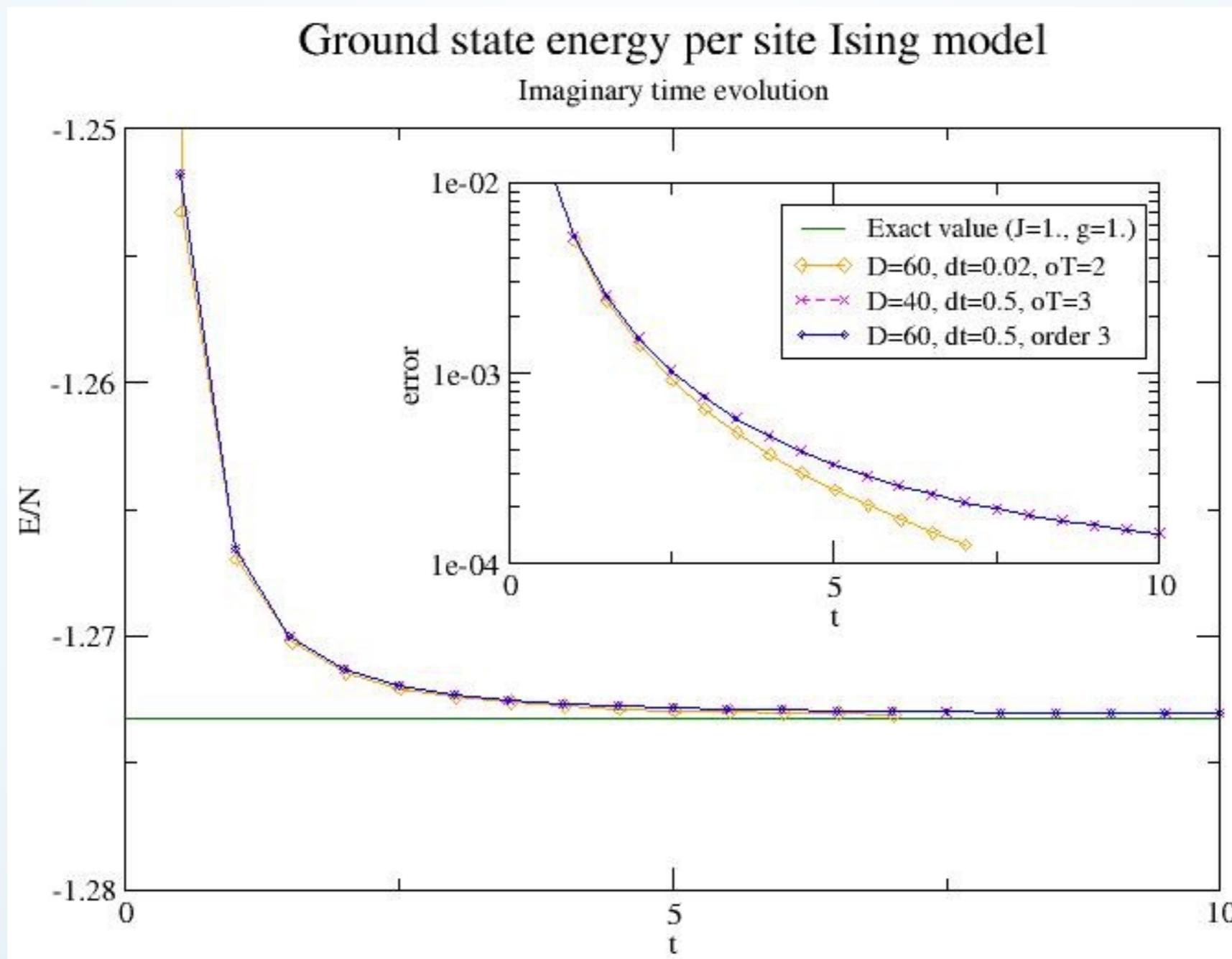
$$|\Phi_0\rangle = \sum c_n |E_n\rangle$$

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

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

BASIC ALGORITHMS

imaginary time evolution \Rightarrow ground state



BASIC ALGORITHMS

simulate time evolution

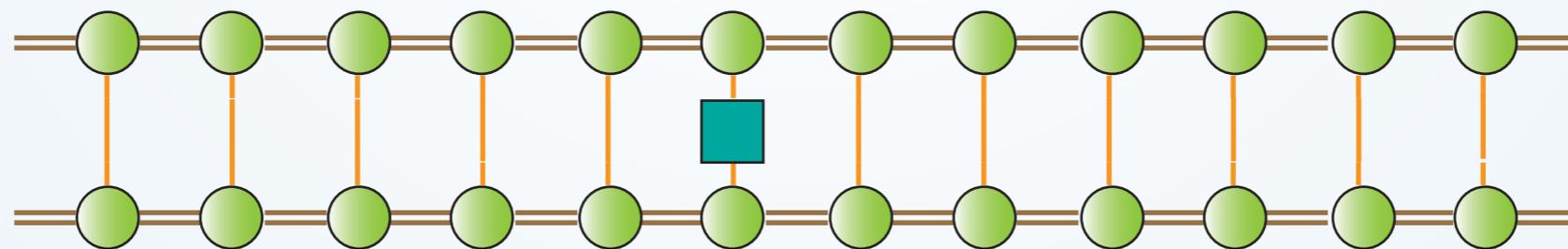
works for real and imaginary time

imaginary time for ground states,
thermal equilibrium

but out of equilibrium entanglement can grow fast!

Osborne, PRL 2006

Schuch et al., NJP 2008

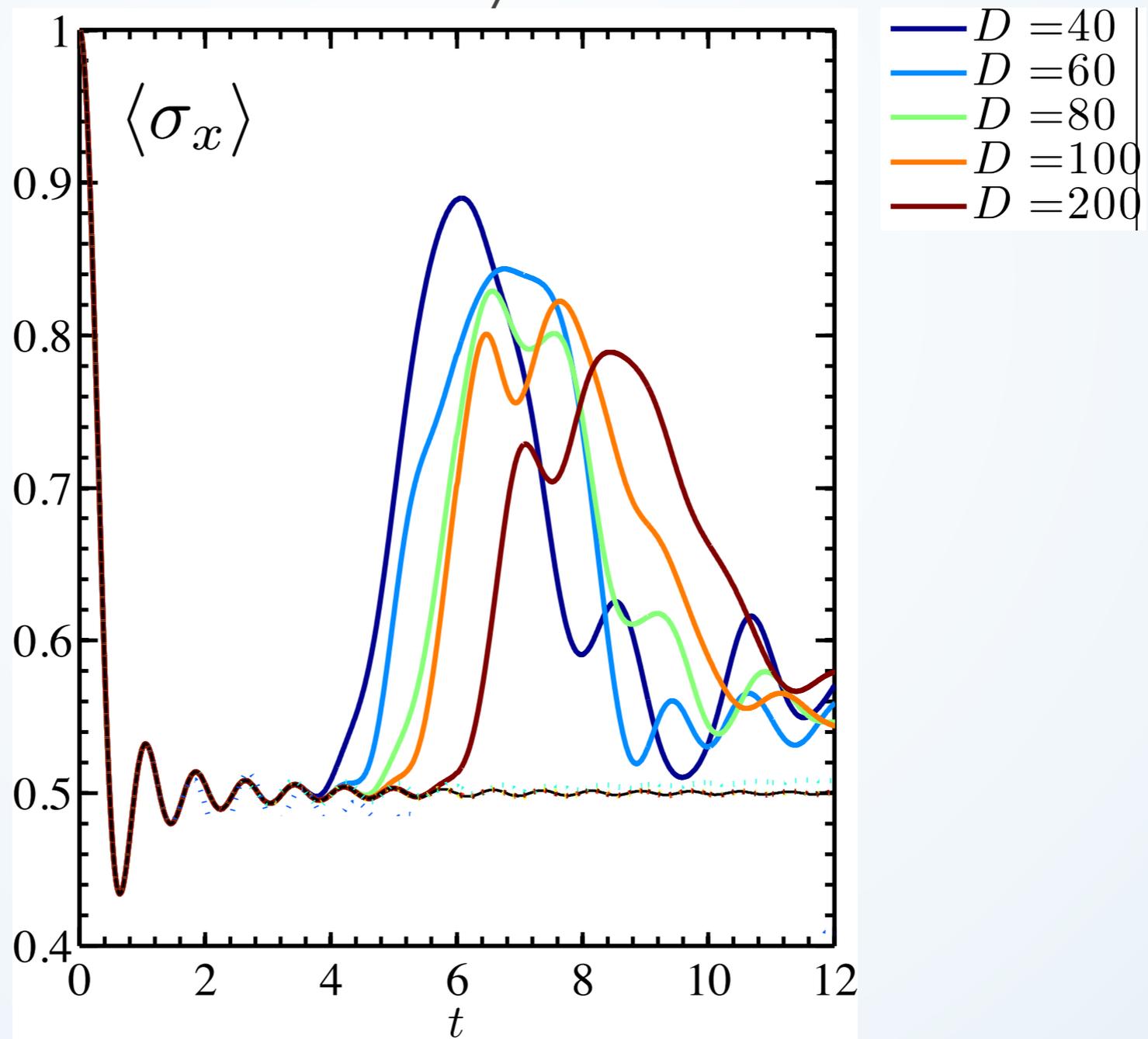


compute
observables

TEBD
t-DMRG

BASIC ALGORITHMS

real time dynamics

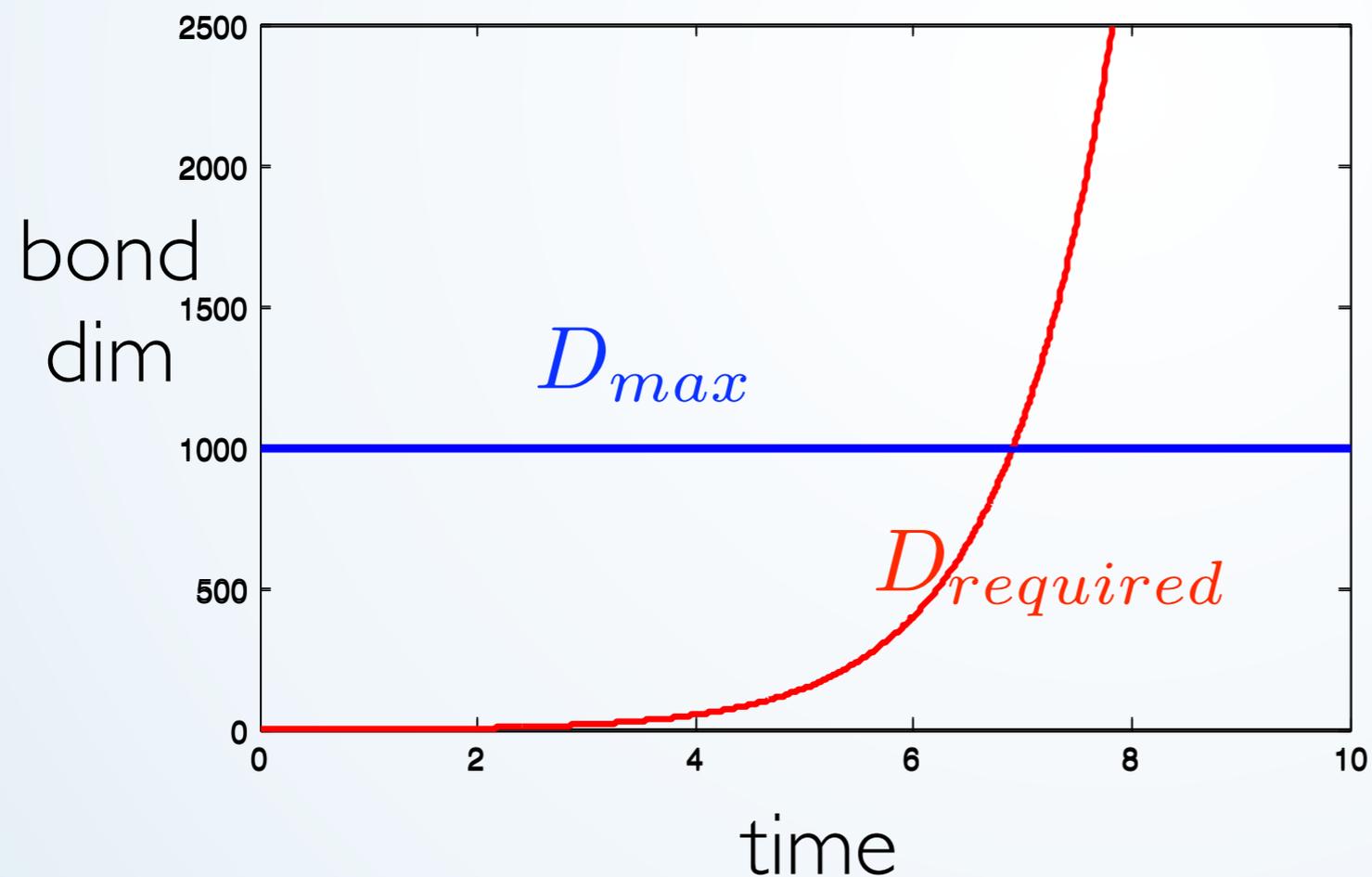


ENTANGLEMENT AND TIME EVOLUTION

ENTANGLEMENT GROWTH

Entropy of evolved state may grow linearly

Osborne, PRL 2006
Schuch et al., NJP 2008



required bond for
fixed precision

$$D \sim e^{at}$$

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 Ann. Phys. 2019

SOME OTHER APPLICATIONS

MIXED STATES

open systems, thermal...

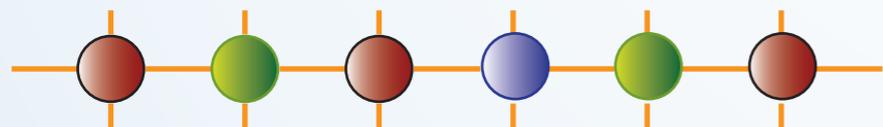
MIXED STATES

similar problems...

equilibrium \rightarrow thermal states

imaginary time evolution

time-dependent \rightarrow real time evolution



unitary $\rho(t) = U(t)\rho(0)U(t)^\dagger$

non-unitary $\frac{d\rho(t)}{dt} = \mathcal{L}(\rho)$

THERMAL STATES

THERMAL STATES

Gibbs ensemble as imaginary time evolution

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

goal: approximate as MPO

efficient!

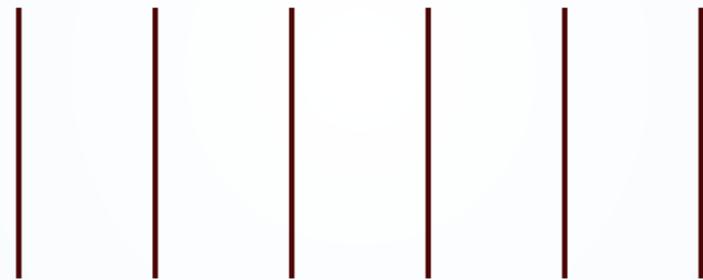
Hastings PRB 2006
Molnar et al PRB 2015

use Suzuki-Trotter expansion for exponential

$$e^{-\beta H} = e^{-\beta H} \mathbb{1} = \left(e^{-\frac{\beta}{M} H} \right)^M \mathbb{1}$$

THERMAL STATES

purification natural



vectorize

$$e^{-\beta H} = e^{-\beta H} \mathbb{1} = \left(e^{-\frac{\beta}{M} H} \right)^M \mathbb{1}$$

THERMAL STATES

purification natural

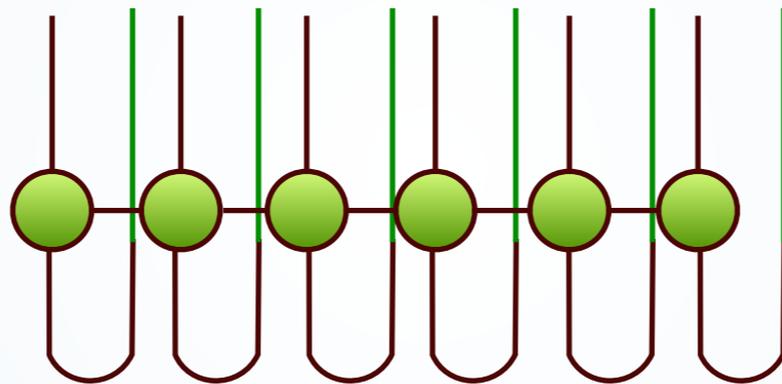


vectorize

$$e^{-\beta H} = e^{-\beta H} \mathbb{1} = \left(e^{-\frac{\beta}{M} H} \right)^M \mathbb{1}$$

THERMAL STATES

purification natural



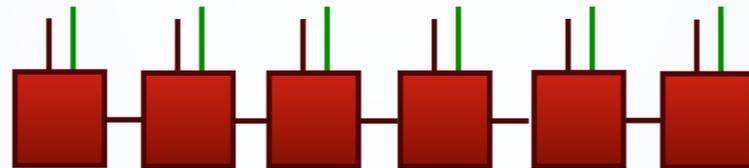
vectorize

$$e^{-\beta H} = e^{-\beta H} \mathbb{1} = \left(e^{-\frac{\beta}{M} H} \right)^M \mathbb{1}$$

THERMAL STATES

purification natural

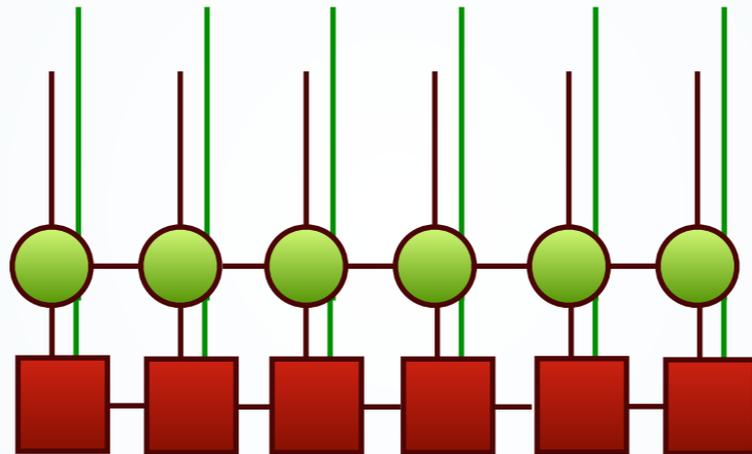
vectorize



$$e^{-\beta H} = e^{-\beta H} \mathbb{1} = \left(e^{-\frac{\beta}{M} H} \right)^M \mathbb{1}$$

THERMAL STATES

purification natural

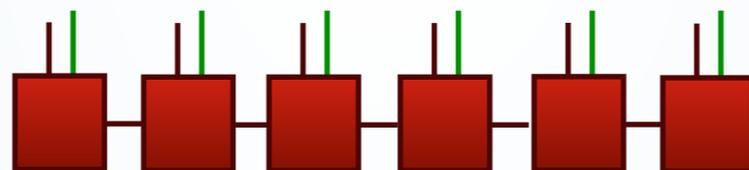


vectorize

$$e^{-\beta H} = e^{-\beta H} \mathbb{1} = \left(e^{-\frac{\beta}{M} H} \right)^M \mathbb{1}$$

THERMAL STATES

purification natural



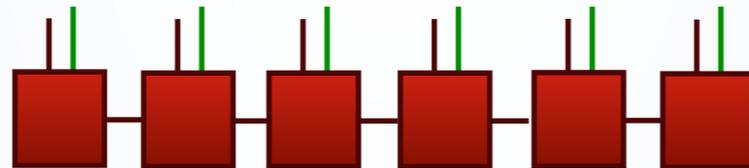
vectorize

THERMAL STATES

purification natural

$$\rho(\beta) \propto \rho(\beta/2)\rho(\beta/2)^\dagger$$

vectorize

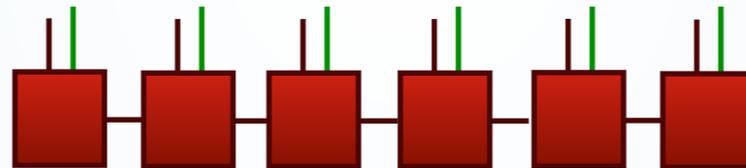


THERMAL STATES

purification natural

$$\rho(\beta) \propto \rho(\beta/2)\rho(\beta/2)^\dagger$$

vectorize



combining real time evolution can compute thermal
response functions

Barthel, NJP 2013

alternative method: METTS [White, PRL 2009](#)

[Binder, Barthel, PRB 2015](#)

OPEN SYSTEMS

OPEN SYSTEMS

non-unitary dynamics

Real-time evolution produces

$$\frac{d\rho(t)}{dt} = \mathcal{L}(\rho) \longrightarrow \mathcal{L}(\rho_S) = 0 \quad \text{a steady state}$$

fixed point of
Liouvillian map

dissipative QC
dissipative QPT

We can approximate it as a MPO

simulating long
time evolution
~imaginary time evolution

variationally
~DMRG

OPEN SYSTEMS

non-unitary dynamics

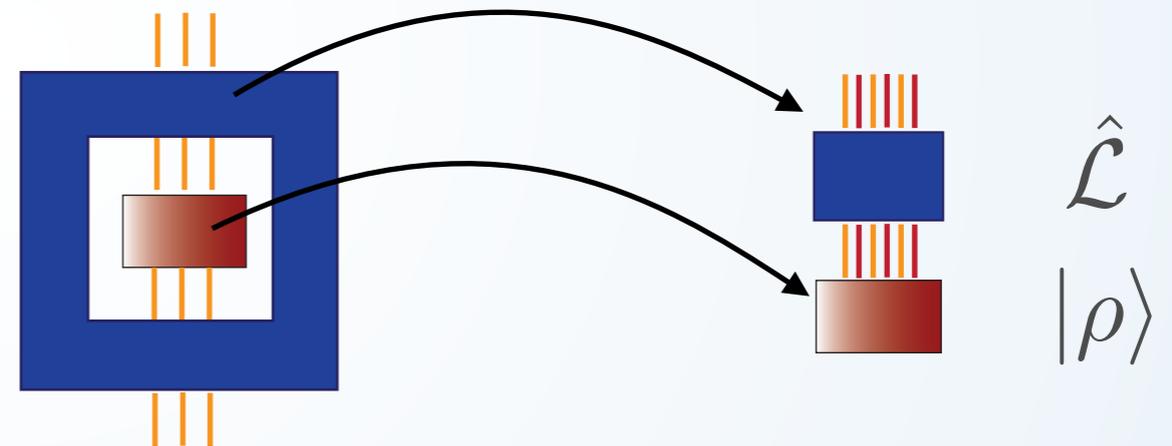
Dynamics determined by Liouvillian

$$\frac{d\rho}{dt} = \mathcal{L}(\rho)$$

vectorize $|\rho\rangle$

superoperator $\hat{\mathcal{L}}$

$$|\rho(t)\rangle = e^{\mathcal{L}t} |\rho(0)\rangle$$



NESS

fixed point of evolution

$$\hat{\mathcal{L}}|\rho\rangle = 0$$

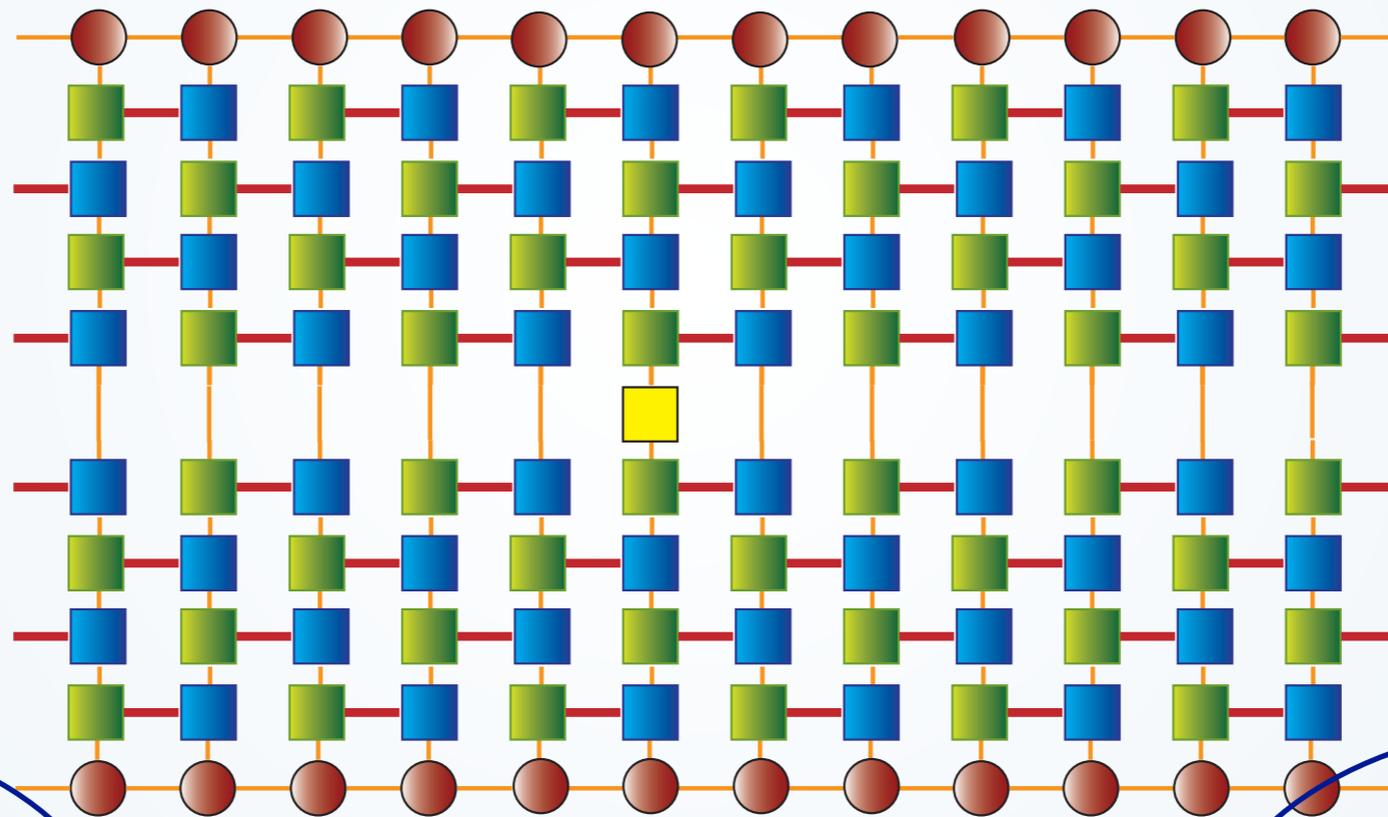
SOME ALTERNATIVES FOR REALTIME EVOLUTION

avoid representing the
state as MPS

ALTERNATIVELY...

time dependent
observables as TN

problem is contracting
the network



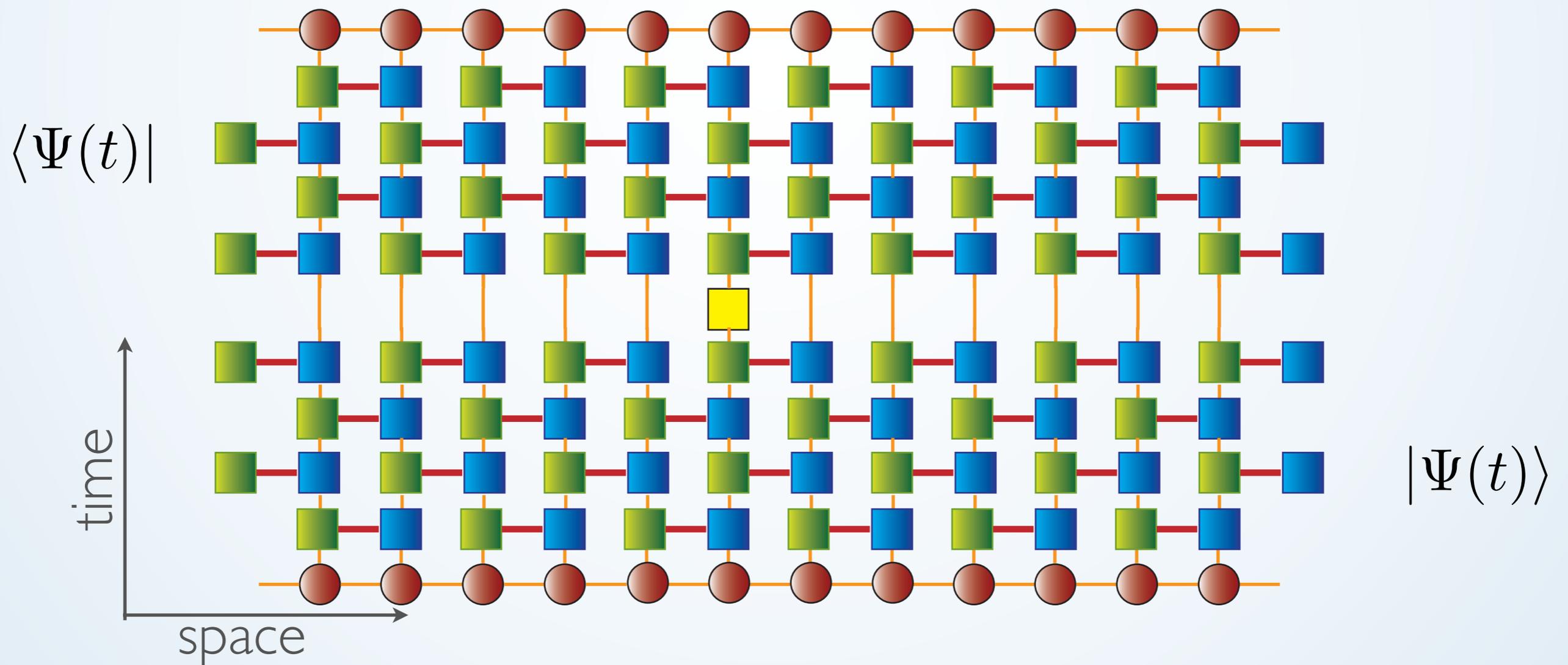
TN describe
observables, not
states

exact contraction
not possible
#P complete

key: *entanglement* in TN

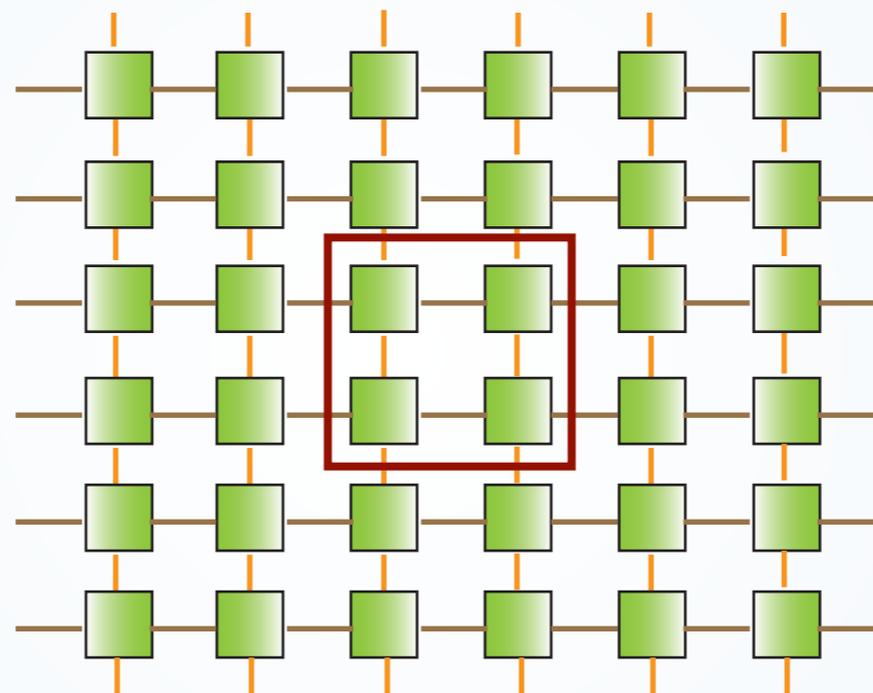
OBSERVABLE AS TN

$$\langle \Psi(t) | O | \Psi(t) \rangle$$



tensor networks may describe partition functions (observables)

need to contract a TN

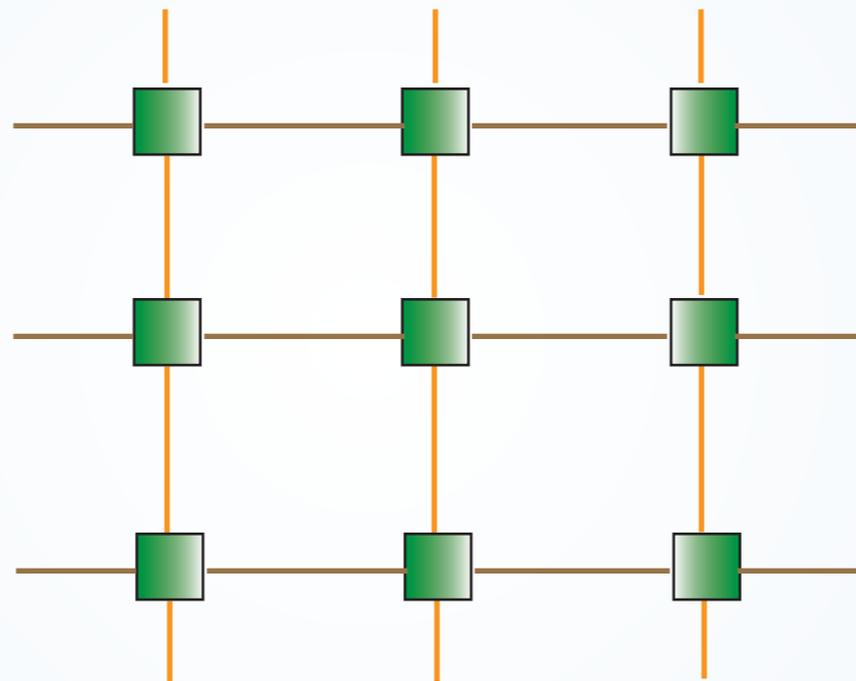


TRG approaches

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

tensor networks may describe partition functions (observables)

need to contract a TN

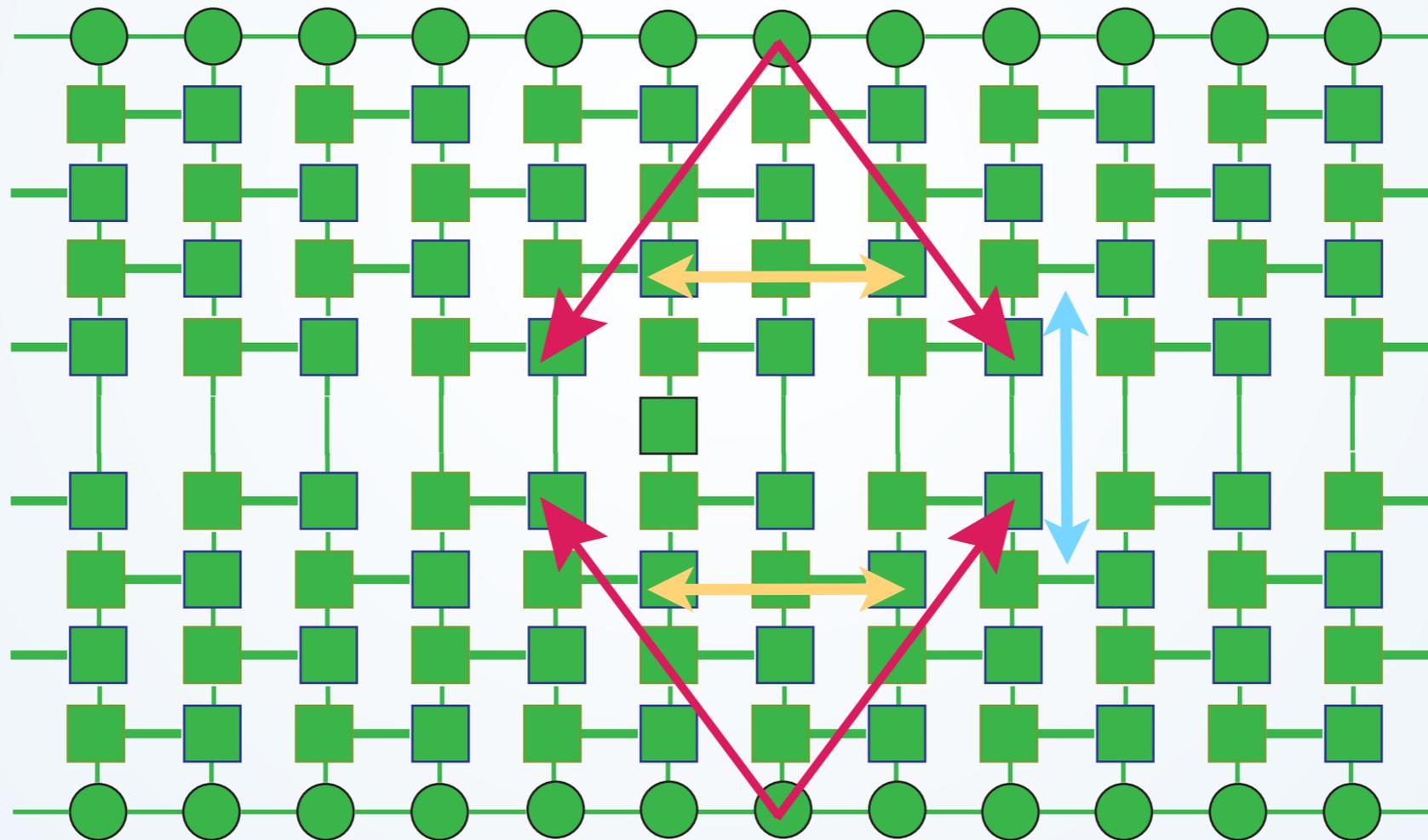


TRG approaches

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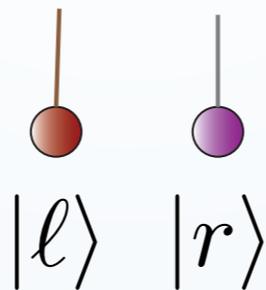
OBSERVABLE AS TN

intuition: model free propagating excitations

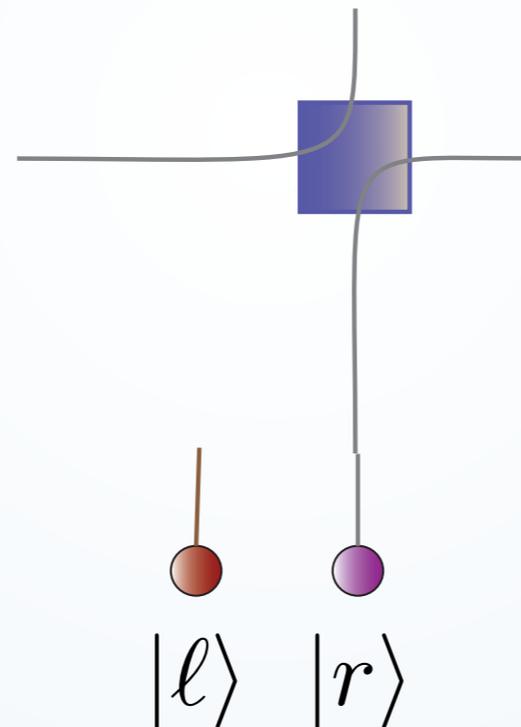


Toy Tensor Network model helps to understand entanglement in the network

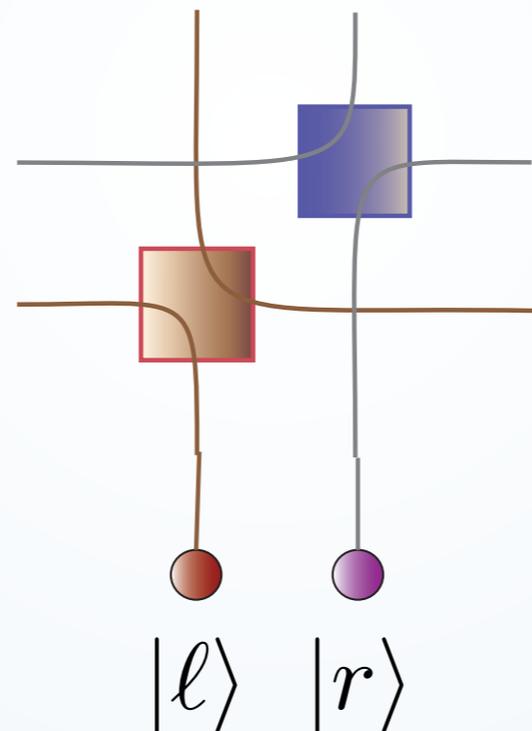
TOY MODEL TN



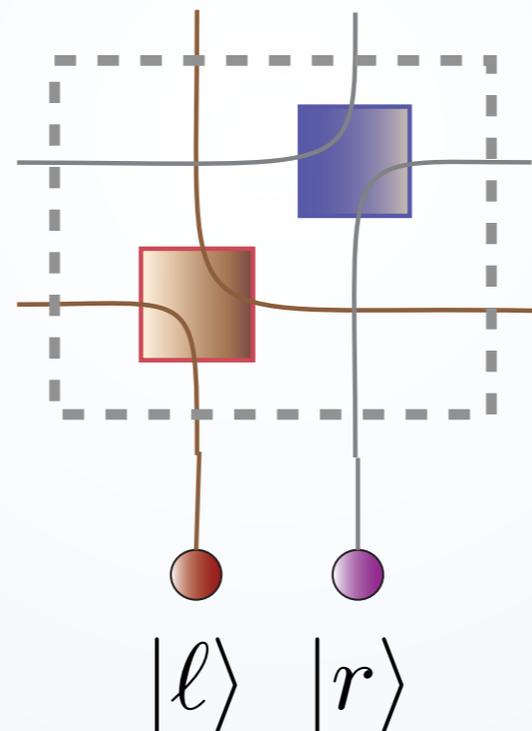
TOY MODEL TN



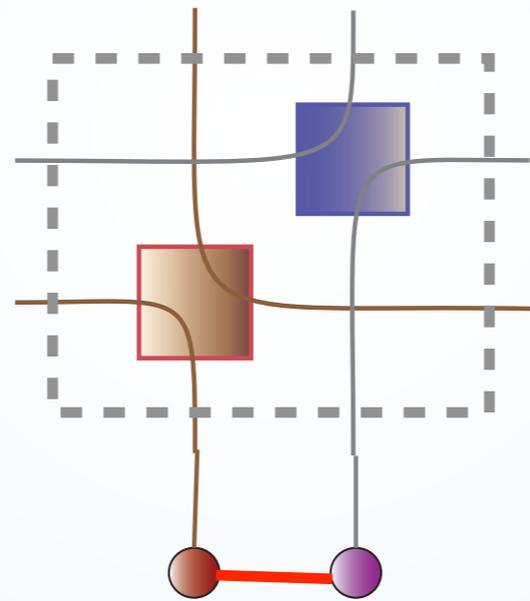
TOY MODEL TN



TOY MODEL TN

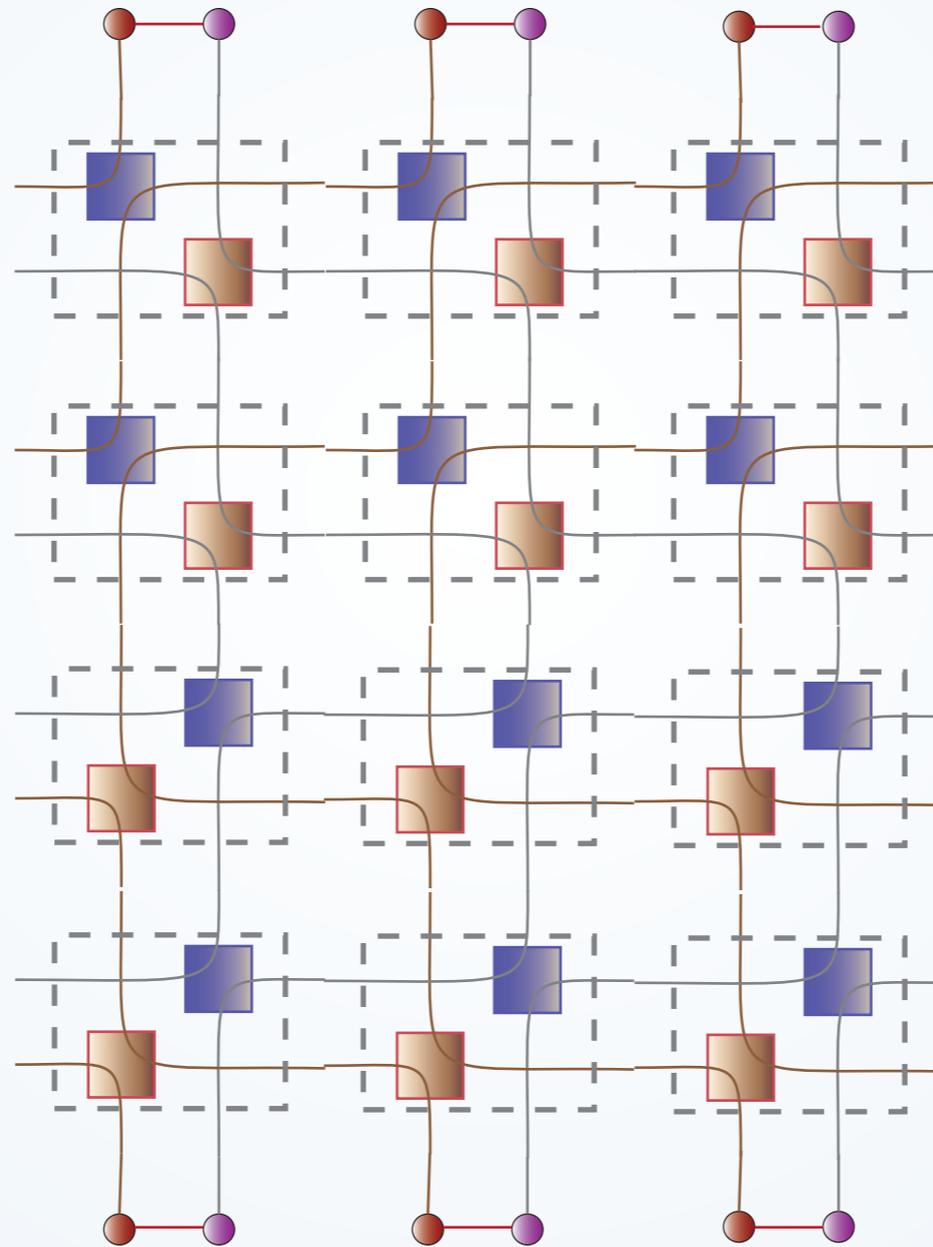


TOY MODEL TN



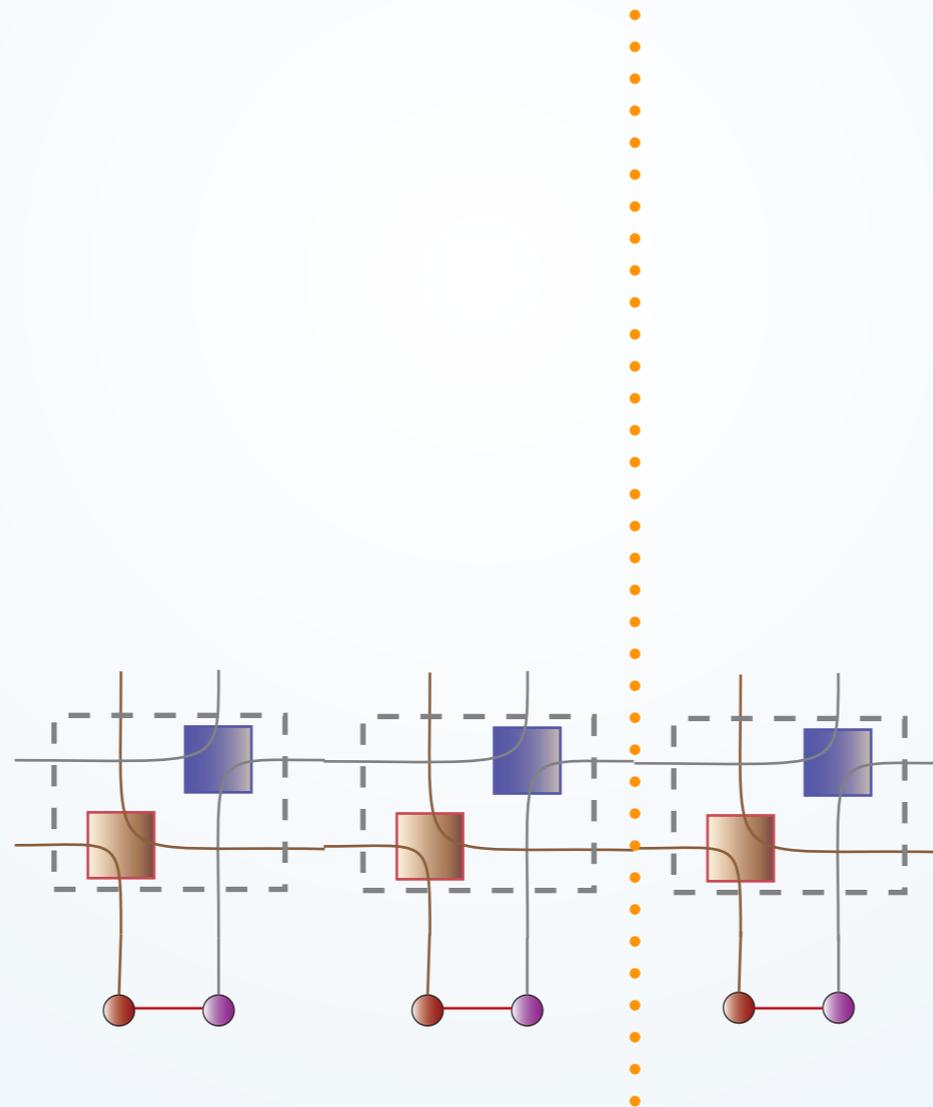
$$|\ell\rangle \otimes |0\rangle + |0\rangle \otimes |r\rangle$$

TOY MODEL TN



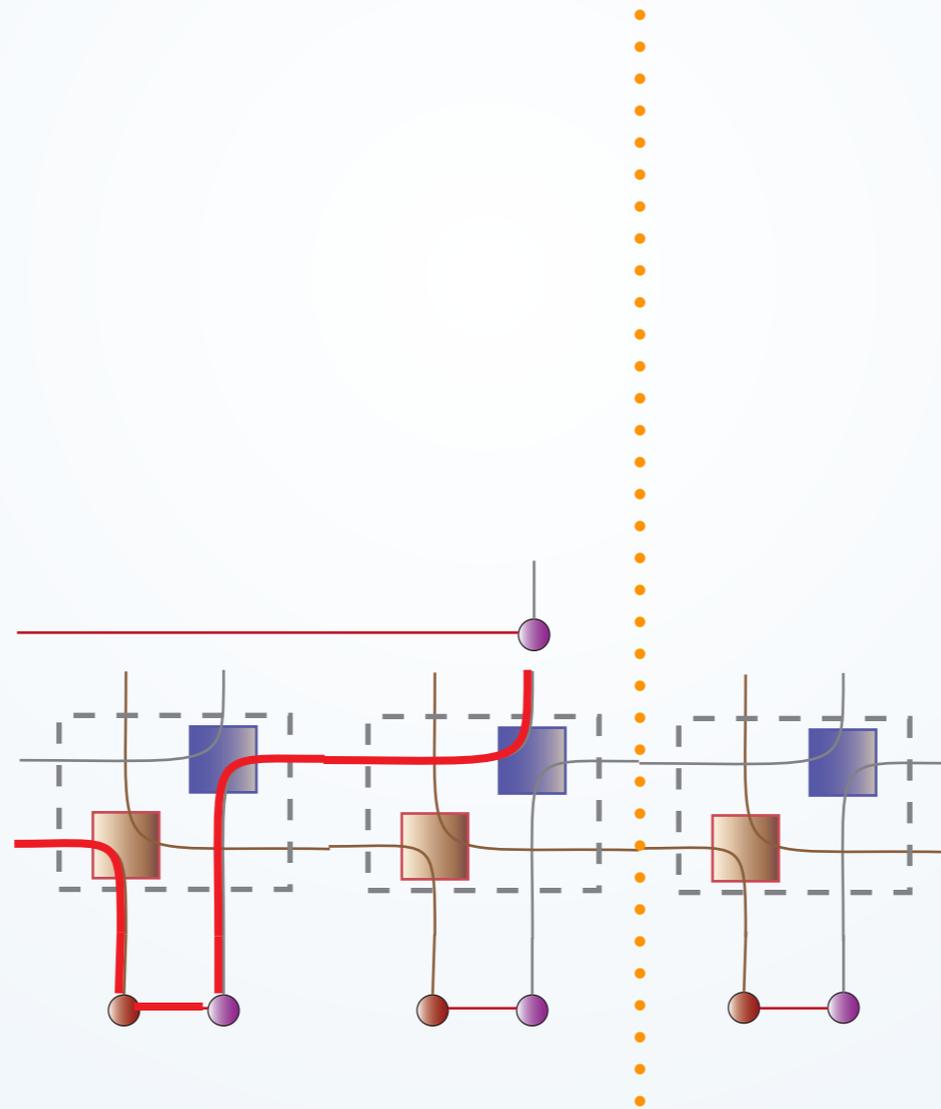
MCB, Hastings, Verstraete, Cirac, PRL 2009
Müller-Hermes, Cirac, MCB, NJP 2012

TOY MODEL TN



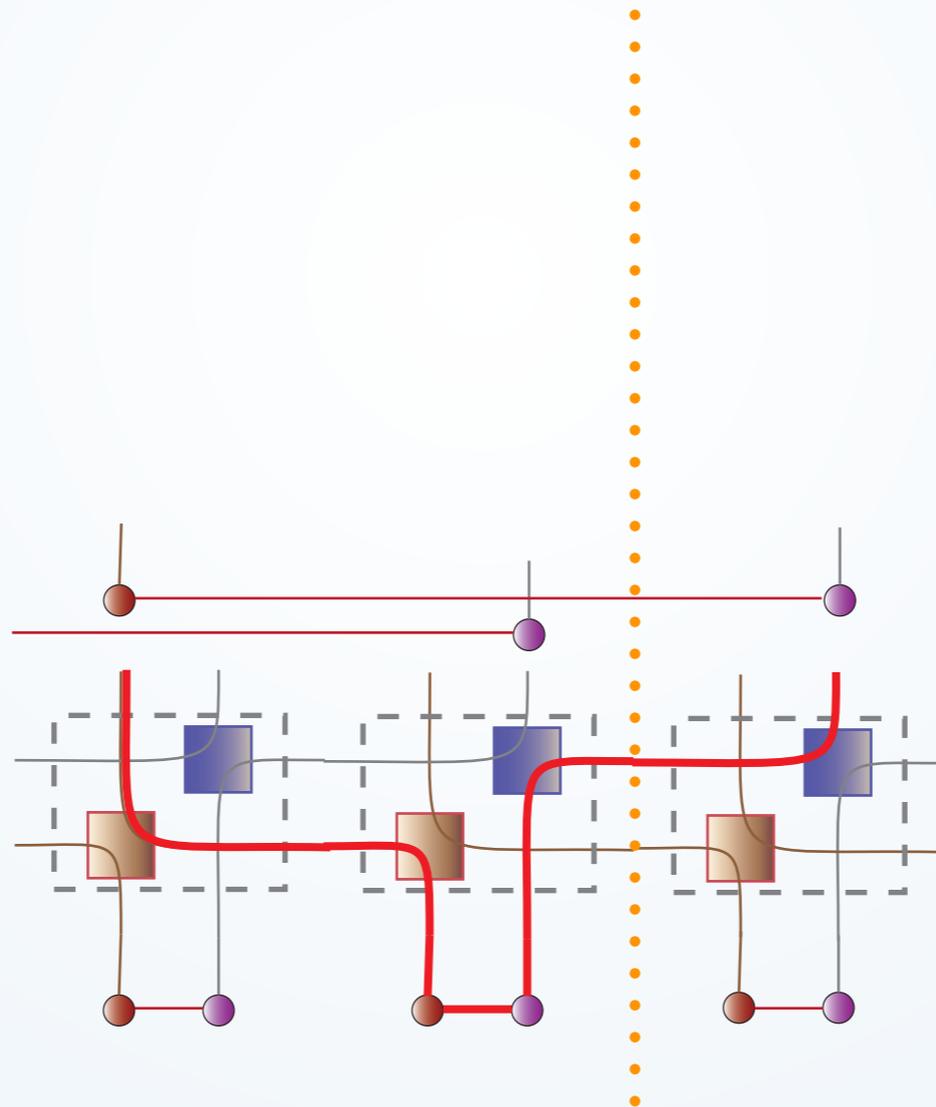
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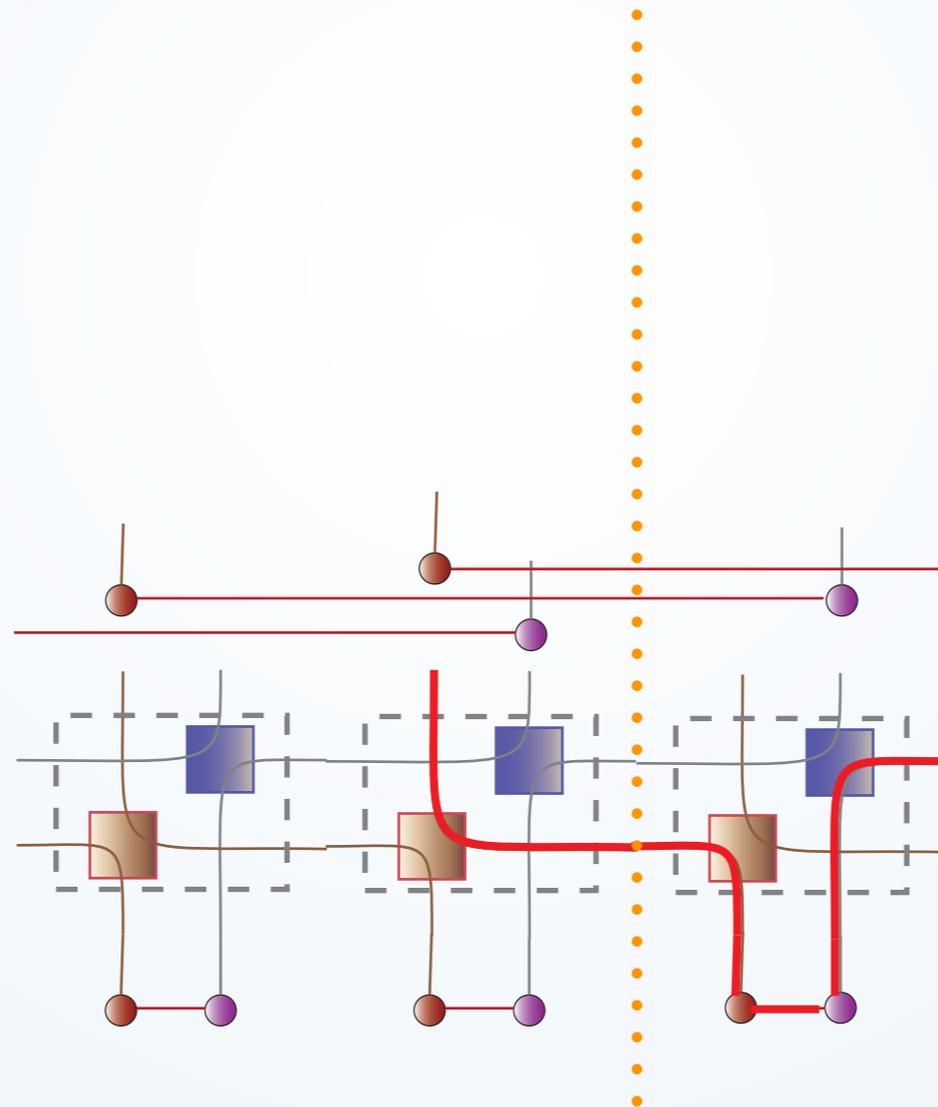
MCB, Hastings, Verstraete, Cirac, PRL 2009
Müller-Hermes, Cirac, MCB, NJP 2012

TOY MODEL TN



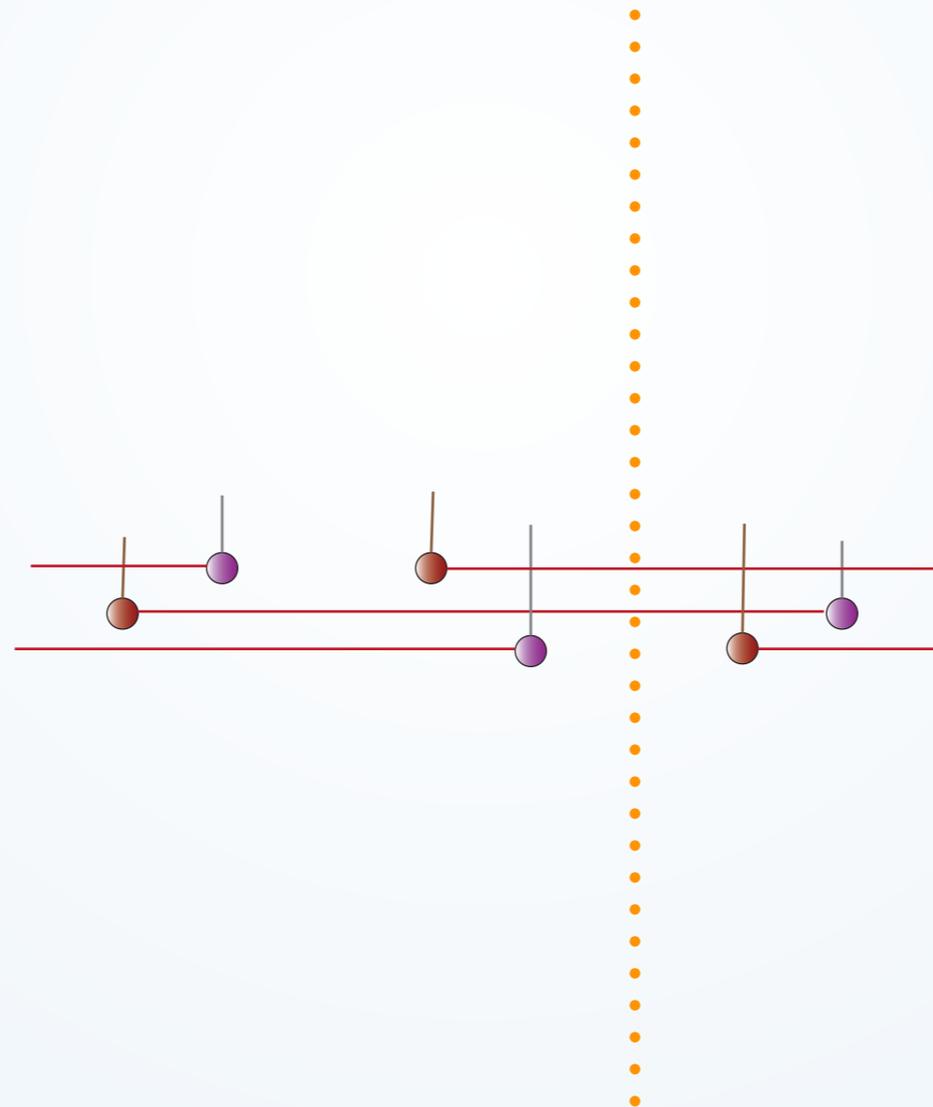
MCB, Hastings, Verstraete, Cirac, PRL 2009
Müller-Hermes, Cirac, MCB, NJP 2012

TOY MODEL TN



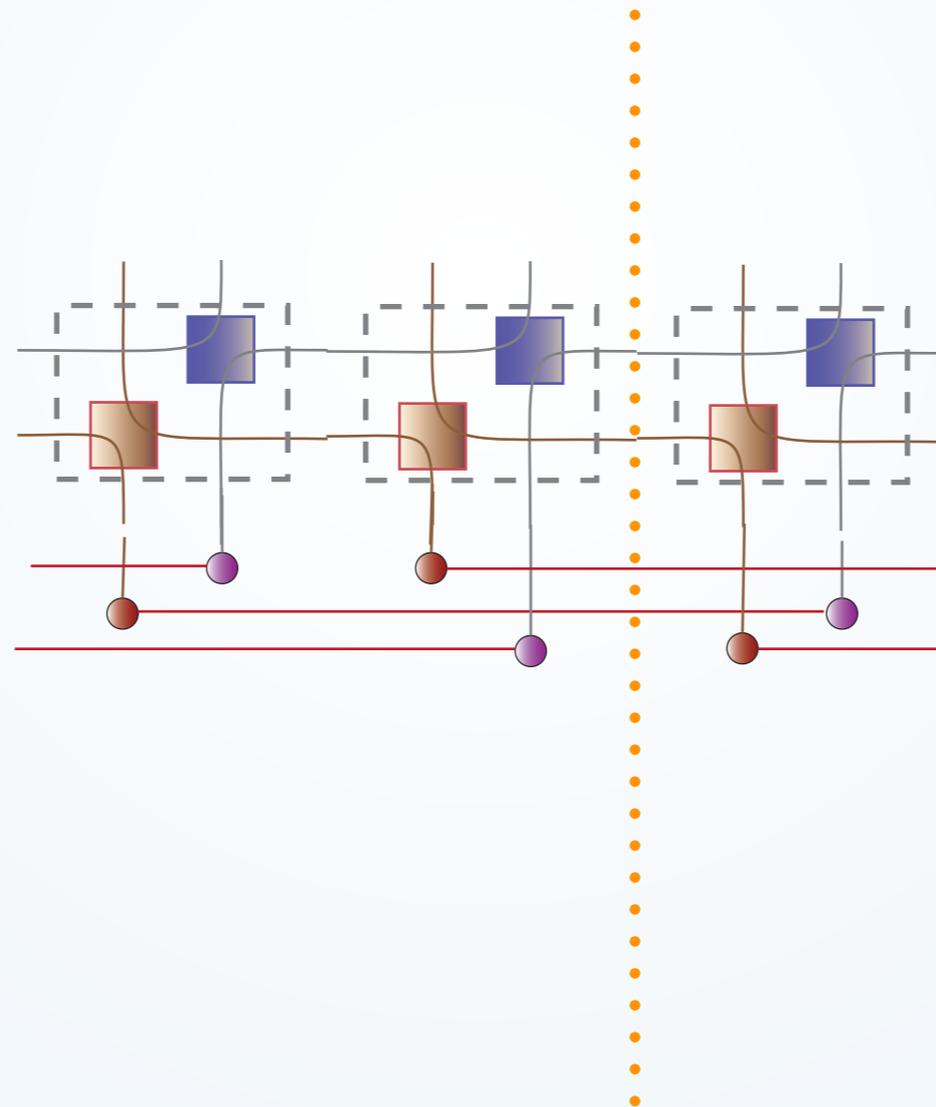
MCB, Hastings, Verstraete, Cirac, PRL 2009
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TOY MODEL TN



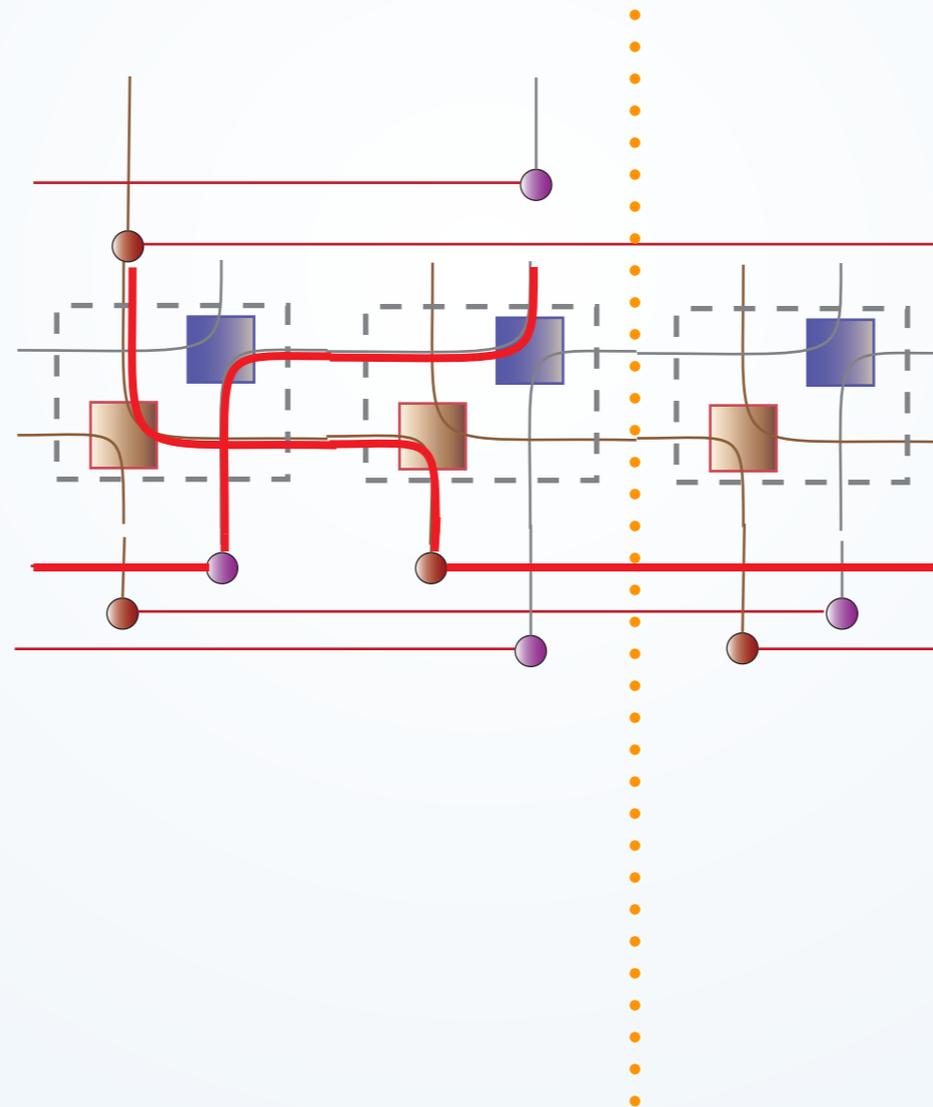
MCB, Hastings, Verstraete, Cirac, PRL 2009
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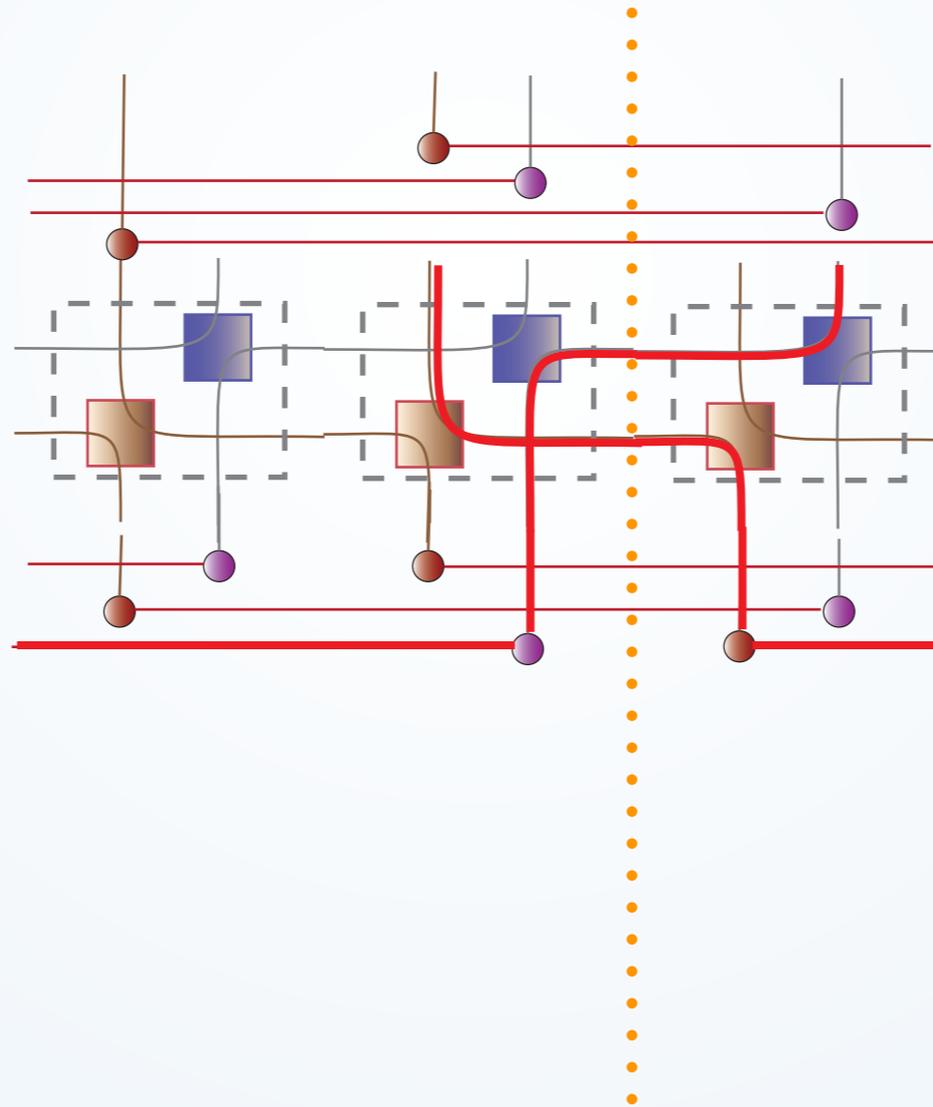
MCB, Hastings, Verstraete, Cirac, PRL 2009
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TOY MODEL TN



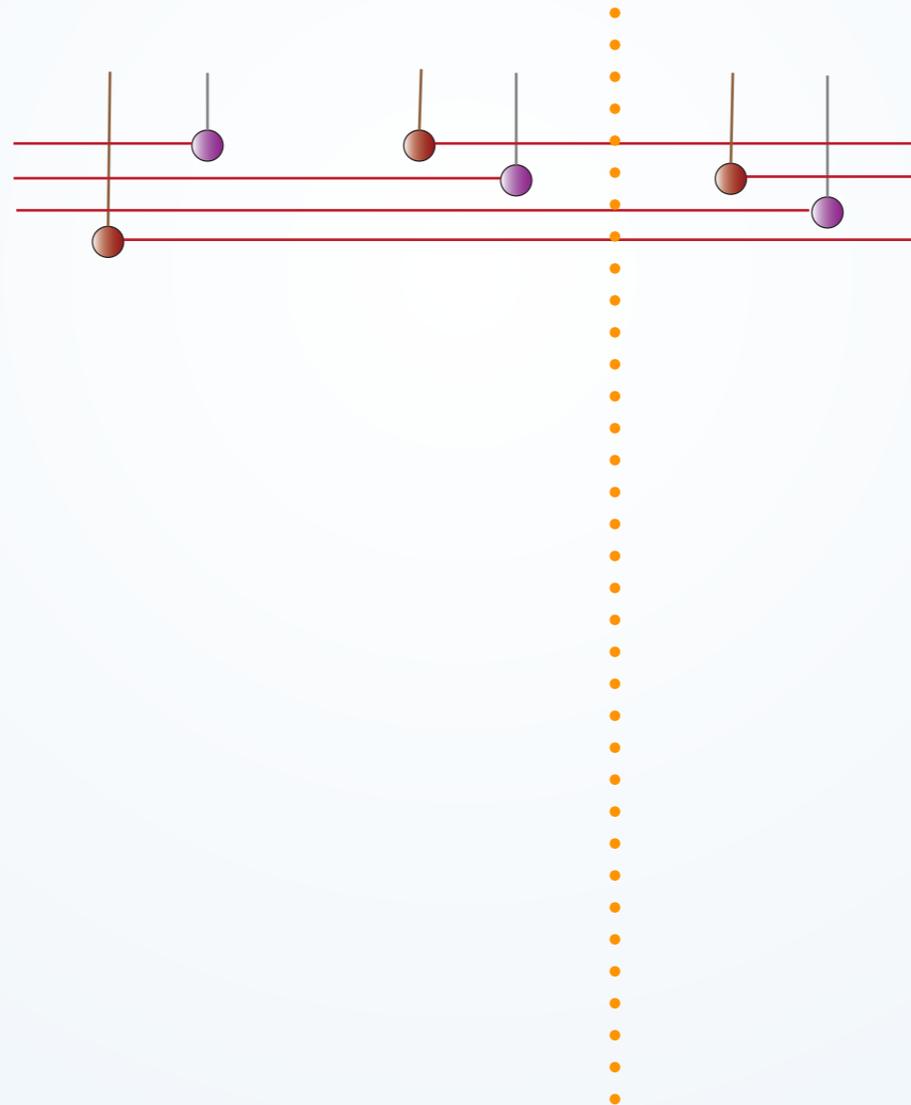
MCB, Hastings, Verstraete, Cirac, PRL 2009
Müller-Hermes, Cirac, MCB, NJP 2012

TOY MODEL TN



MCB, Hastings, Verstraete, Cirac, PRL 2009
Müller-Hermes, Cirac, MCB, NJP 2012

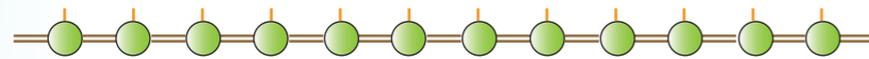
TOY MODEL TN



MCB, Hastings, Verstraete, Cirac, PRL 2009
Müller-Hermes, Cirac, MCB, NJP 2012

various evolution algorithms

evolving the (pure state) ansatz



entanglement can grow fast!

Vidal, PRL 2003, PRL 2007

White, Feiguin, PRL 2004

Daley et al., 2004

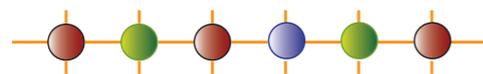
Haegeman et al., 2011

Osborne, PRL 2006

Schuch et al., NJP 2008

evolving operators: Heisenberg picture

Hartmann et al, PRL 2009

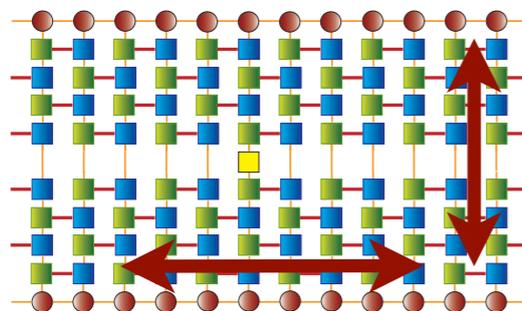


also for mixed states

operator space entanglement

Prosen Pizorn, PRL 2008

observables as TN to contract



different *entanglement* quantities

MCB, Hastings, Verstraete, Cirac, PRL 2009

Müller-Hermes et al., NJP 2012

Hastings, Mahajan 2014

Frías-Pérez, MCB 2201.08402

THERMALIZATION

a question we would like to solve

THERMALIZATION

Closed quantum system initialized out of equilibrium

does it thermalize?

do local observables
reach thermal
equilibrium values?

independent of
details of initial state?

predicted by
statistical mechanics?

analytical techniques: exactly solvable systems

GGE

Rigol et al. PRL 2007
Cramer et al. PRL 2008
Calabrese et al. PRL 2011
Ilievski et al. PRL 2015

THERMALIZATION

Closed quantum system initialized out of equilibrium

does it thermalize?

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reach thermal
equilibrium values?

independent of
details of initial state?

predicted by
statistical mechanics?

non-integrable systems

Deutsch PRA91
Srednicki PRE94
Rigol et al. Nature 2008

ETH mechanism
time scales?

numerical
simulations of real
time evolution

global quench in 1D

entanglement
barrier

TNS challenge:
getting around this
limitation

$$D_{\min}(t) \sim e^{\alpha t}$$

$$S(t) \propto t$$

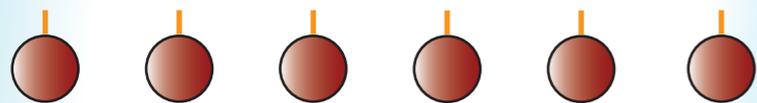
Osborne, PRL 2006
Schuch et al., NJP 2008

some recent progress
Dubai JPhysA 2017
Leviatan et al. 2017
White et al PRB 2018
Surace et al. 2018

 **work in
progress!**
Yang et al. PRL 2020
Lui et al PRX Quantum 2021
Frías-Pérez, MCB 2201.08402

$t = 0$

product state

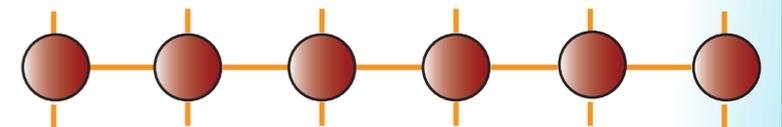


easy to write as MPS

local
observables

$t = \infty$

thermal states

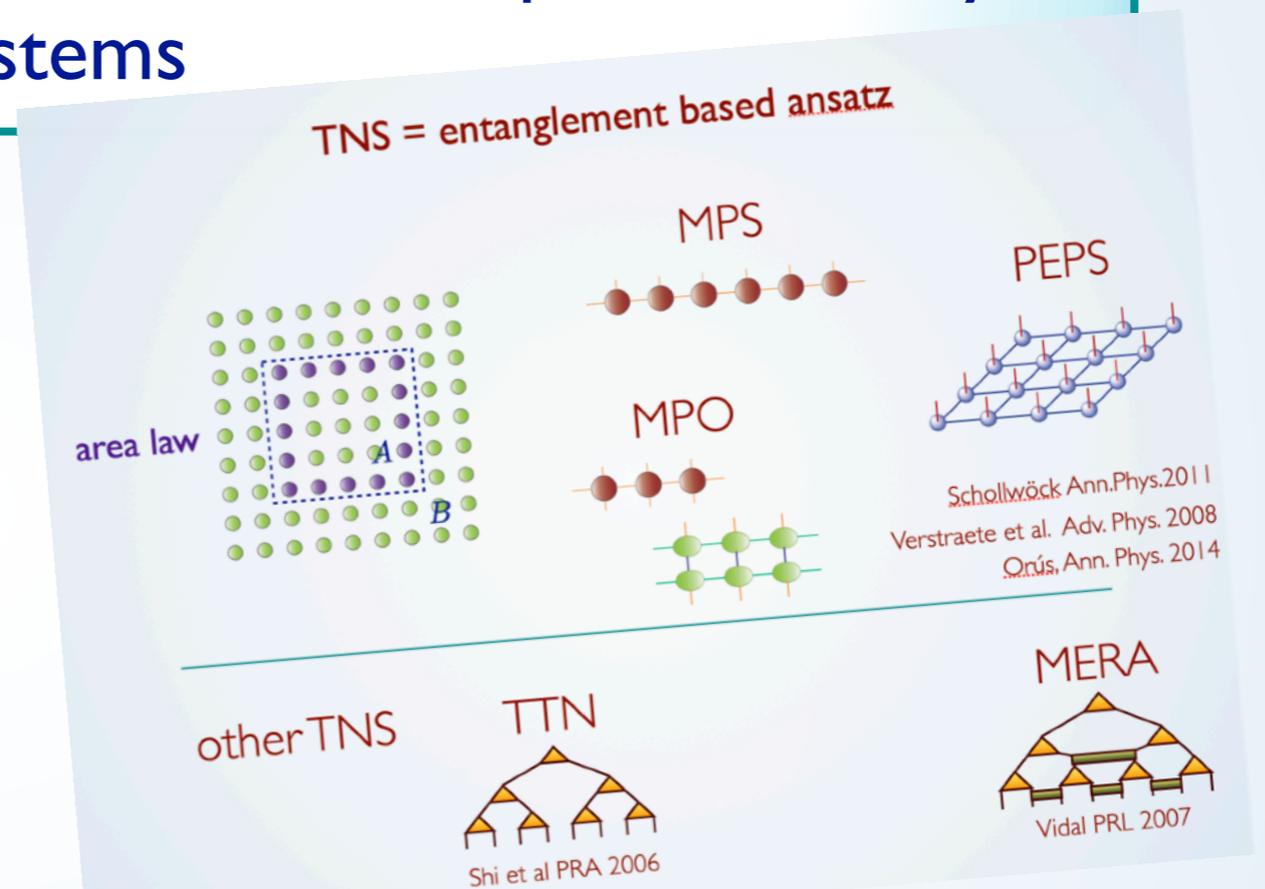


well approximated as MPO

to conclude...

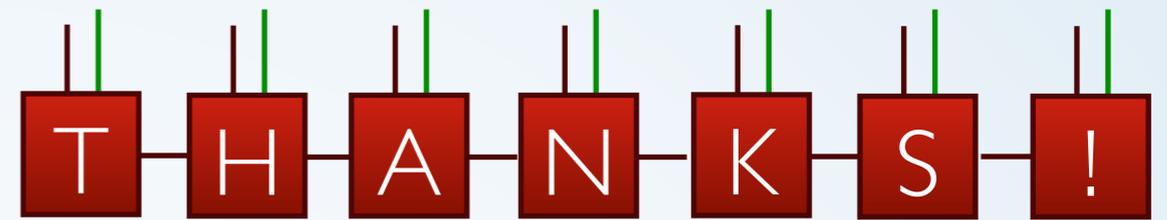
TNS: (quantum inspired) methods to describe quantum many-body systems

NOTES:



efficient algorithms to find ground states, thermal states

simulating time evolution/arbitrary quantum circuits requires
truncation \Rightarrow limited



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](https://arxiv.org/abs/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](https://arxiv.org/abs/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](https://arxiv.org/abs/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](https://arxiv.org/abs/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](https://arxiv.org/abs/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](https://arxiv.org/abs/1710.03733)

Introduction to Tensor Network Methods: Numerical simulations of low-dimensional many-body quantum
systems, S. Montangero, Springer, 2018.



Max Planck Institut
of Quantum Optics
(Garching)



March 2022

THANKS!



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