Tensor Network States: ground states and time evolution of spin systems

M. C. Bañuls
Max Planck Institut für Quantenoptik
Garching (Germany)

Why Tensor Network States

Long time evolution with MPS

Tensor Network States: MPS, PEPS and others

A short incomplete review

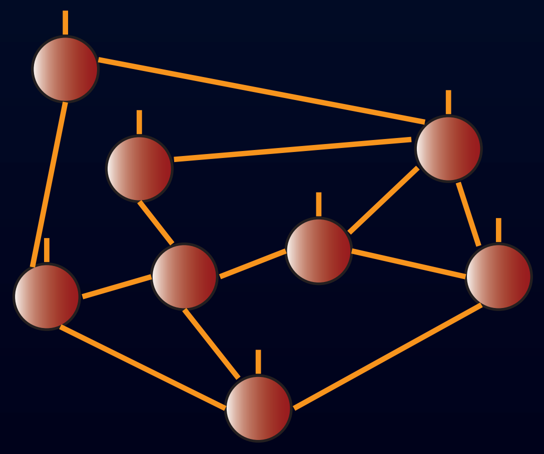
What are TNS?

- TNS = Tensor Network States

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

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

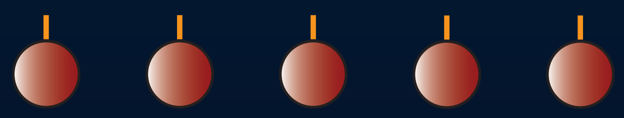
N-legged tensor



A TNS has only a polynomial number of parameters

What are TNS?

- A particular example



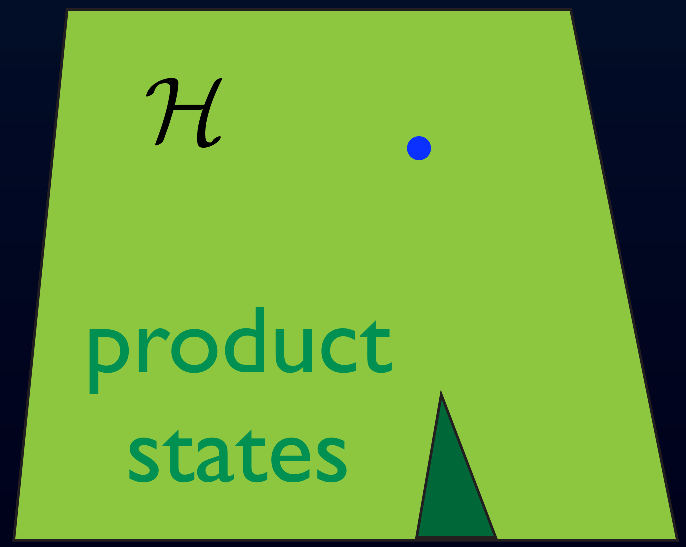
Mean field approximation

Can still produce good results in some cases

Why should TNS be useful?

- States appearing in Nature are peculiar

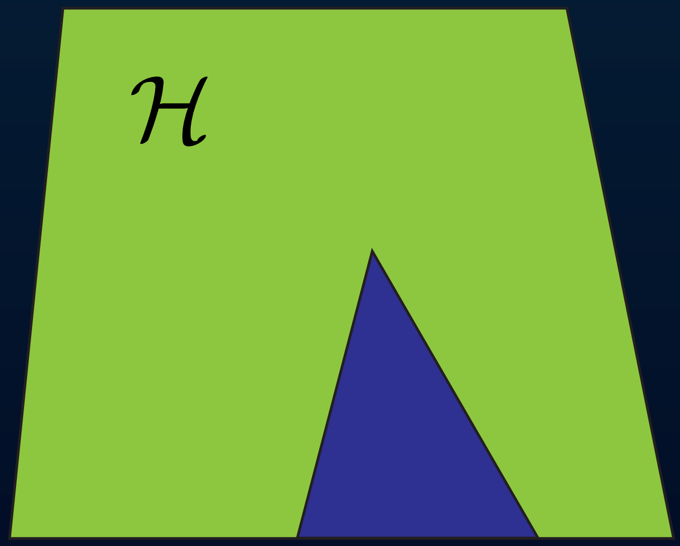
State at random
from Hilbert space is
not close to product



We look for the
particular corner of
the Hilbert space

Why should TNS be useful?

- Thermal states of nearest neighbour Hamiltonians described by small number of parameters



$$H = \sum_i h_{i,i+1}$$

$d^2 \times d^2$

$$\rho \sim \mathrm{e}^{-H/T}$$

specifies the state with a small number of parameters

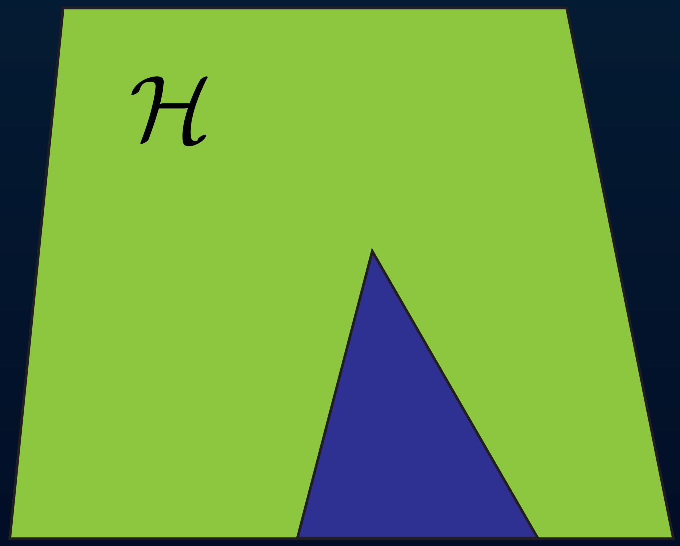
Why should TNS be useful?

- The goal is to find good descriptions of physical states

  ➡ efficient representation

  ➡ computable observables

  ➡ (variational) algorithms

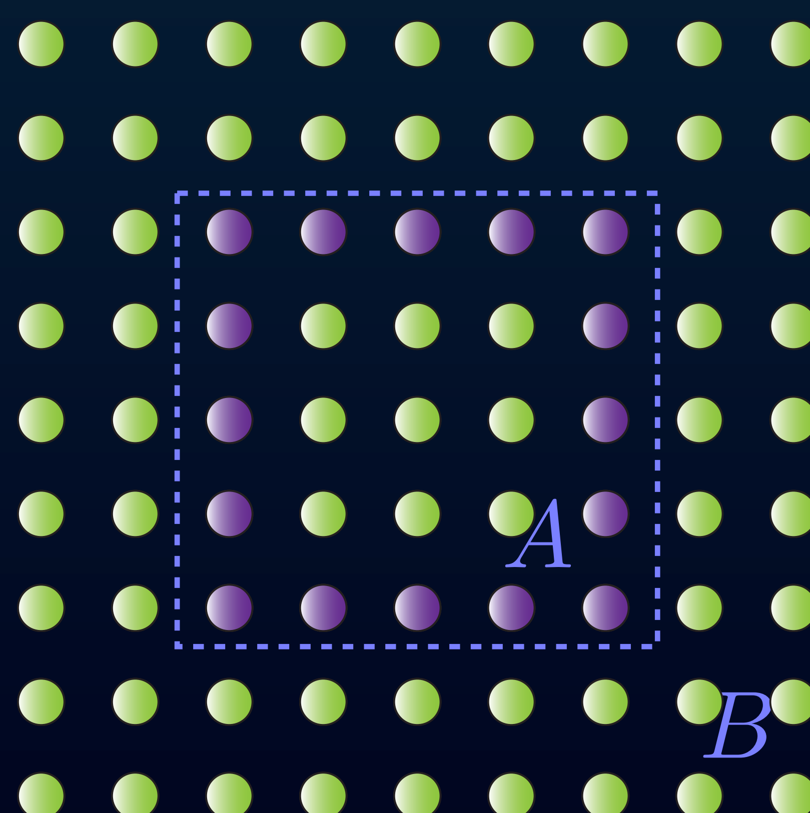


Finding a good ansatz

- Which properties characterize ground states of relevant Hamiltonians?

Area law

finite range
gapped
Hamiltonians



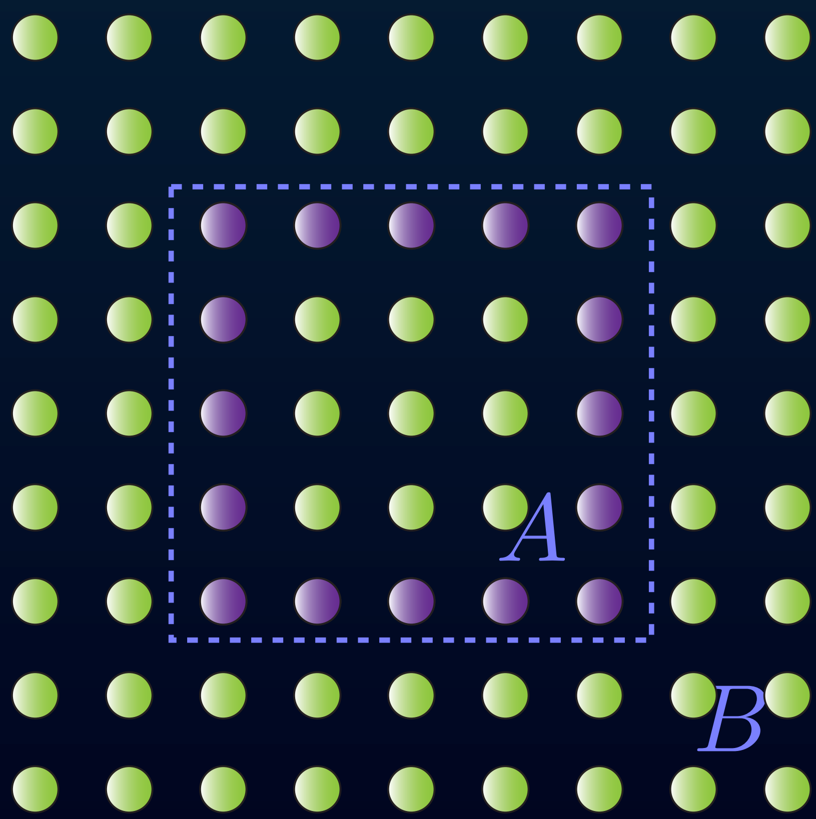
$$S_A = -\mathrm{tr}(\rho_A \log \rho_A)$$

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

Finding a good ansatz

- Which properties characterize ground states of relevant Hamiltonians?

Area law



➡ observed for known Hamiltonians

➡ proven in 1D Hastings 2007

➡ in critical systems, only log corrections

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

Calabrese, Cardy 2004

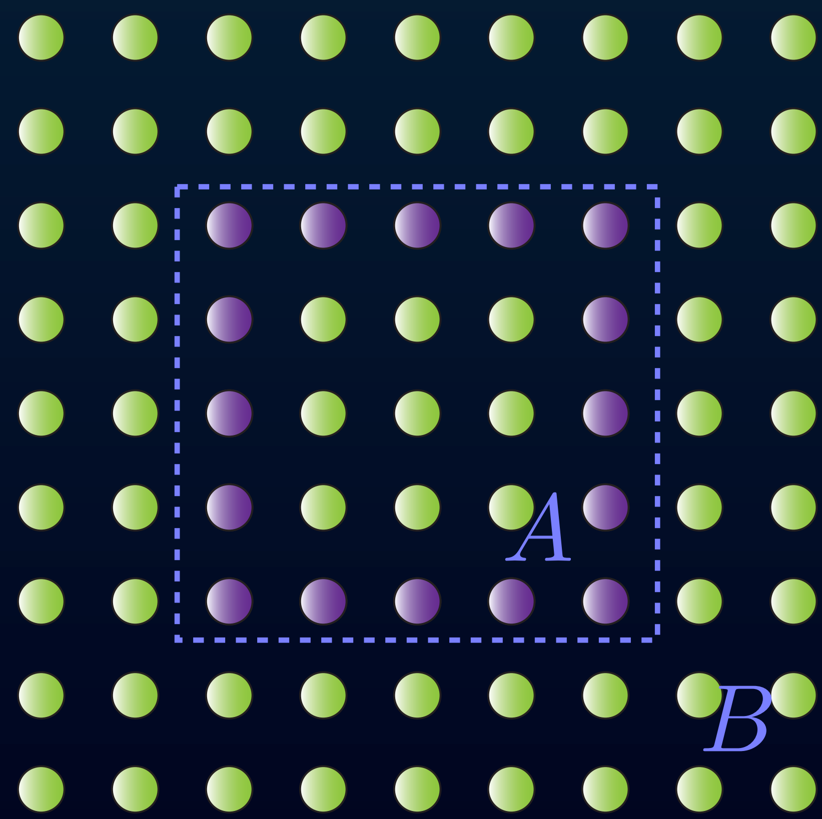
Wolf 2006

Finding a good ansatz

- Which properties characterize ground states of relevant Hamiltonians?

Area law

- ➡ rigorously proven for thermal states
- ➡ in any dimension



$$I(A:B) =$$
$$= S(\rho_A) + S(\rho_B) - S(\rho_{AB})$$

$$I(A:B)_{\max} \propto \frac{1}{T}|\delta A|$$

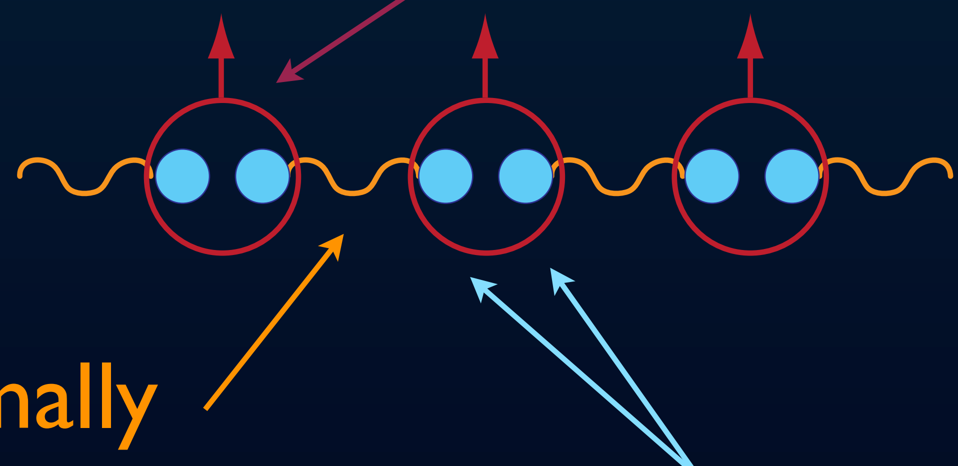
Wolf, Verstraete, Hastings, Cirac, PRL 2008

MPS and PEPS

- States which fulfill the area law by construction

project onto the physical degrees of freedom d

1D



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

maximally entangled state

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

virtual particles

D

number of parameters

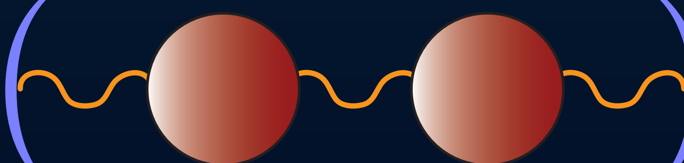
NdD^2

Verstraete, Porras, Cirac, PRL 2004

MPS and PEPS

- States which fulfill the area law by construction

1D

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

local projectors
cannot increase
the entropy

MPS and PEPS

- States which fulfill the area law by construction

1D

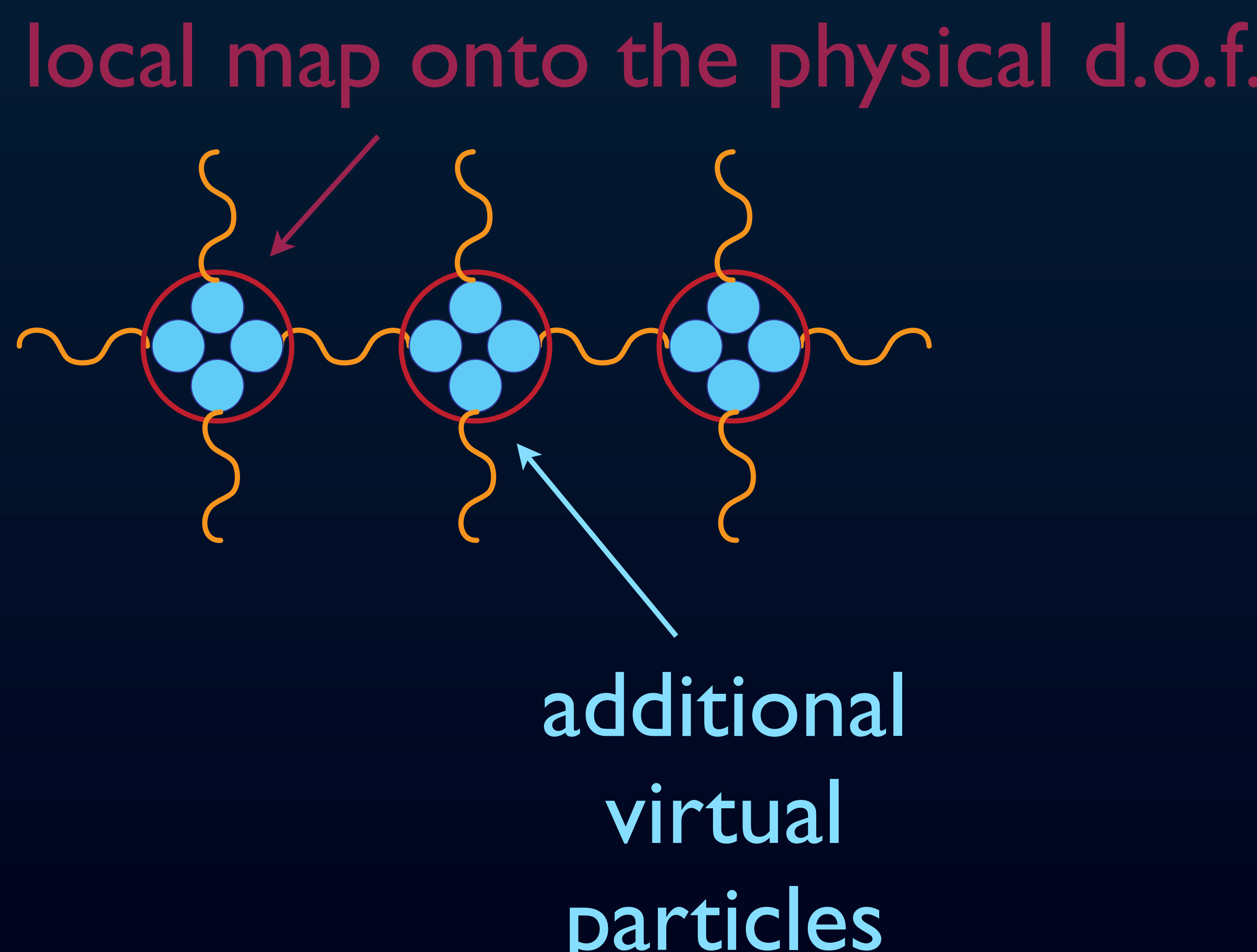
$\leq S\Big($  $\Big) = S\Big($  $\Big)$

$$= 2\log D$$

MPS and PEPS

- States which fulfill the area law by construction

higher D

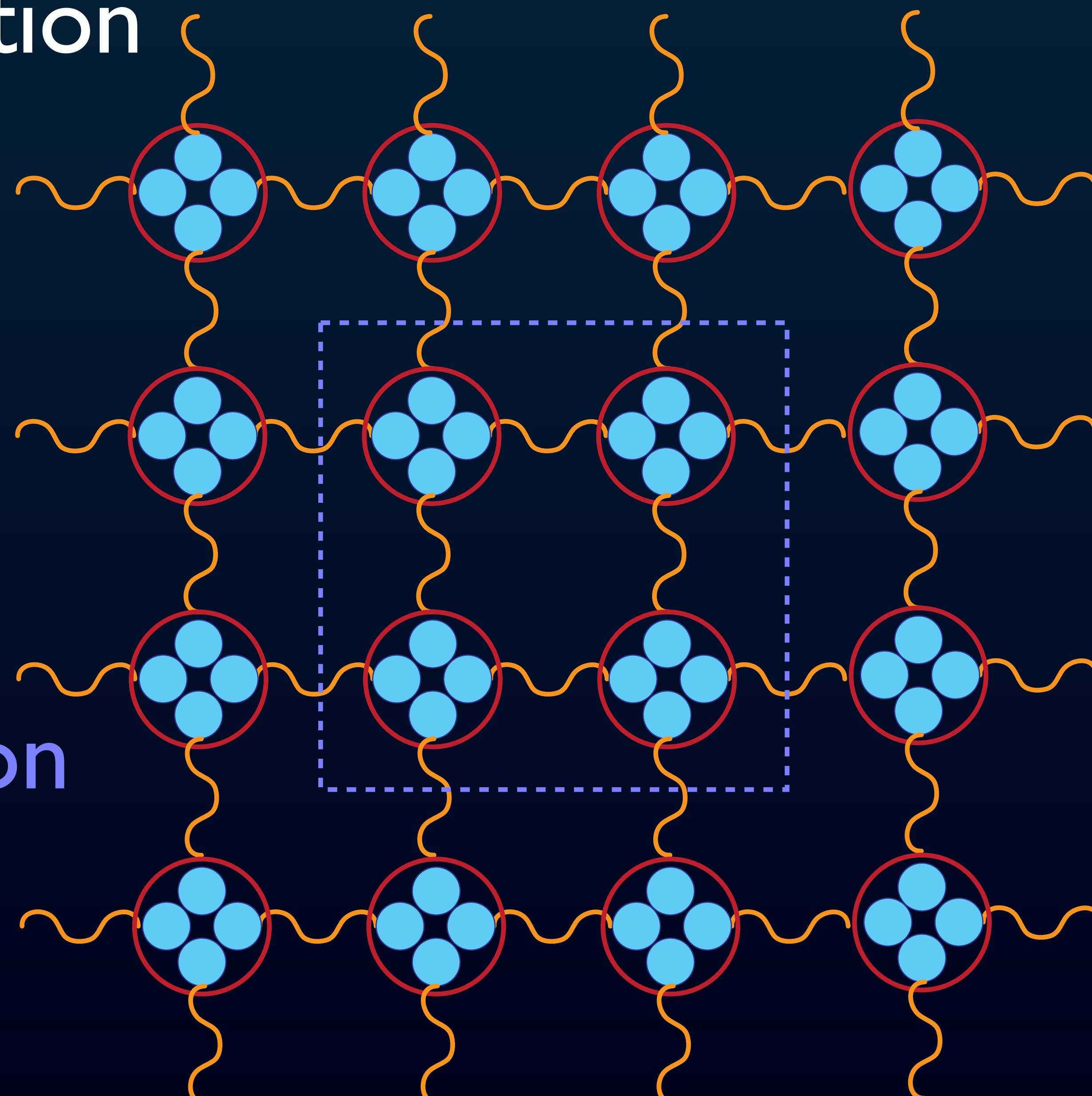


Verstraete, Cirac, 2004

MPS and PEPS

- States which fulfill the area law by construction

higher D



Entropy of a region bounded by the number of cut bonds

Verstraete, Cirac, 2004

MPS and PEPS

- Also formal results known

➡ MPS and PEPS are complete families

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

MPS and PEPS

- Also formal results known
  - ➡ one dimensional
    - gapped finite range Hamiltonian ⇒ area law (ground state) Hastings, J. Stat. Phys. 2007
    - area law ⇒ MPS efficient approximation Verstraete, Cirac, PRB 2006
  - ➡ higher dimensions
    - finite range, finite T ⇒ PEPS efficiently approximate thermal state Hastings, PRB 2006

MPS and PEPS

provide
accurate and efficient descriptions
of ground and thermal states of
finite range Hamiltonians

Relation to RG

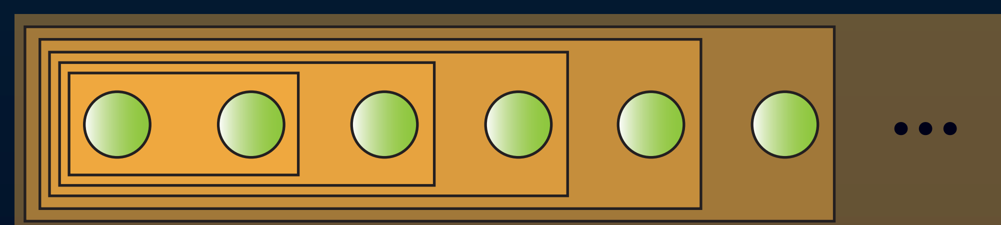
- Real space renormalization produce MPS

$$|\alpha_{M+1}\rangle = \sum A^i_{\beta\alpha} |\beta_M\rangle \otimes |i\rangle_{M+1}$$

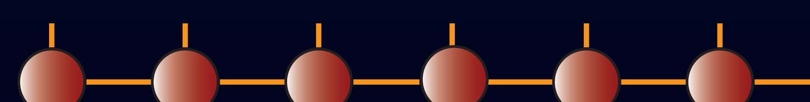
truncation method

Relation to RG

- Real space renormalization produce MPS



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



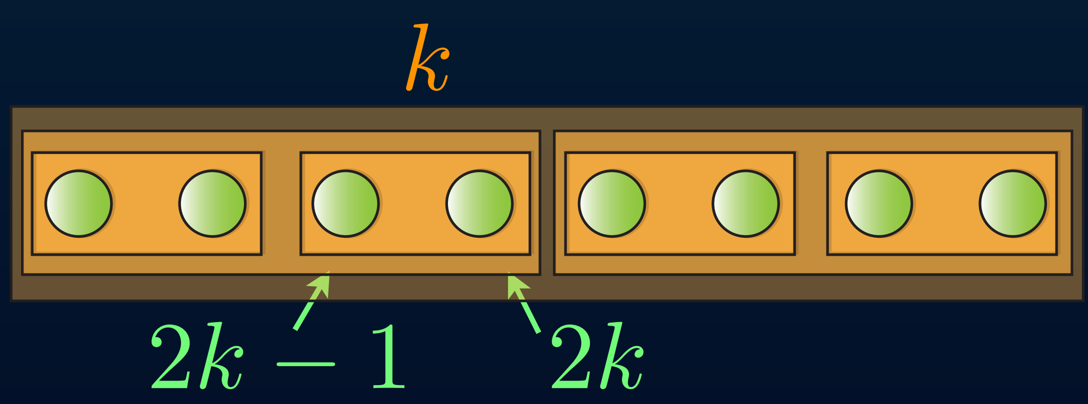
Relation to RG

- Real space renormalization produce MPS
  - ➡ different truncation methods
    - states of minimal energy for the subsystem ⇒ Wilson's NRG
    - variational minimization of over MPS ⇒ DMRG

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

Relation to RG

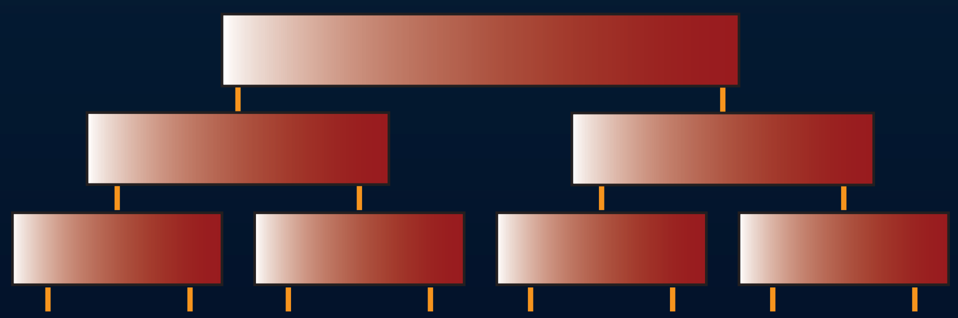
- Other renormalization procedures give rise to different TNS



$$|n\rangle_k = \sum T^n_{mp} |m\rangle_{2k-1} \otimes |p\rangle_{2k}$$

Relation to RG

- Other renormalization procedures give rise to different TNS



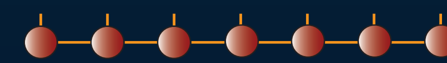
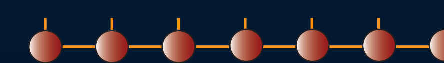
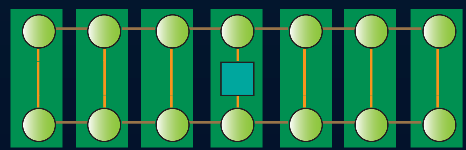
tree tensor states
TTS

➡ efficient contraction

➡ violate area law

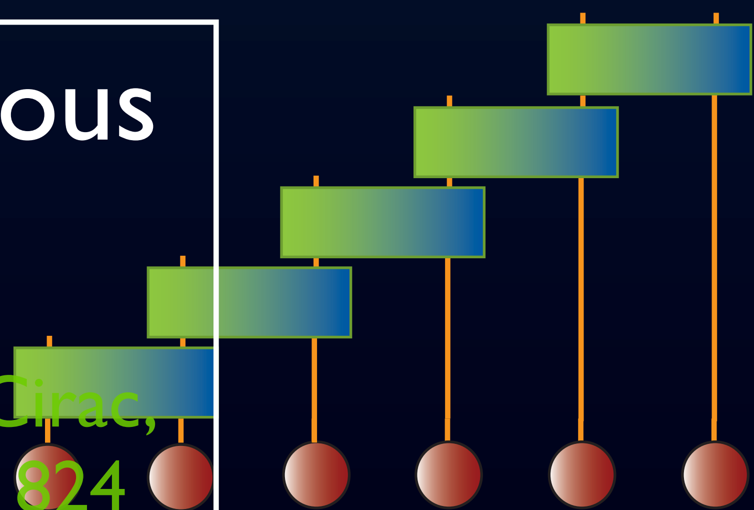
  - logarithmically

Some more properties of MPS

- Efficient algorithms
  - ➡ ground states $|E_0\rangle \simeq$ 
  - ➡ approximate a state by a MPS $|\Psi\rangle \simeq$ 
  - ➡ compute expectation values 
- Can be efficiently prepared

Continuous limit

Verstraete, Cirac, arXiv:1002.1824



Schön et al., PRL 2005

PEPS

- Generalization of MPS
  - ➡ incorporate area law

    Verstraete, Cirac, 2004
  - ➡ approximate interesting states

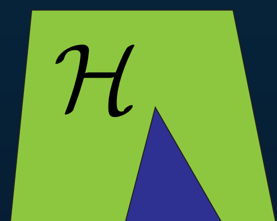
    Hastings, PRB 2007
- Prepare them is hard

  Schuch, Wolf, Verstraete, Cirac, PRL 2007
- Cannot be contracted efficiently
  - approximate contraction

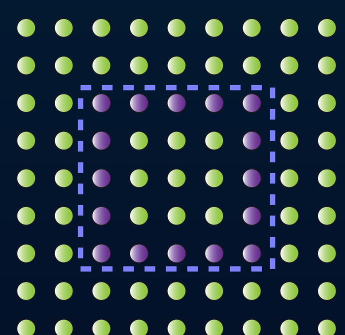
PEPS

- Efficient algorithms
  - ➡ ground states Murg, Verstraete, Cirac, PRA 2009
  - ➡ time evolution Murg, Verstraete, Cirac, PRA 2007
- Infinite lattices Jordan, Orús, Vidal, Verstraete, Cirac, PRL 2008
  Bauer, Vidal, Troyer, J. Stat. Mech 2009
- Fermionic systems
  Kraus, Schuch, Verstraete, Cirac, 2009
  Corboz, Orús, Bauer, Vidal, 2009
- Limited to small bond dimension
  - RG techniques Levin, Nave, PRL 2007
    Levin, Wen, PRB 2008
    Kao, Sandvik, 2009

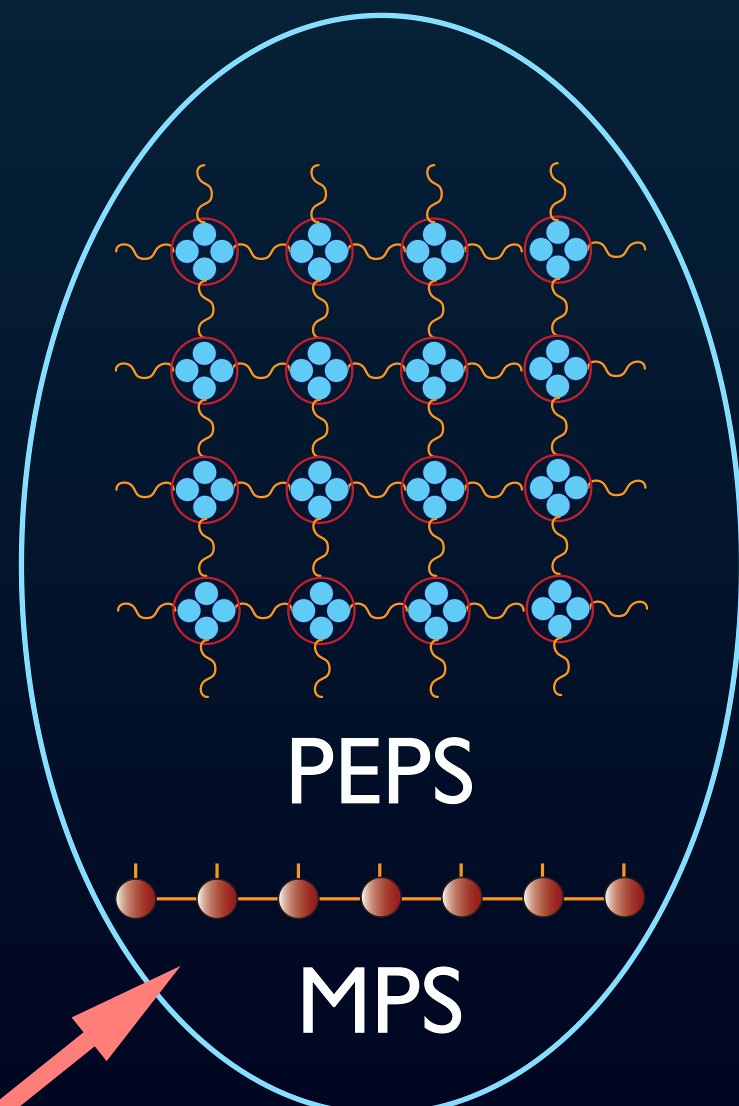
Summarizing



GS and thermal states of finite range H

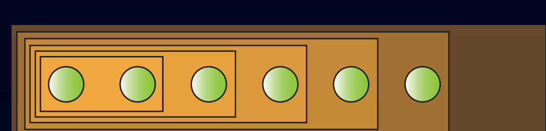


area law



approximate efficiently GS and thermal states of finite range H

successful variational algorithms



renormalization procedures

other TNS

Cirac, Verstraete, J. Phys. A 2009
Verstraete, Murg, Cirac, Adv. Phys. 2008

Long-time evolution with MPS

M. C. Bañuls, M. B. Hastings, F. Verstraete, J. I. Cirac

What can be studied with MPS

- Ground states properties with MPS
  - finite chains → very successful approach

    White, PRL 1992
    Schollwöck, RMP 2005
  - infinite chains → with translational invariance

    Östlund, Rommer, PRL 1995
    Vidal, PRL 2007

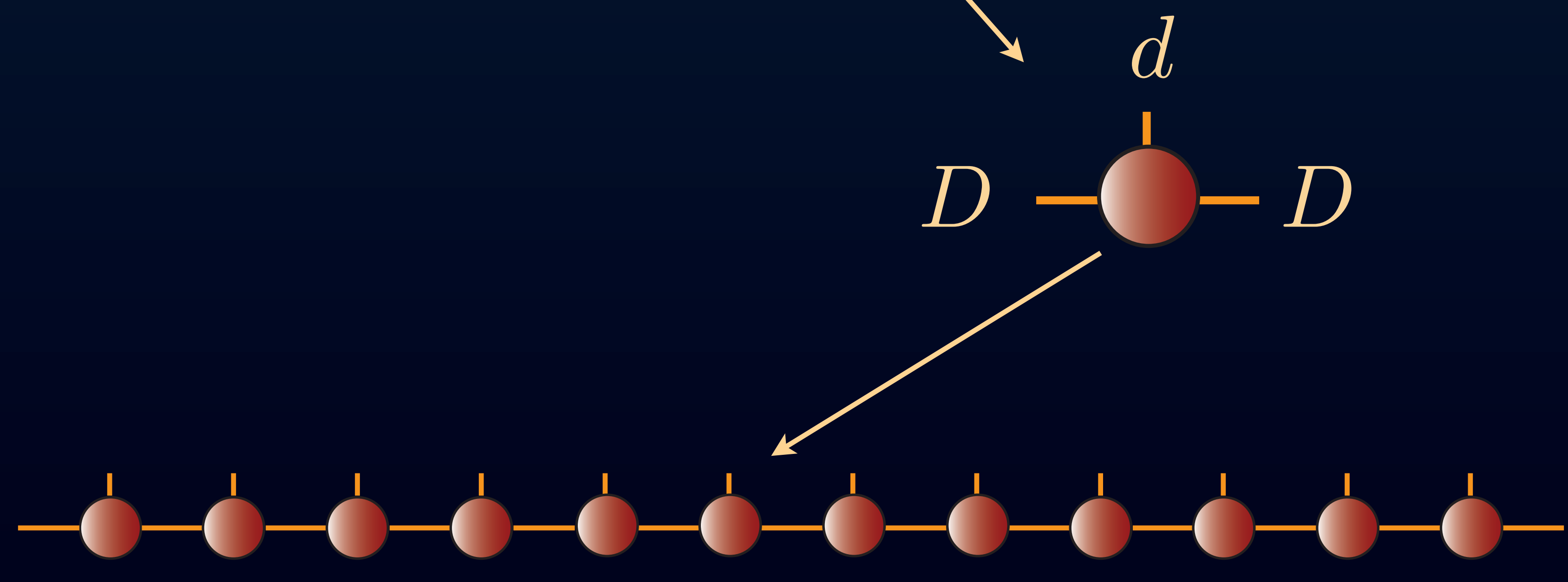
What can be studied with MPS

- Time evolution with MPS
  - finite chains   Vidal, PRL 2003
    White, Feiguin, PRL 2004
    Daley et al., 2004
  - infinite (TI) chains $\Rightarrow$ iTEBD method
    Vidal, PRL 2007
  - but limited to short times

Standard method

➡ Start with a MPS

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



Standard method

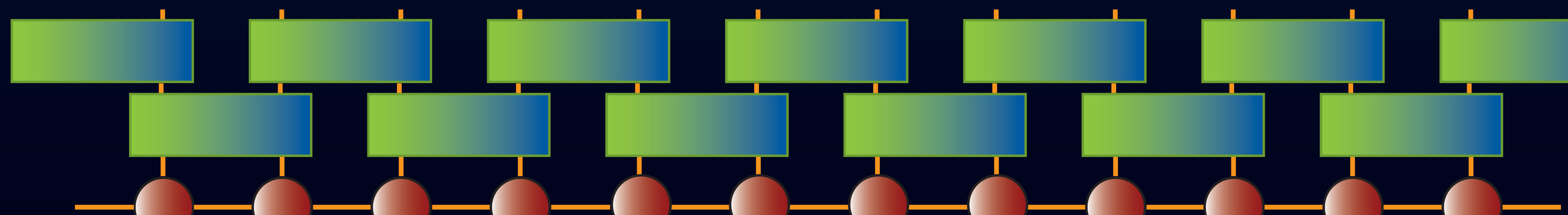
➡ Start with a MPS

- Apply evolution operator

  ➡ discrete time steps $U(t) \rightarrow [U(\delta)]^M$

  ➡ nearest-neighbour $H = H_e + H_o$

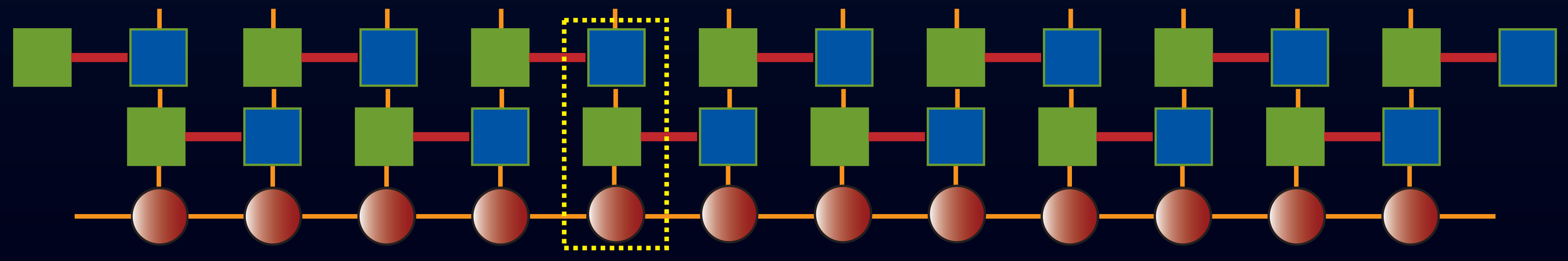
  ➡ Trotter $U(\delta) = e^{-iH_e\delta} e^{-iH_o\delta}$



Standard method

➡ Start with a MPS

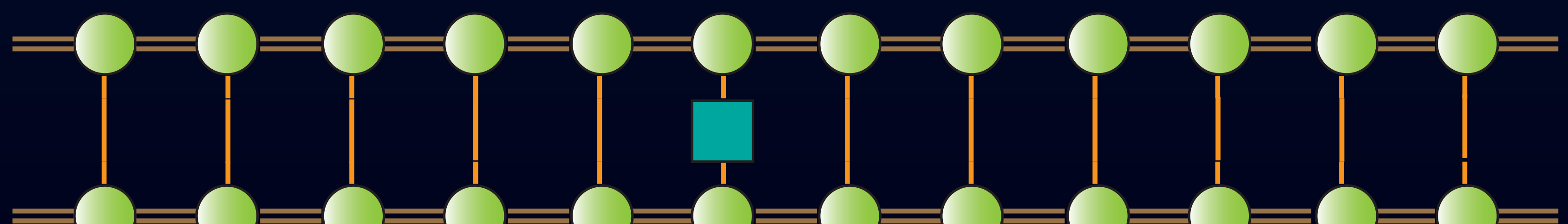
- Apply evolution step
- Obtain a MPS with larger bond
- Truncate D



Standard method

➡ Start with a MPS

- Apply evolution step
- Obtain a MPS with larger bond
- Truncate D



Standard method

- Problem: only short times
- Entropy of evolved state may grow linearly

Osborne, PRL 2006
Schuch et al., NJP 2008

➡ required bond for fixed precision

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

  - truncation error becomes dominant

    ➡ results deviate abruptly from the exact

  - increasing D by factor gets only constant improvement

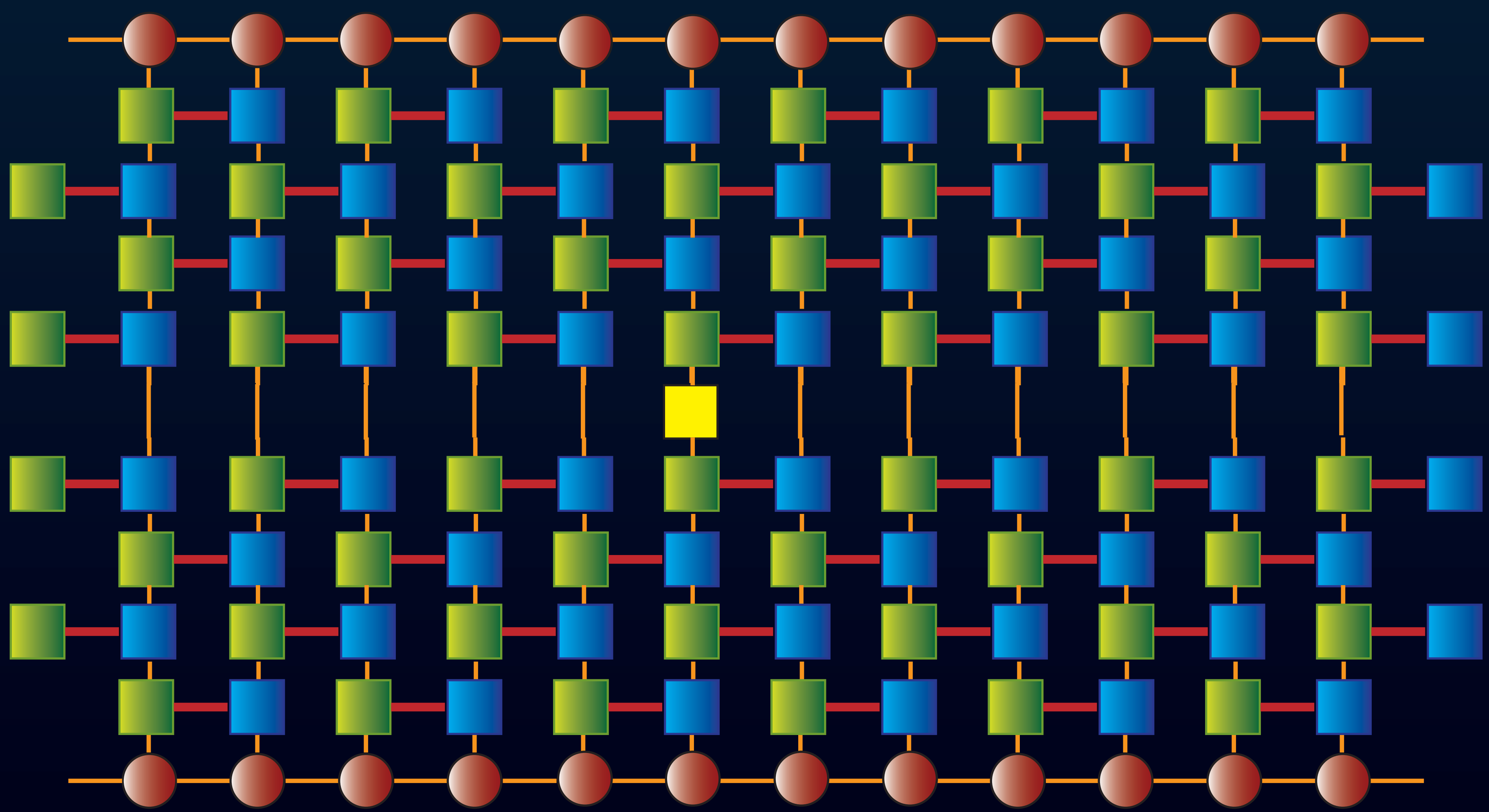
Transverse method

- Compute dynamical quantities
- For infinite chains
  - No extrapolation from finite size
- Avoid explicit truncation of the bond dimension along the evolution

M.C.B., M. Hastings, F. Verstraete, J.I. Cirac, PRL 2009

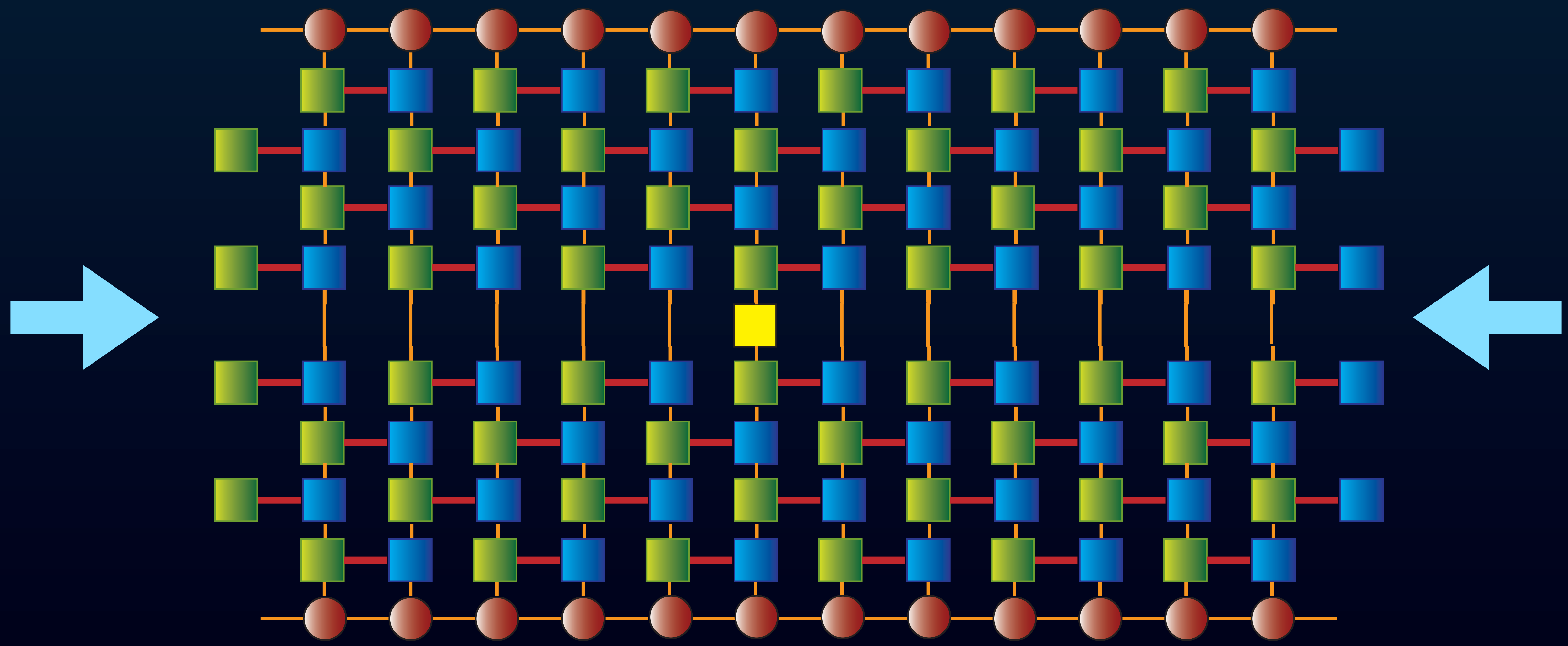
Transverse method

1. Start with MPS
2. Apply evolution steps
3. Apply an operator
4. Contract



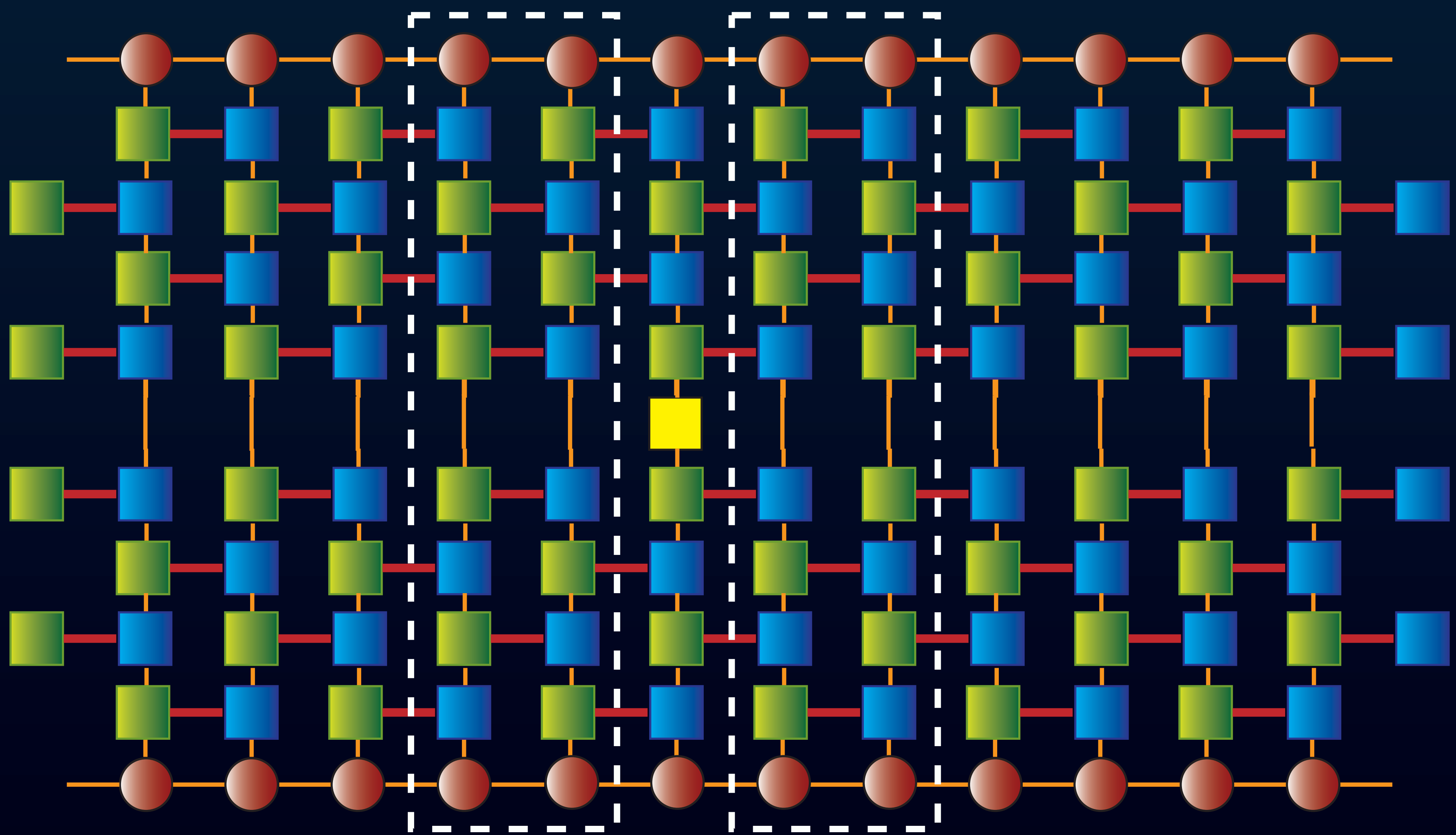
Transverse method

- Infinite in the space direction, finite in time direction
- Reduce to 2D finite network



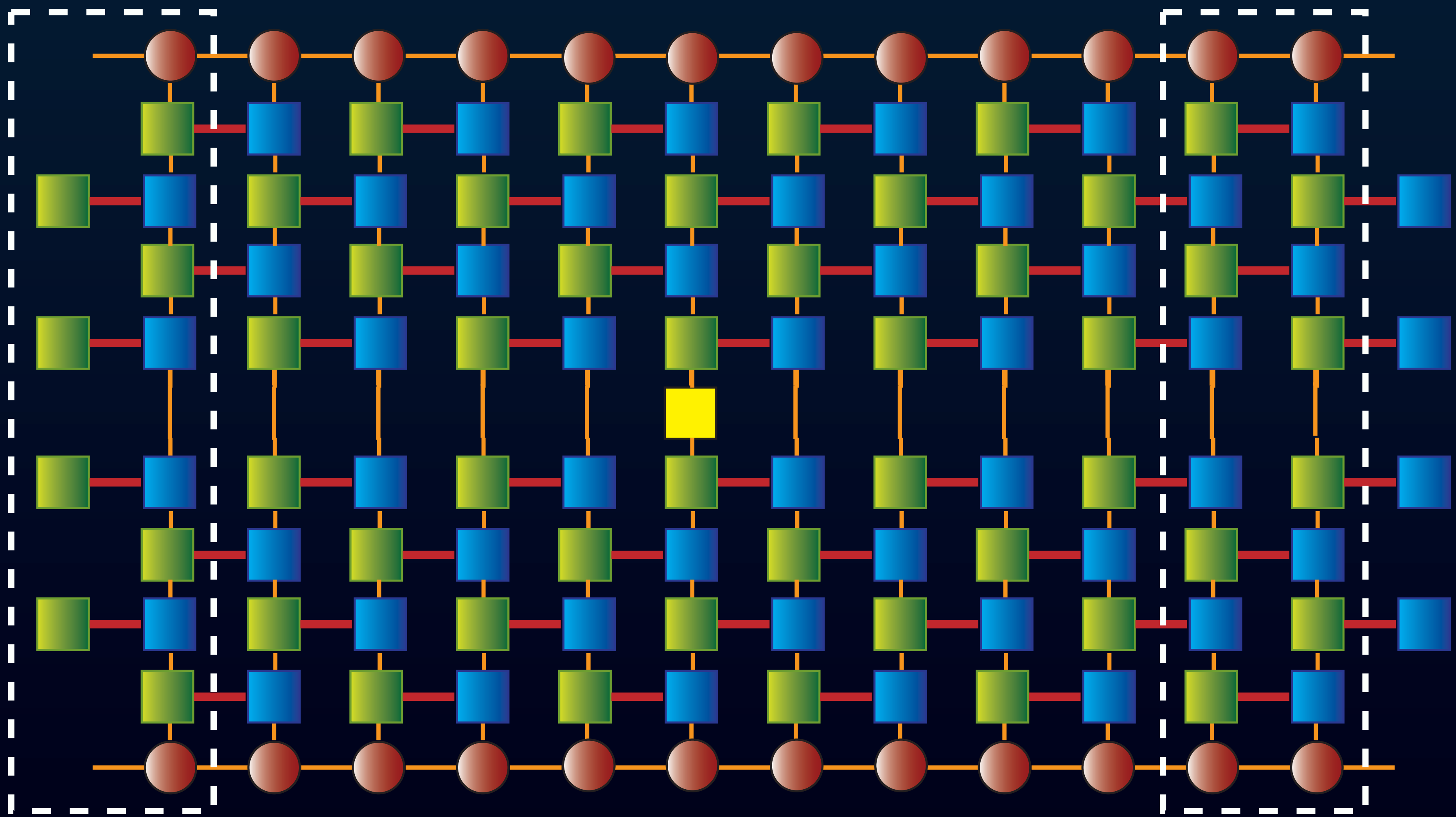
Transverse method

- TI $\Rightarrow$ Repeated contraction of same operator
    - transfer matrix of evolved MPS



Transverse method

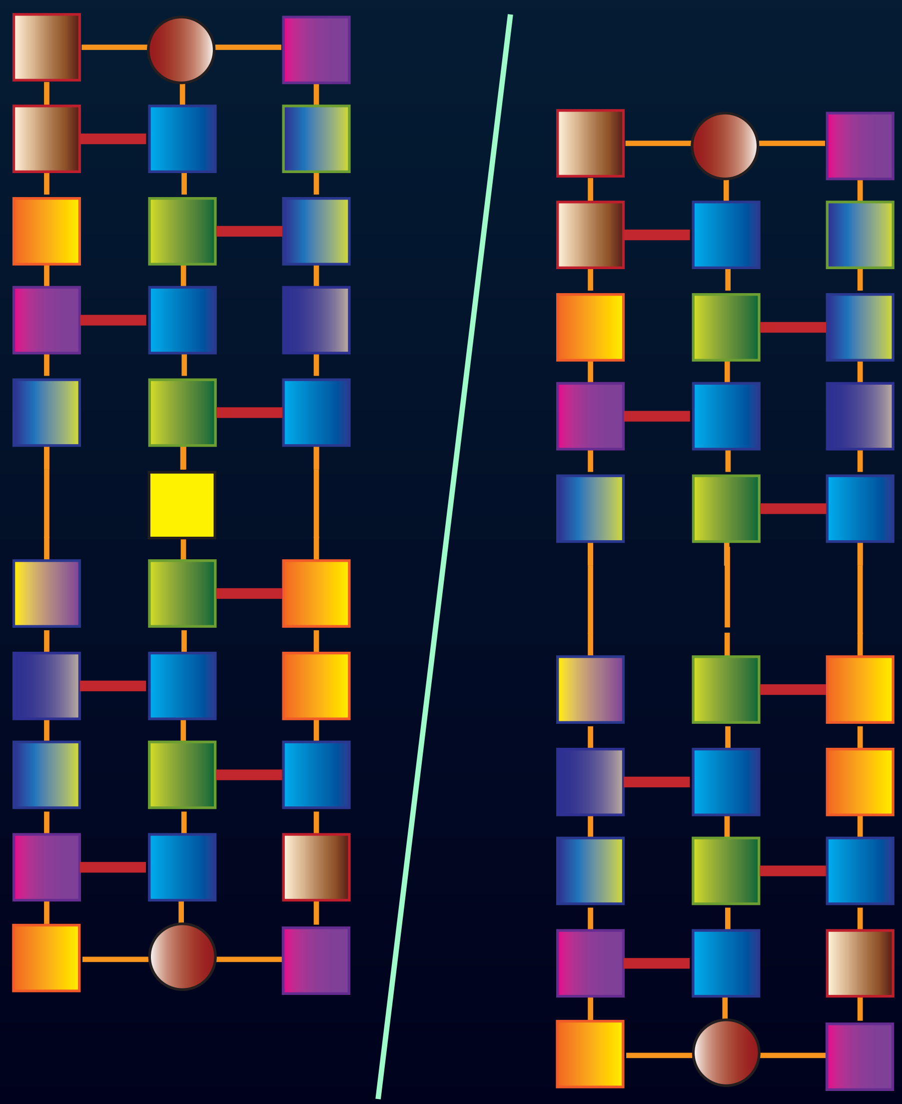
- If non-degenerate $E^n \xrightarrow[n\to\infty]{} \lambda^n |R\rangle\langle L|$
- Effectively substitute half networks by left and right eigenvectors



Transverse method

- Up to normalization

$$\langle O(t) \rangle =$$



Real time evolution

- Benchmark: Ising model

$$H = -\sum_i \left(\sigma_z^i \sigma_z^{i+1} + g\sigma_x^i\right)$$

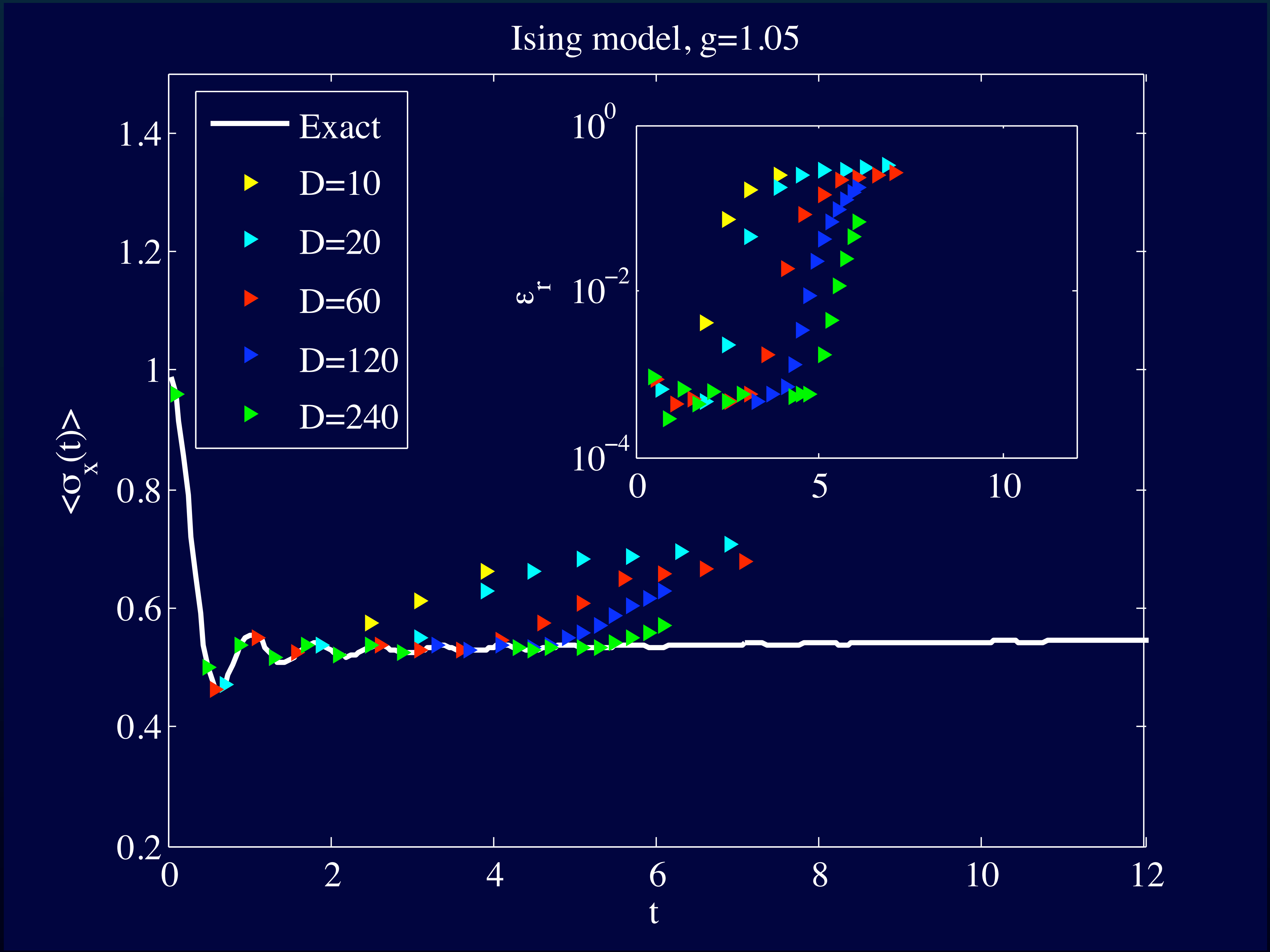
  - exactly solvable

- Start in product state

$$|\Psi_0\rangle \sim \otimes_i (|0\rangle + |1\rangle)$$

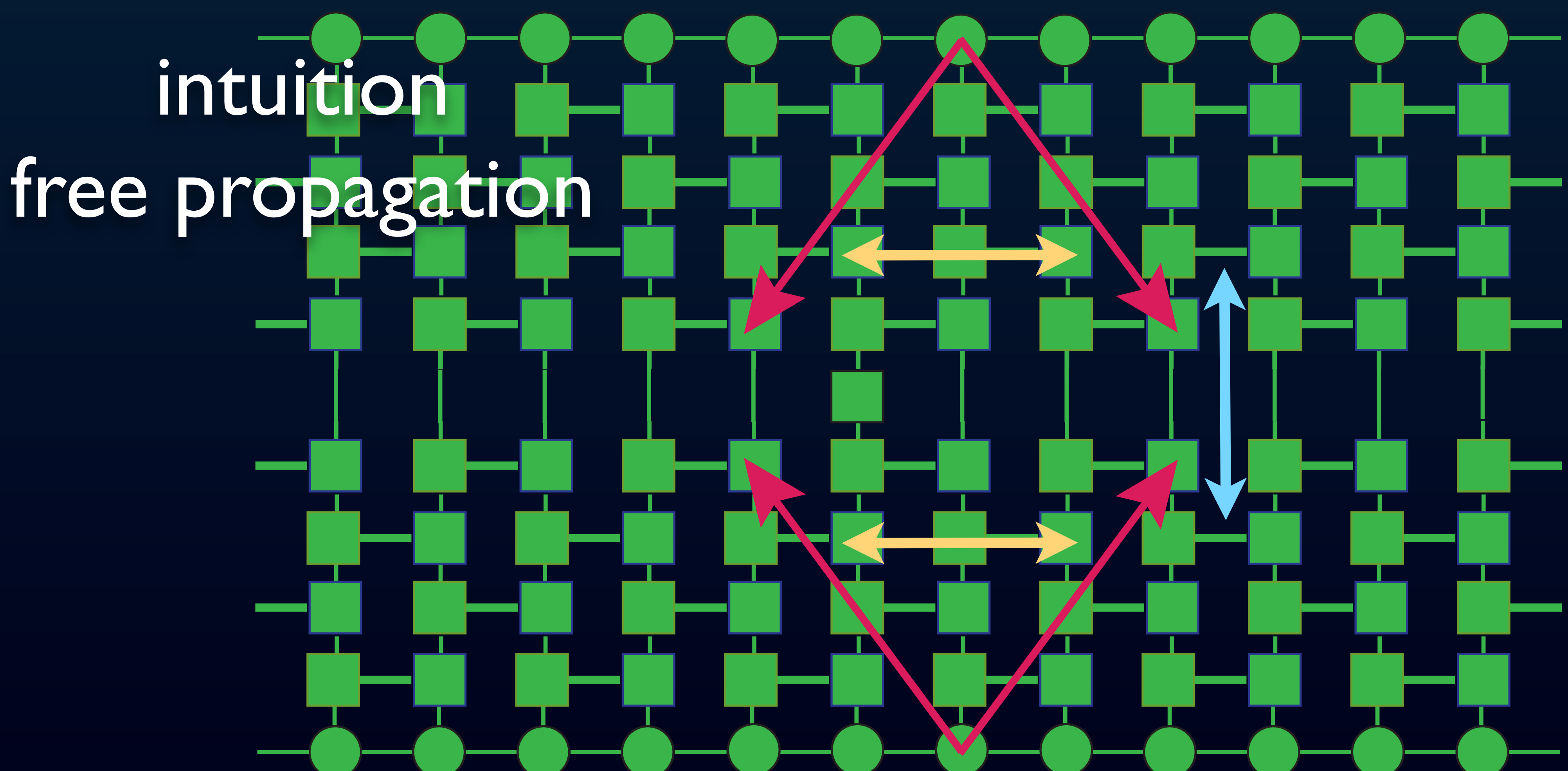
- Evolve with *g=1.05* ⇒ magnetization $\langle \sigma_x(t) \rangle$

Real time evolution



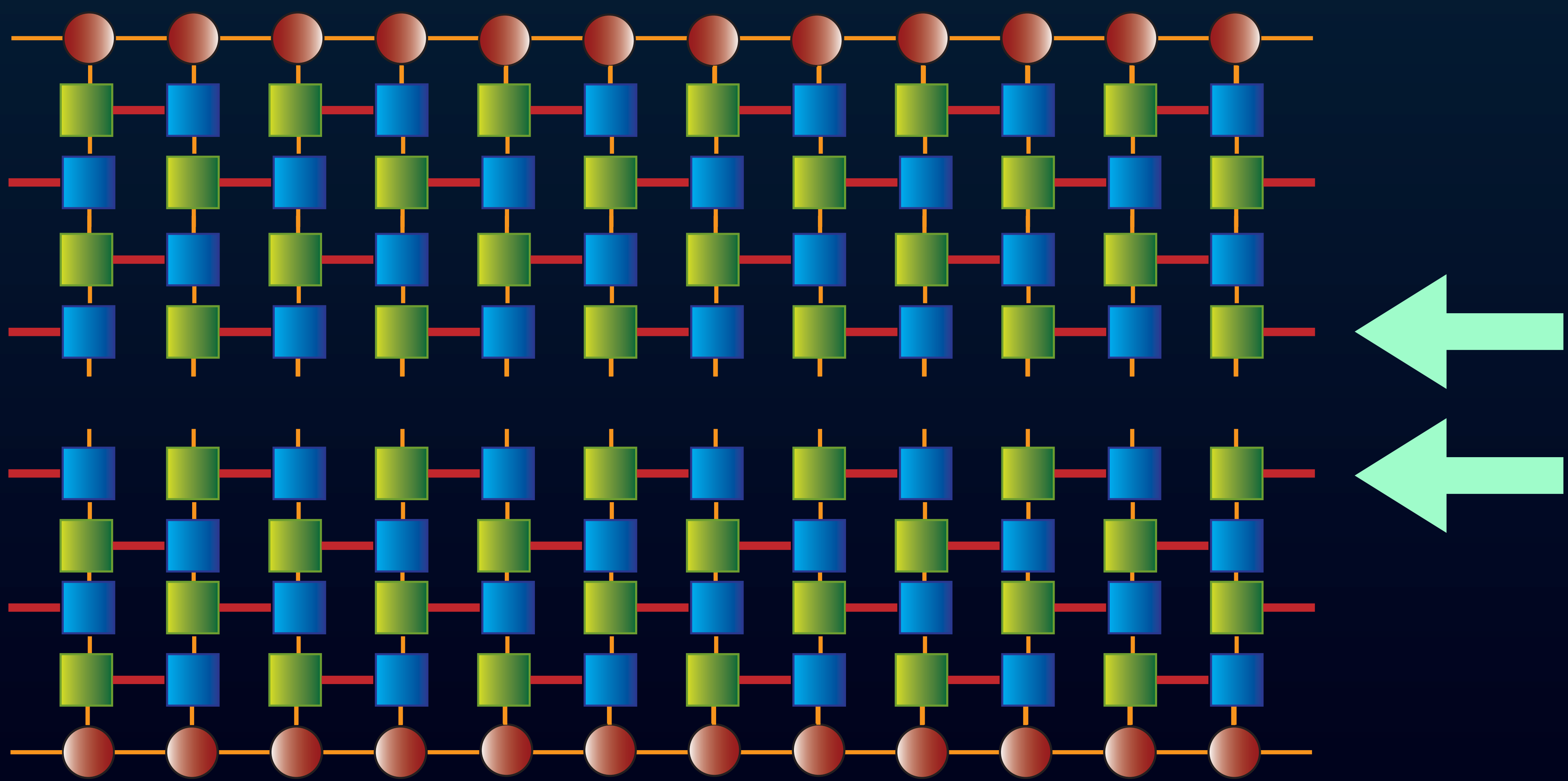
But...

- Not all sites along the time direction are independent



But...

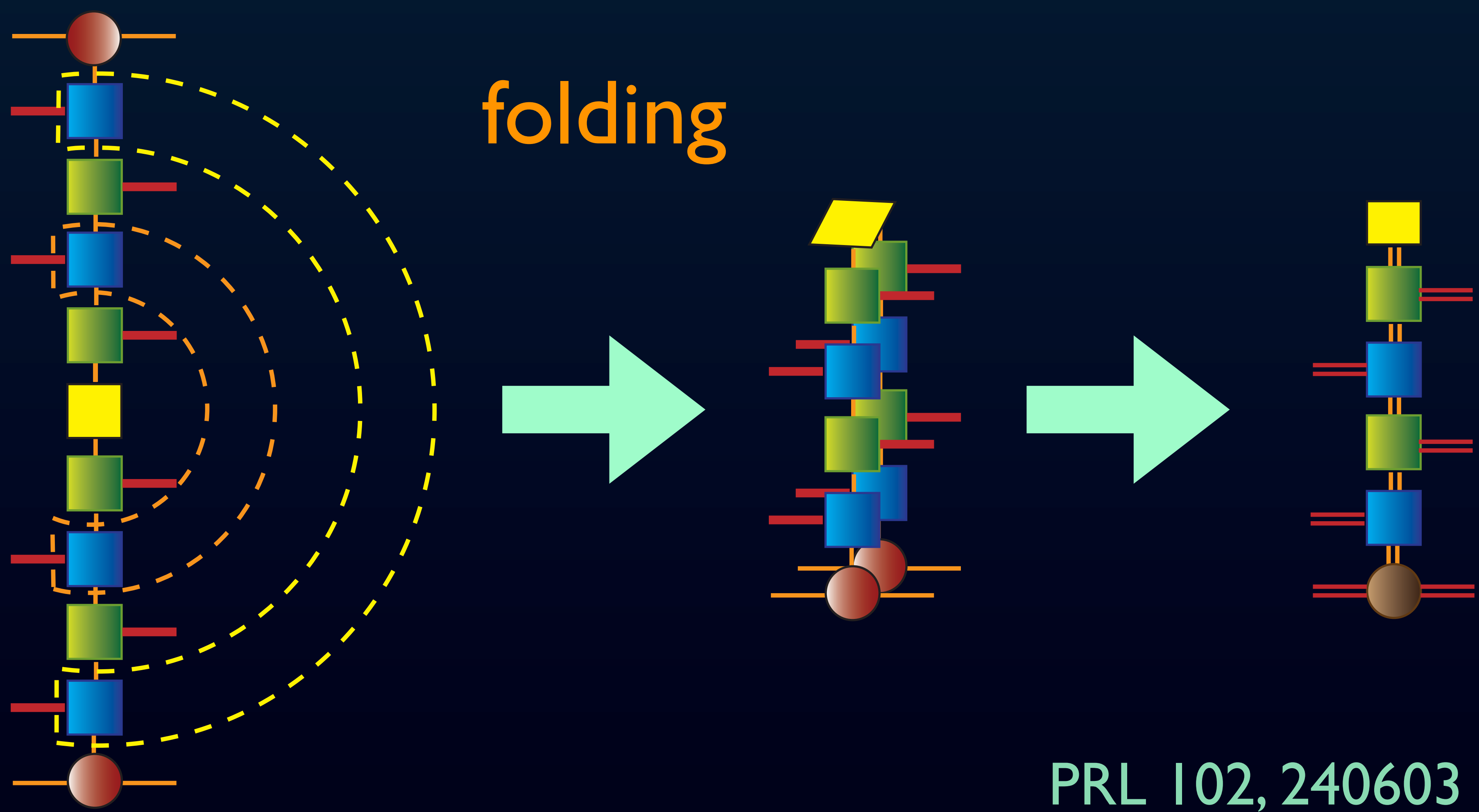
- Not all sites along the time direction are independent



PRL 102, 240603 (2009)

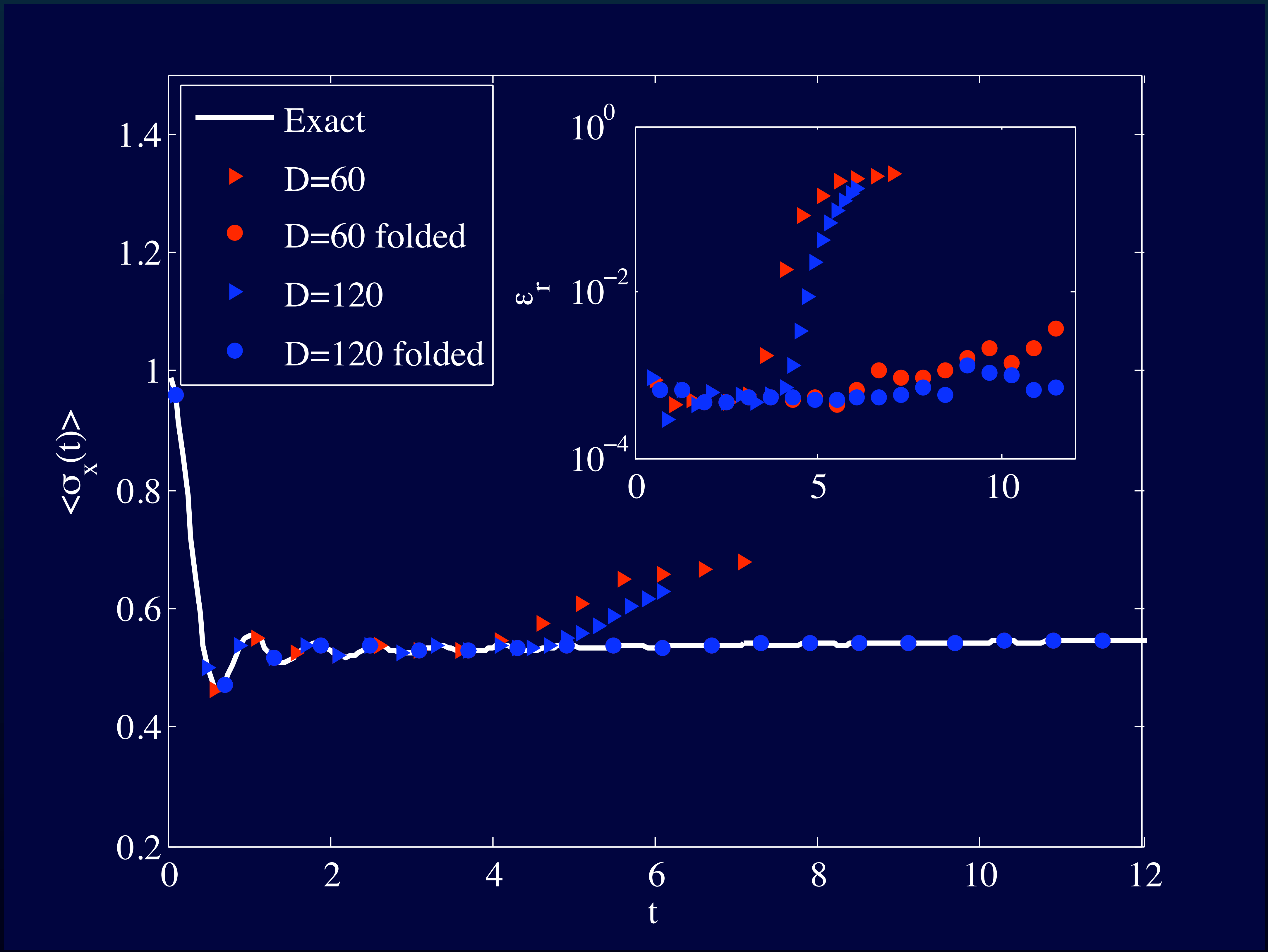
Folded transverse method

- Bring together sites corresponding to the same time step
  - largest correlations expected



PRL 102, 240603 (2009)

Ising model



Exact
D=60
D=60 folded
D=120
D=120 folded
$\langle\sigma_x(t)\rangle$
t
0
2
4
6
8
10
12
0.2
0.4
0.6
0.8
1
1.2
1.4
ε_r
10^0
10^{-2}
10^{-4}
0
5
10

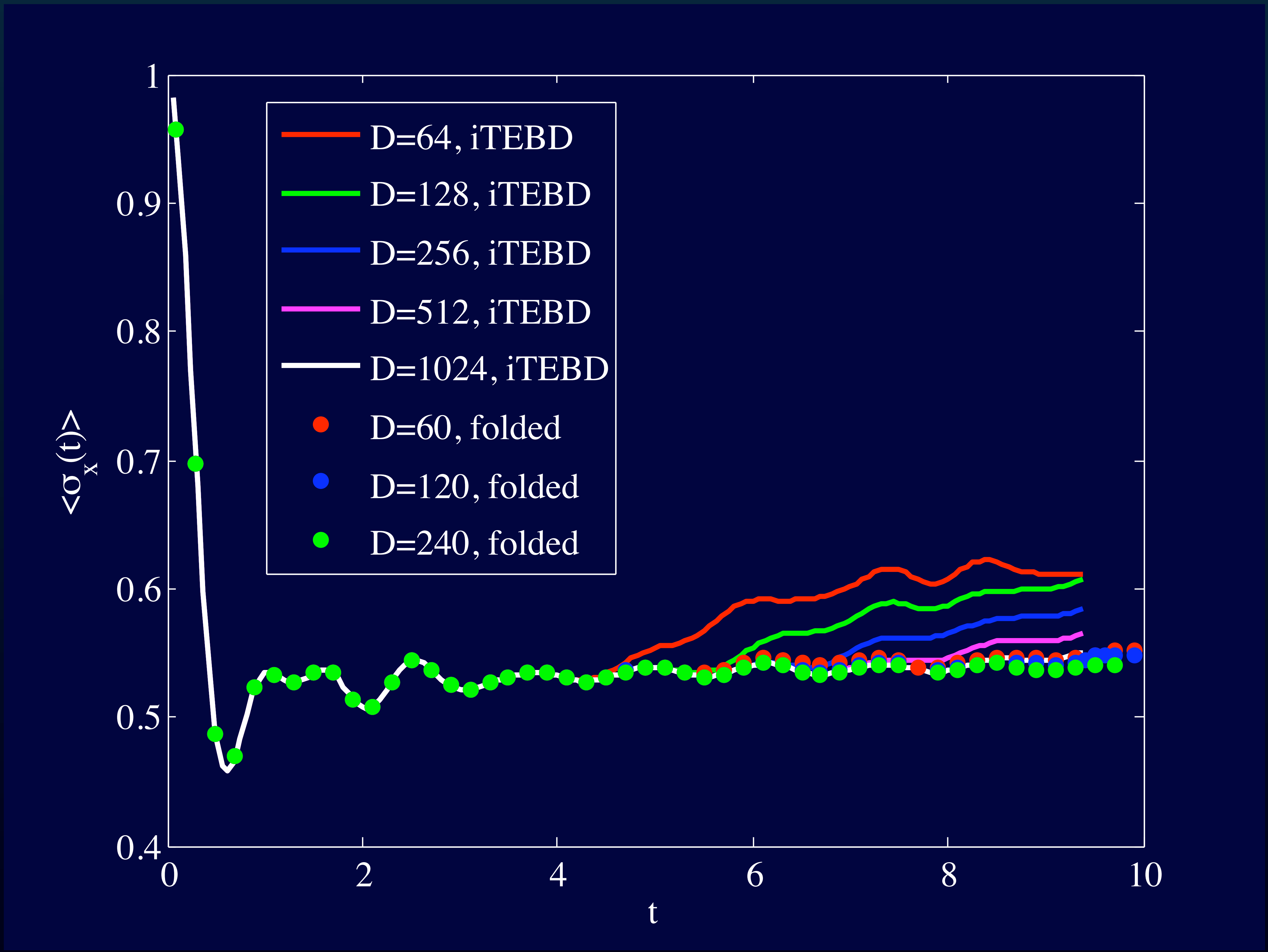
Non-integrable model

- More general: non-integrable model
  - Ising chain plus parallel field

$$H = -\sum_i \left(\sigma_z^i \sigma_z^{i+1} + g\sigma_x^i + h\sigma_z^i\right)$$

  - No exact results $\Rightarrow$ Compare with iTEBD method

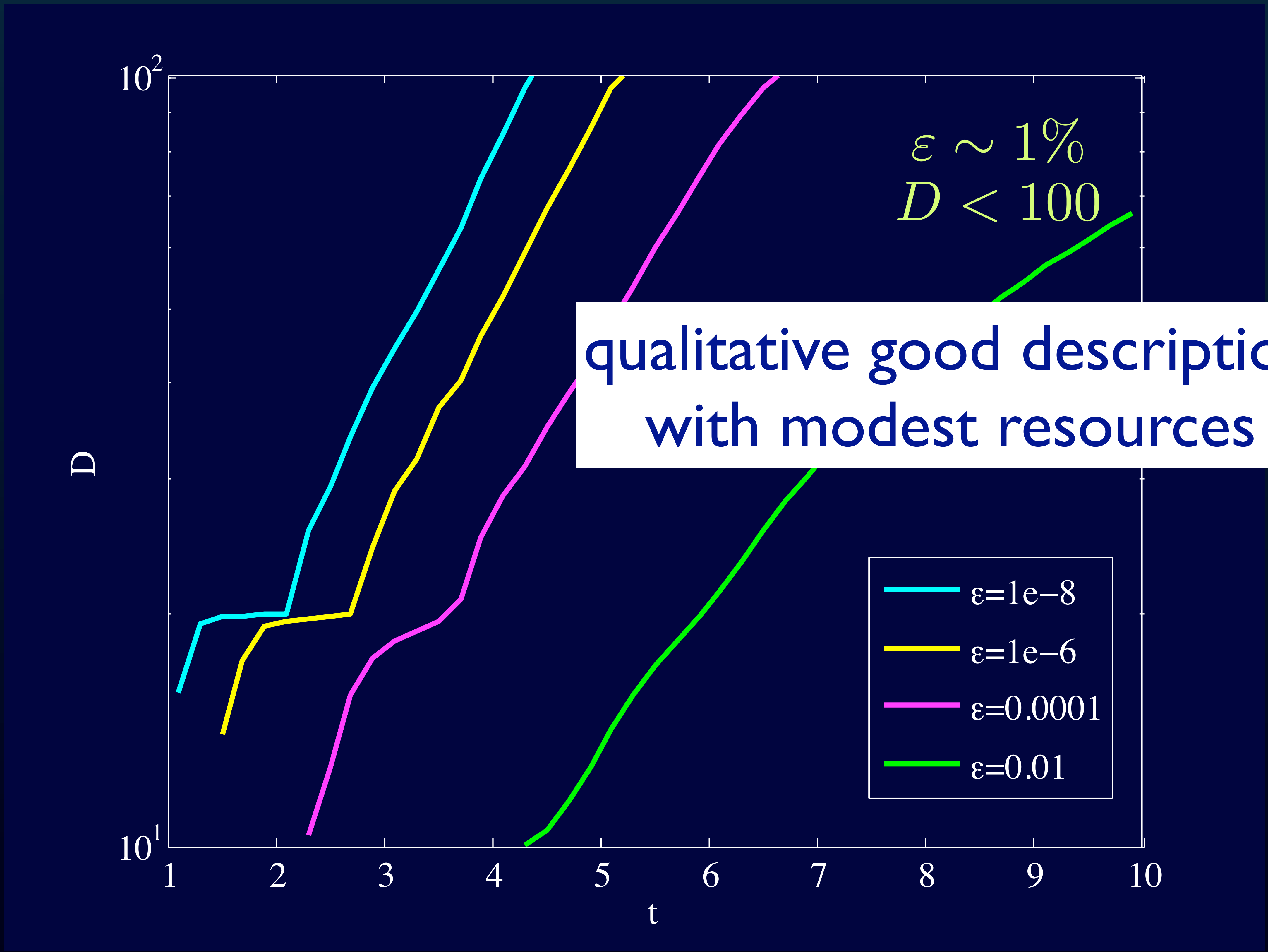
Non-integrable model



Folded transverse method

- With same D, much longer t
- Look at truncation errors
  - Compare eigenvector with highest D to its truncated versions
  - Which D do we need for a fixed truncation error?

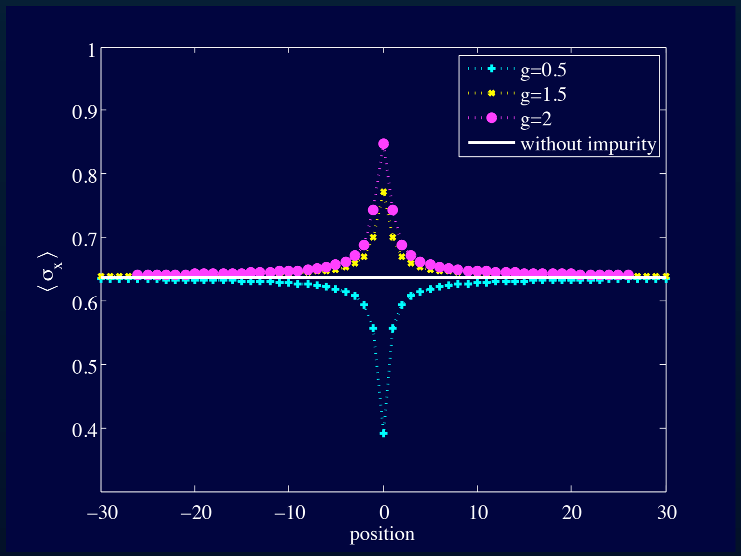
Folded transverse method



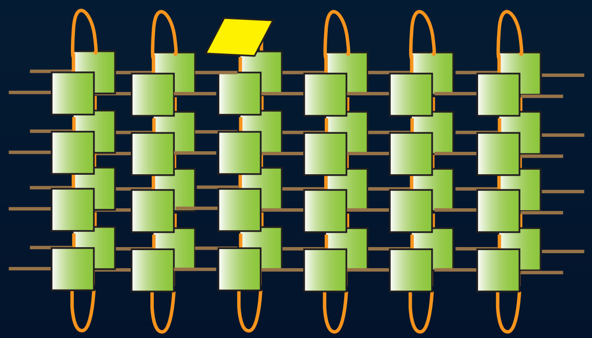
qualitative good description
with modest resources

Applications

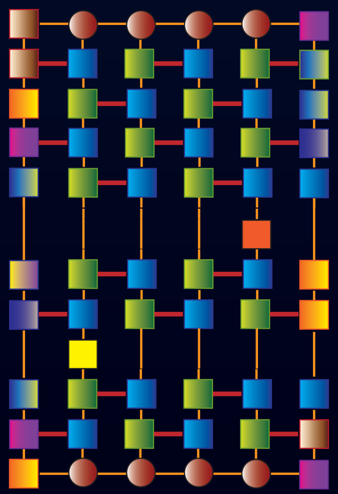
1. Impurity models



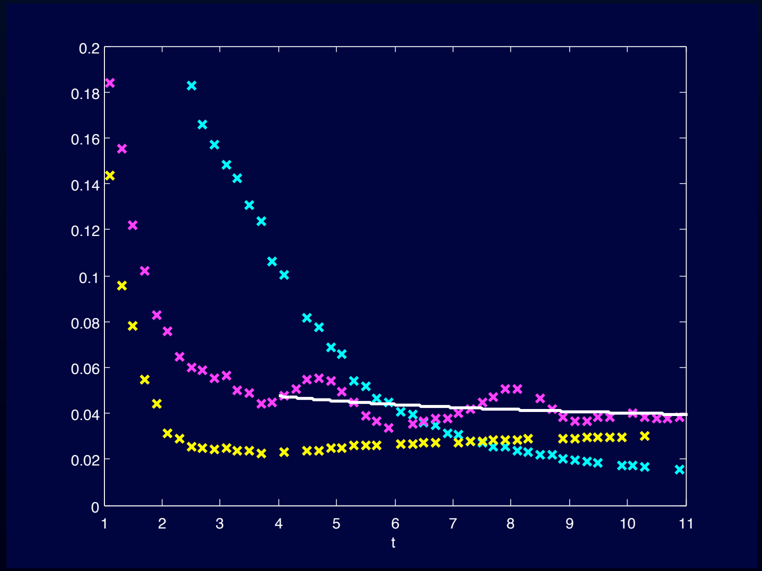
3. Thermal states



2. Dynamical correlators



4. Thermalization



Outlook

- Transverse method
  - dynamical quantities in infinite chains
  - correlations at different times
  - can deal with impurity models
- Folded variant
  - much longer times than existing methods
  - qualitative description at very large times
- Applications
  - thermalization
  - physical impurity problems, dynamics of QPT, finite chains, ...