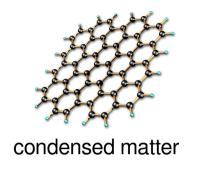
# Matrix Product States and Tensor Network States

Norbert Schuch

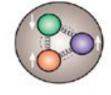
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#### **Overview**

Quantum many-body systems are all around!







quantum chemistry

high-energy physics

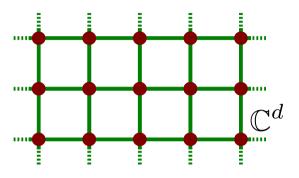
- Can exhibit complex quantum correlations (=multipartite entanglement)
  - → rich and unconventional physics, but difficult to understand!
- Quantum information and Entanglement Theory:
   Toolbox to characterize and utilize entanglement

Aim: Study strongly correlated quantum many-body systems from the perspective of quantum information + entanglement theory.

# Entanglement structure of quantum many-body states

## **Quantum many-body systems**

- Wide range of quantum many-body (QMB) systems exists
- Our focus: spin models (=qudits) on lattices:

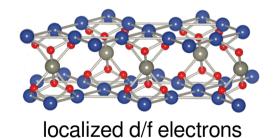


**local** interactions

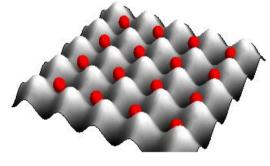
$$H = \sum_{\langle ij 
angle} h_{ij}$$

... typically transl. invariant

• Realized in many systems:



half-filled band



quantum simulators, e.g. optical lattices

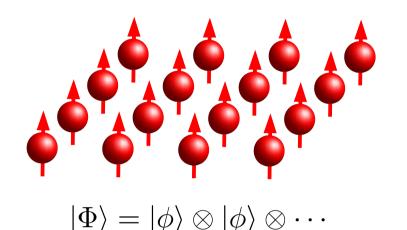
• Expecially interested in the **ground state**  $|\Psi_0\rangle$ ,

i.e., the lowest eigenvector  $H |\Psi_0\rangle = E_0 |\Psi_0\rangle$ 

(It is the "most quantum" state, and it also carries relevant information about excitations.)

# **Mean-field theory**

- In many cases, entanglement in QMB systems is negligible
- System can be studied with product state ansatz



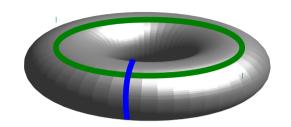
$$H = \sum_{\langle ij 
angle} h_{ij}$$
 "mean field theory"

Consequence of "monogamy of entanglement" (→ de Finetti theorem)

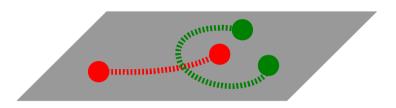
- Behavior fully characterized by a single spin  $|\phi\rangle$  a local property (order parameter) → Landau theory of phases
- Behavior insensitive to boundary conditions, topology, ...

## **Exotic phases and topological order**

Systems exist which cannot be described by mean field theory



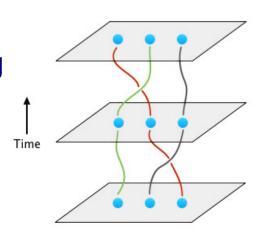
degeneracy depends on global properties



system supports exotic excitations ("anyons")

... e.g. Kitaev's "Toric Code".

- → impossible within mean-field ansatz
- → ordering in entanglement
- → To understand these systems: need to capture their entanglement!
- Useful as quantum memories and for topological quantum computing



# The physical corner of Hilbert space

- How can we describe entangled QMB states?
- ullet general state of N spins:

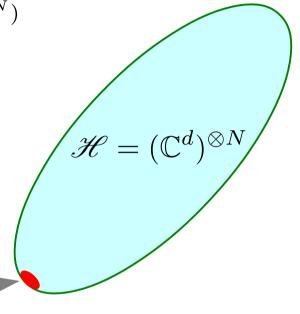
$$|\Psi_0\rangle = \sum_{i_1,\dots,i_N} c_{i_1\cdots i_N} |i_1,\dots,i_N\rangle \in (\mathbb{C}^d)^{\otimes N} = \mathbb{C}^{(d^N)}$$

exponentially large Hilbert space!

• but then again ...

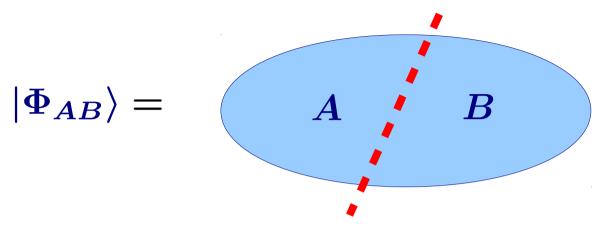
$$H = \sum_{\langle ij \rangle} h_{ij}$$
 has only  $O(N)$  parameters

- $\rightarrow$  ground state  $|\Psi_0\rangle$  must live in a small "physical corner" of Hilbert space!
- Is there a "nice" way to describe states in the physical corner?
  - → use entanglement structure!



## **Entanglement**

Consider bipartition of QMB system into A and B



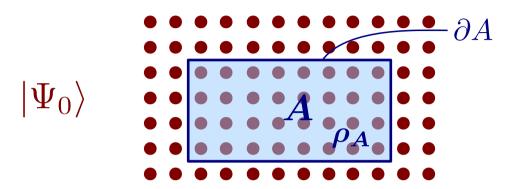
Schmidt decomposition 
$$|\Phi_{AB}\rangle = \sum_{k} \sqrt{p_k} |\alpha_k\rangle_A |\beta_k\rangle_B \quad (|\alpha_k\rangle, |\beta_k\rangle \text{ ONB})$$

- Schmidt coefficients  $p_k$  characterize bipartite entanglement more disorder  $\rightarrow$  more entanglement
- Measure of entanglement:

Entanglement entropy 
$$E(\Phi_{AB}) = S(
ho_A) = -\sum p_k \log p_k$$

## **Entanglement structure: The area law**

How much is a region of a QMB system entangled with the rest?

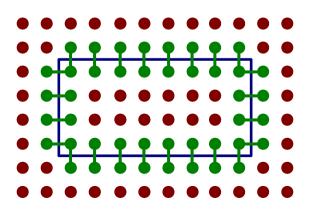


• entanglement entropy  $S(\rho_A)$  of a region scales as boundary (vs. volume)

"area law" for entanglement

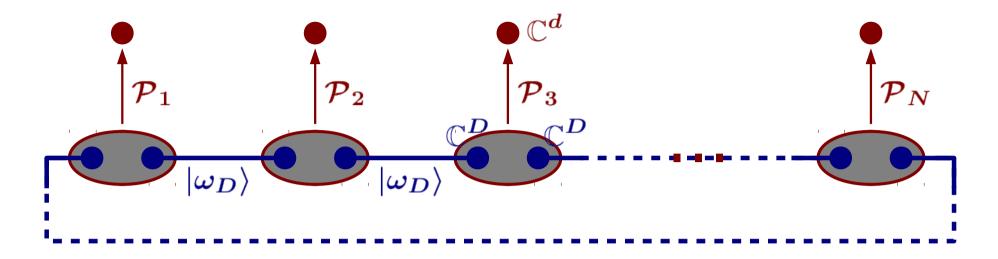
(for Hamiltonians with a **spectral gap**; but approx. true even without gap)

 Interpretation: entanglement is distributed locally



# **One dimension: Matrix Product States**

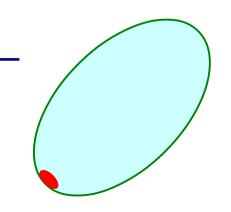
#### An ansatz for states with an area law



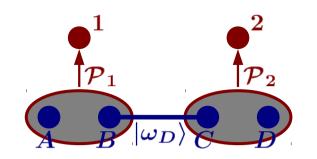
- each site composed of two **auxiliary particles** ("virtual particles") forming max. entangled **bonds**  $|\omega_D\rangle := \sum_{i=1}^D |i,i\rangle$  (D: "bond dimension")
- apply linear map ("projector")  $\mathcal{P}_k : \mathbb{C}^D \times \mathbb{C}^D \to \mathbb{C}^d$

$$\Rightarrow |\psi\rangle = ({\cal P}_1\otimes \cdots \otimes {\cal P}_N)|\omega_D
angle^{\otimes N}$$

- satisfies area law by construction
- state characterized by  $\mathcal{P}_1, \dots, \mathcal{P}_N \to NdD^2$  parameters
- ullet family of states: enlarged by increasing D



#### **Formulation in terms of Matrix Products**



$$\mathcal{P}_{s} = \sum_{i,\alpha,\beta} A_{\alpha\beta}^{[s],i} |i\rangle\langle\alpha,\beta|$$

$$A^{[s],i}: D\times D \text{ matrices}$$

$$(\mathcal{P}_{1} \otimes \mathcal{P}_{2})|\omega_{D}\rangle = \left[\sum_{i,\alpha,\beta} A_{\alpha\beta}^{[1],i}|i\rangle_{1}\langle\alpha,\beta|_{AB}\right] \left[\sum_{j,\gamma,\delta} A_{\gamma\delta}^{[2],j}|j\rangle_{2}\langle\gamma,\delta|_{CD}\right] \left[\sum_{k}|k,k\rangle_{BC}\right]$$

$$= \sum_{i,j,\alpha,\delta} \left[\sum_{\beta} A_{\alpha\beta}^{[1],i}A_{\beta\delta}^{[2],j}\right]|i,j\rangle_{12}\langle\alpha,\delta|_{AD} \qquad \beta = \gamma$$

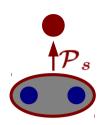
$$= \sum_{i,j,\alpha,\delta} (A^{[1],i}A^{[2],j})_{\alpha\delta}|i,j\rangle_{12}\langle\alpha,\delta|_{AD}$$

• iterate this for the whole state  $|\psi\rangle=(\mathcal{P}_1\otimes\cdots\otimes\mathcal{P}_N)|\omega_D\rangle^{\otimes N}$ :

$$|\psi\rangle = \sum_{i_1,...,i_N} [A^{[1],i_1}A^{[2],i_2}\cdots A^{[N],i_N}]|i_1,...,i_N\rangle$$
 "Matrix Product State" (MPS)

(or 
$$|\psi\rangle = \sum_{i_1,\dots,i_N} \langle l|A^{[1],i_1}A^{[2],i_2}\cdots A^{[N],i_N}|r\rangle|i_1,\dots,i_N\rangle$$
 for open boundaries)

#### Formulation in terms of Tensor Networks



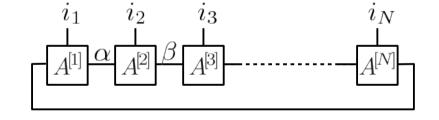
$$\mathcal{P}_s = \sum_{i,\alpha,\beta} A_{\alpha,\beta}^{[s],i} |i\rangle\langle\alpha,\beta|$$

$$\mathcal{P}_{s} = \sum_{i=0}^{s} A_{\alpha,\beta}^{[s],i} |i\rangle\langle\alpha,\beta| \qquad A_{\alpha\beta}^{[s],i} \equiv \alpha - A_{\alpha\beta}^{[s]} - \beta$$

Tensor Network notation:

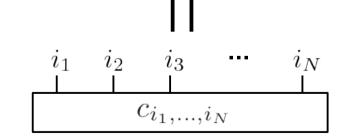
$$A^{i}_{\alpha\beta} \equiv \alpha - A - \beta \qquad \qquad \sum_{\beta} A^{i}_{\alpha\beta} B^{j}_{\beta\gamma} \equiv \alpha - A - B - \gamma$$

$$\operatorname{tr}[A^{[1],i_1}A^{[2],i_2}\cdots A^{[N],i_N}] = A^{[1]} \alpha A^{[2]} \beta A^{[3]} - \cdots$$



Matrix Product States can be written as

$$|\Psi_0\rangle = \sum_{i_1,...,i_N} c_{i_1,...,i_N} |i_1,\ldots,i_N\rangle$$
 with

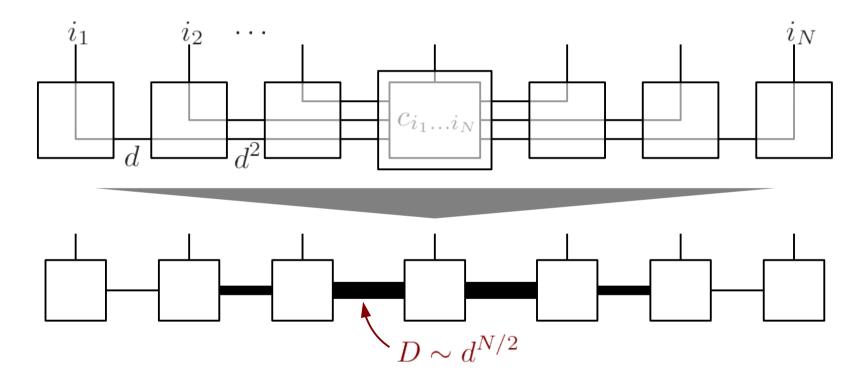


"Tensor Network States"

## **Completeness of MPS**

• MPS form a complete family – every state can be written as an MPS:

$$|\psi\rangle = \sum_{i_1,\dots,i_N} c_{i_1\dots i_N} |i_1,\dots,i_N\rangle$$

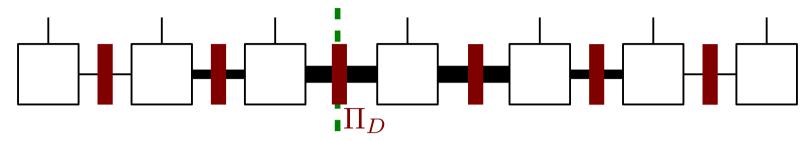


• Can be understood in terms of **teleporting**  $|\psi\rangle$  using the entangled bonds



# **Approximation by MPS**

General MPS with possibly very large bond dimension



Schmidt decomposition across some cut:

$$|\Phi_{AB}\rangle = \sum_{k} \sqrt{p_k} |\alpha_k\rangle |\beta_k\rangle$$

• Project onto  $\boldsymbol{D}$  largest Schmidt values  $p_1, \dots, p_D$ :

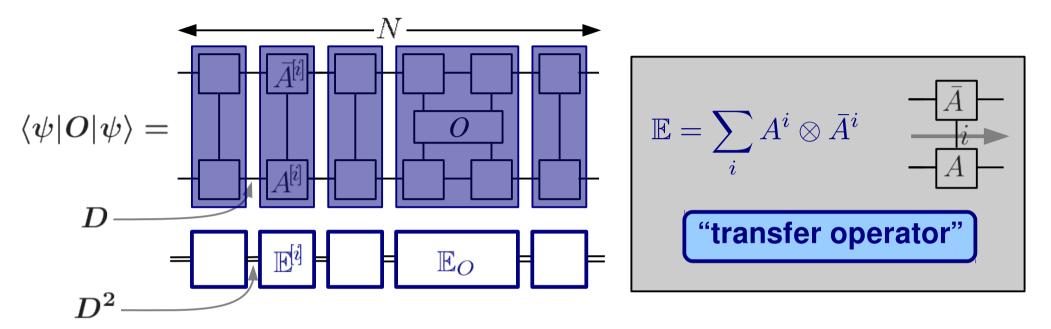
$$\rightarrow \operatorname{error} \ \epsilon(D) = \sum_{k>D} p_k$$

- Rapidly decaying  $p_k$  ( $\leftrightarrow$  bounded entropy): total error  $\sim \text{poly}(N, 1/D)$
- Efficient approximation of states with area law (and thus ground states)

Matrix Product States can efficiently approximate states with an area law, and ground states of (gapped) one-dimensional Hamiltonians.

## **Computing properties of MPS**

• Given an MPS  $|\psi\rangle$ , can we compute exp. values  $\langle\psi|O|\psi\rangle$  for local O?

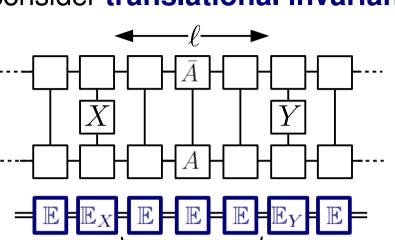


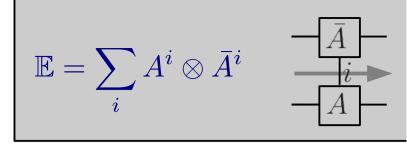
$$\langle \psi | O | \psi \rangle = [\mathbb{E}^{[1]} \mathbb{E}^{[2]} \cdots \mathbb{E}^{[k-1]} \mathbb{E}_O \mathbb{E}^{[k+2[} \cdots \mathbb{E}^{[N]}]$$

- computing  $\langle \psi | O | \psi \rangle$  = multiplication of  $D^2 \times D^2$  matrices
  - ightarrow computation time  $\propto N \cdot D^6 = poly(N)$
- OBC scaling:  $D^4$  [and if done properly, even  $D^5$  (PBC) and  $D^3$  (OBC)]

# The transfer operator

consider translational invariant system:





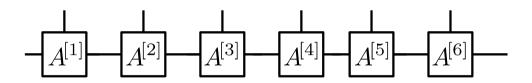
$$\mathbb{E} = \sum_{k} \lambda_k |r_k\rangle \langle l_k|$$

$$\mathbb{E}^{\ell} = \sum_{k} \lambda_{k}^{\ell} |r_{k}\rangle\langle l_{k}|$$

- spectrum of transfer operator governs scaling of correlations
  - (a) largest eigenvalue unique: exponential decay of correlations
  - (b) largest eigenvalue degenerate: long-range correlations
- ullet uniqueness of purification:  ${\mathbb E}$  contains all non-local information about state
- $\mathbb{E} = \sum A^i \otimes \bar{A}^i$  is Choi matrix of quantum channel  $\mathcal{E}: \rho \mapsto \sum A^i \rho(A^i)^\dagger$

## **Numerical optimization of MPS**

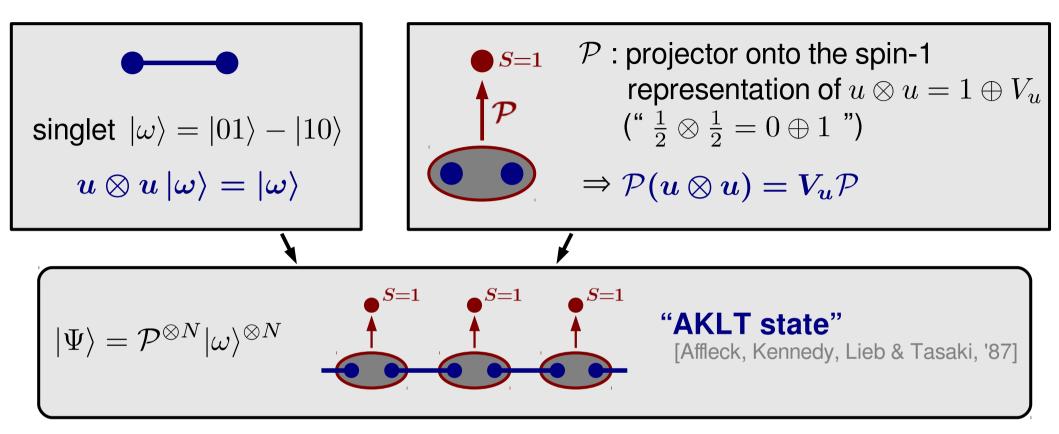
- MPS approximate ground states efficiently
- expectation values can be computed efficiently
- can we efficiently find the  $|\psi\rangle$  which minimizes  $\langle\psi|H|\psi\rangle$ ?



- various methods:
  - DMRG: optimize sequentially  $A^{[1]}, A^{[2]}, \ldots$  & iterate
  - gradient methods: optimize all  $A^{[s]}$  simultaneously
  - hybrid methods
  - ...  $\langle \psi | H | \psi \rangle$  is quadratic in each  $A^{[s]} \rightarrow$  each step can be done efficiently
- hard instances exist (NP-hard), but methods practically converge very well
- provably working poly-time method exists

MPS form the basis for powerful variational methods for the simulation of one-dimensional spin chains

## Example: The AKLT state - a rotationally invariant model



• Resulting state is **invariant under** SU(2) (=spin rotation) by construction:

$$V_u^{\otimes N} |\Psi\rangle = (V_u \mathcal{P})^{\otimes N} |\omega\rangle^{\otimes N} = (\mathcal{P}(u \otimes u))^{\otimes N} |\omega\rangle^{\otimes N} = \mathcal{P}^{\otimes N} |\omega\rangle^{\otimes N} = |\Psi\rangle$$

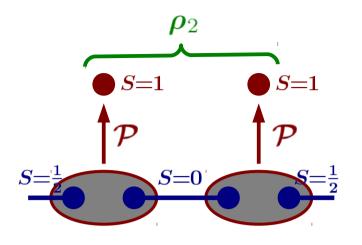
Can construct states w/ symmetries by encoding symmetries locally

#### The AKLT Hamiltonian

consider 2 sites of AKLT model

2 sites have spin 
$$1 \otimes 1 = 0 \oplus 1 \oplus X$$

#### impossible!



• 
$$h := \Pi_{S=2} : h \ge 0$$
, and  $h|\Psi_{AKLT}\rangle = 0$ 

$$\Rightarrow \ket{\Psi_{ ext{AKLT}}}$$
 is a (frustration free) **ground state** of  $H = \sum h_i$ 

(frustration free = it minimized each  $h_i$  individually)

#### "parent Hamiltonian"

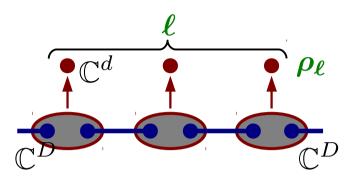
ullet *H* inherits spin-rotation symmetry of state by construction

(specifically, 
$$h_i = \frac{1}{2} \left[ \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \frac{1}{3} (\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 \right] + \frac{1}{3}$$
)

- One can prove:  $|\Psi_{\rm AKLT}\rangle$  is the **unique ground state** of H
  - H has a **spectral gap** above the ground state

#### **Parent Hamiltonians**

• A parent Hamiltonian can be constructed for any MPS:



 $ho_\ell$  lives in  $d^\ell$ -dimensional space

 ${\cal D}^2$  possible boundary conditions

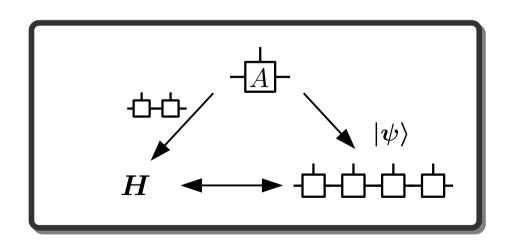
choose  $\ell$  s.th.  $d^{\ell} > D^2 \to \rho_{\ell}$  doesn't have full rank

- Construct parent Hamiltonian  $h=1-\Pi_{\ker(
  ho_\ell)}$  ,  $H=\sum h$
- Can prove:
  - has unique ground state
  - has a spectral gap above the ground state
- This + ability of MPS to approximate ground states of general Hamiltonians
  - → MPS form right framework to study physics of 1D QMB systems

## **MPS** and symmetries

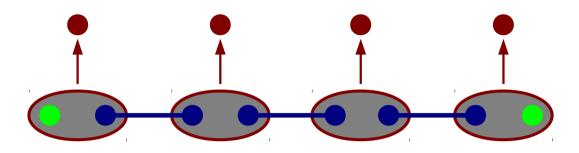
Symmetries in MPS can always be encoded locally

• Symmetries are inherited by the parent Hamiltonian!



#### **Fractionalization**

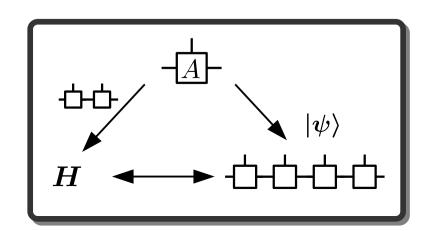
• Consider AKLT model on chain with open boundaries



- all choices of boundaries are **ground states** of parent Hamiltonian
  - ightarrow zero energy "edge excitations" with spin  $S=rac{1}{2}$
- "fractionalization" of physical spin S=1 into  $S=rac{1}{2}$  at the boundary
  - → impossible in mean-field theory
  - → non-trivial "topological" phase ("Haldane phase")

$$- \stackrel{u_g}{-} = V_g - \stackrel{\downarrow}{-} - V_g^{\dagger}$$

- can prove: cannot smoothly connect MPS with integer and half-integer spin at edge
  - → inequivalent phases!

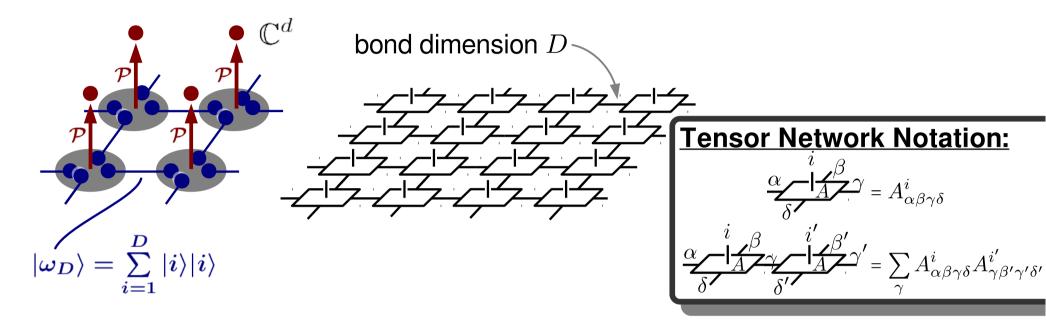


MPS encode physical symmetries locally, and can be used to model physical systems and study their different non-trivial phases.



# Two dimensions: Projected Entangled Pair States

Natural generalization of MPS to two dimensions:



**Projected Entangled Pair States (PEPS)** 

- approximate ground states of local Hamiltonians well
- PEPS form a complete family with accuracy parameter D.
- PEPS can also be defined on other lattices, in three and more dimensions, even on any graph

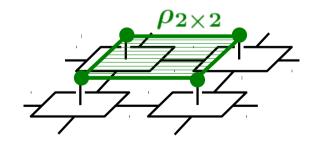
# 2D: Symmetries and parent Hamiltonians

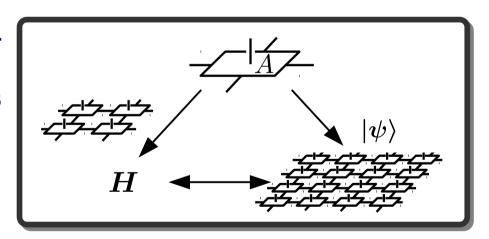
• **symmetries** can be encoded locally in **entanglement** degrees of freedom:

$$= V_g^{\dagger} \bigvee_{V_g}^{\dagger} V_g$$

however, a general characterization of inverse direction is still missing ...
 (but there are partial results)

we can also define parent Hamiltonians

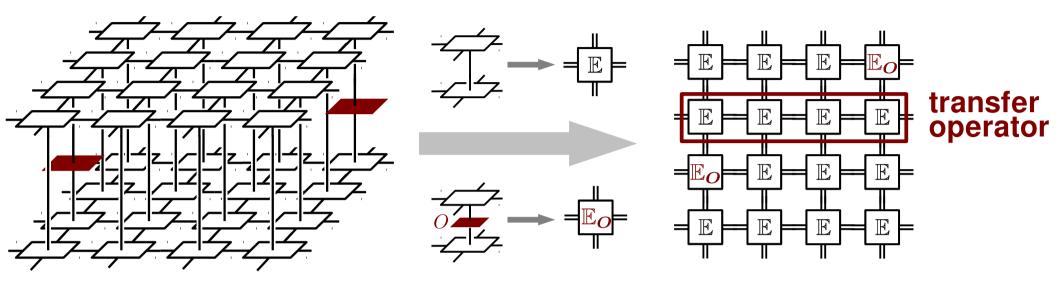




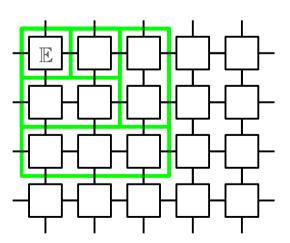
again, a full characterization of ground space and spectral gap is missing ...
 (and again, there are partial results)

## **Computational complexity of PEPS**

• expectation values in PEPS (e.g. correlation functions):



• resembles 1D situation, but ...



... exact contraction is a hard problem (more precisely, #P-hard)

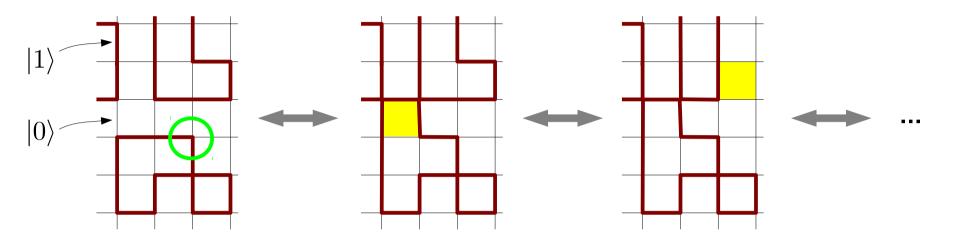
approximation methods necessary – e.g. by again using MPS

Projected Entangled Pair States (PEPS) approximate two-dimensional systems faithfully, can be used for numerical simulations, and allow to locally encode the physics of 2D systems.

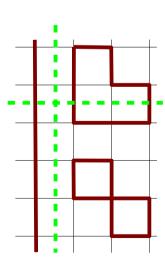


#### The Toric Code model

• Toric Code: ground state = superposition of all loop patterns



- Hamiltonian: (i) vertex term → enforce closed loops
  - (ii) plaquette term → **fix phase** when flipping plaquette
- degenerate ground states:
   labeled by parity of loops around torus
- non-trivial excitations:
  - (i) broken strings (come in pairs)
  - (ii) wrong relative phase (also in pairs)



## Tensor networks for topological states

Tensor network for Toric Code:

$$\frac{A}{A} = \begin{cases}
0 & 1 & 0 & 1 \\
0 & 1 & 0
\end{cases} + \begin{cases}
0 & 0 & 0 \\
1 & 0 & 1
\end{cases} + \dots$$

• Toric Code tensor has  $\mathbb{Z}_2$  symmetry (=even parity):

$$= Z \xrightarrow{Z} Z$$

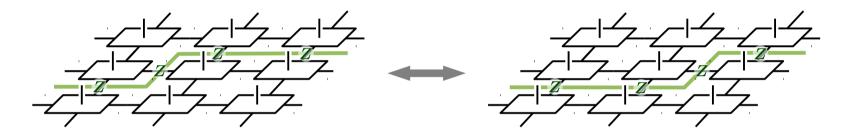
$$Z \xrightarrow{Z} Z$$

What are consequences of such an entanglement symmetry in a PEPS?

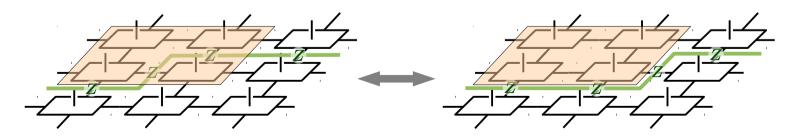
## **Entanglement symmetry and pulling through**

• Symmetry can be rephrased as "pulling-through condition":

pulling-through condition ⇒ Strings can be freely moved!



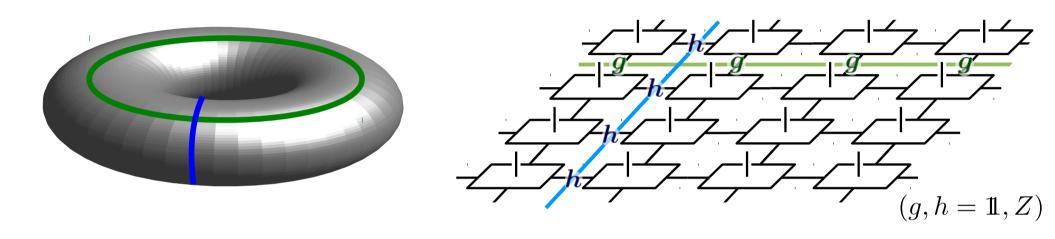
• Strings are invisible locally (e.g. to Hamiltonian)



 Note: Generalization of "pulling-through condition" allows to characterize all known (non-chiral) topological phases

## Topological ground space manifold

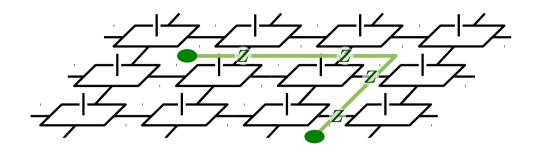
Torus: closed strings yield different ground states



- degeneracy depends on topology (genus): Topological order!
  - → **local characterization** of topological order
  - → parametrization of ground space manifold based on symmetry of single tensor
  - → gives us the tools to explicitly construct & study ground states
  - → works for systems with finite correlation length

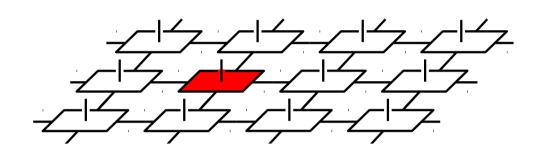
# Symmetries and excitations

- Strings w/ open ends:
  - → endpoints = excitations
  - → excitations come in pairs

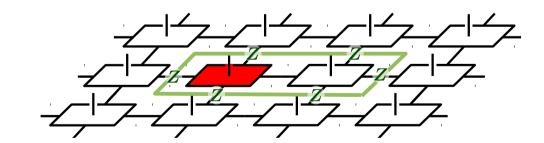


tensors with odd parity:

$$= - z = Z Z$$



- → cannot be created locally
- → must also come in pairs
- these two types of excitations have non-trivial mutual statistics!

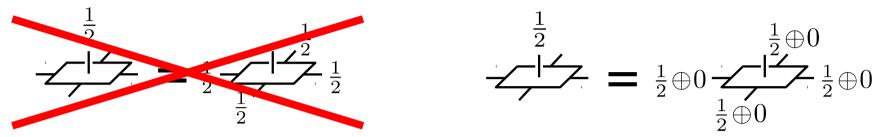


- modeling of anyonic excitations from local symmetries of tensor
- fully local description also at finite correlation length

Topological order in PEPS can be comprehensively modeled based on a local entanglement symmetry.

# Interplay of physical and entanglement symmetries

• spin- $\frac{1}{2}$  model: how can we **encode** SU(2) **symmetry**?



 $\Rightarrow V_q$  must combine integer & half-integer representations!

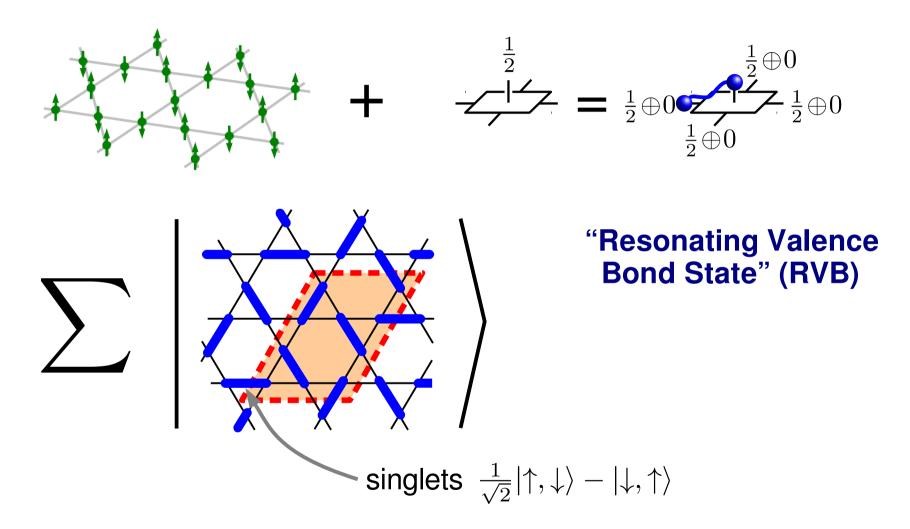
constraint: number of half-integer representations must be odd

$$Z = -Z Z Z Z Z Z Z = \begin{bmatrix} S = \frac{1}{2} \\ -1 \end{bmatrix}$$
 counts half-int. spins

- Entanglement symmetry can emerge from physical symmetries
- Open: Full understanding of interplay between physical and entanglement symmetries!

# **Example: Study of Resonating Valence Bond states**

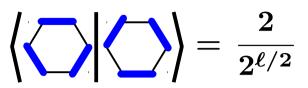
• SU(2) invariant PEPS on the kagome lattice:



• Natural interpretation of  $\mathbb{Z}_2$  constraint: fixed parity of singlets along cut

#### **RVB** and dimer models

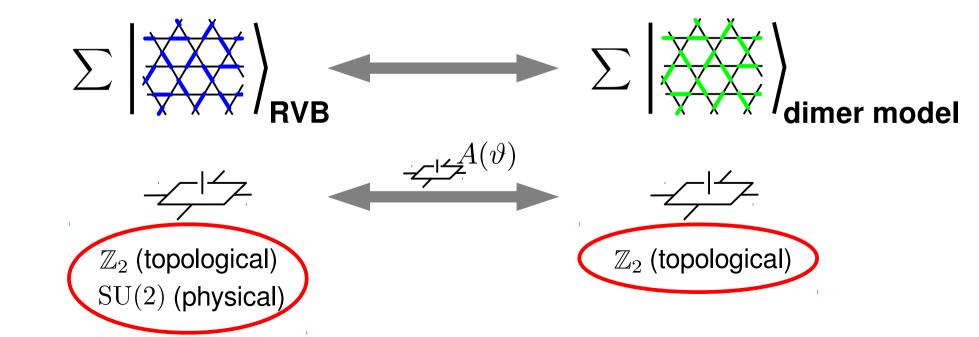
- RVB difficult to study:
  - configurations not orthogonal, negative signs
  - Topological? Magnetically ordered?



- resort to dimer models with orthogonal dimers
  - can be exactly solved
  - topologically ordered

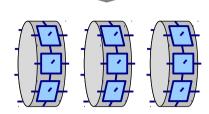
$$\left\langle \left\langle \right\rangle \right| \left\langle \right\rangle \right\rangle = 0$$

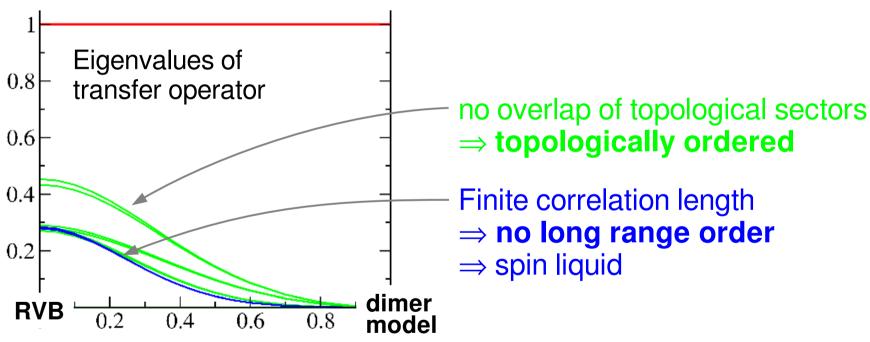
Interpolation in PEPS (w/ smooth Hamiltonian!):



#### Numerical study of the RVB state

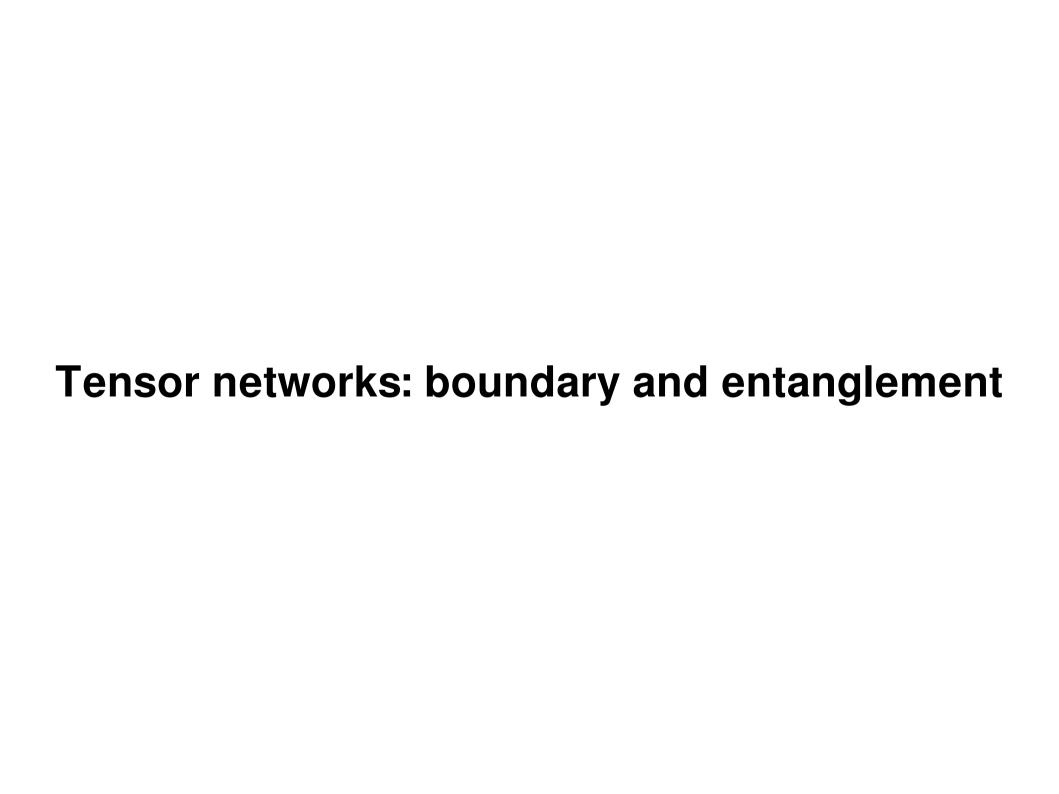
- numerical study of interpolation RVB ↔ dimer model
- "transfer operator": governs all correlation functions
   topological sector labeled by symmetry





- $\Rightarrow$  RVB state on kagome lattice is a  $\mathbb{Z}_2$  topological spin liquid
- can be proven: RVB is (topo. degenerate) ground state of parent Hamiltonian

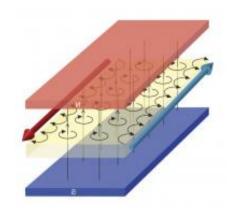
PEPS allow to study the interplay of physical and entanglement symmetries and to separately analyze their effect.



## Edge physics of topological models

Fractional Quantum Hall effect (FQHE):

edge exhibits precisely quantized currents which are robust to any perturbation



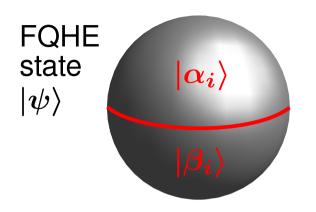
Such a behavior cannot occur in a truly one-dimensional system:

Physics at the edge has an anomaly!

- Origin of anomalous edge physics: presence of topologically entangled bulk!
- Nature of anomaly characterizes topological order in the bulk

## **Entanglement spectra**

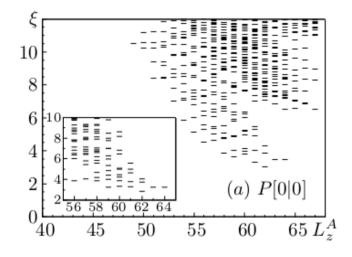
• Entanglement spectra: [Li & Haldane, PRL '08]



$$|\psi\rangle = \sum e^{-E_i} |\alpha_i\rangle \otimes |\beta_i\rangle$$

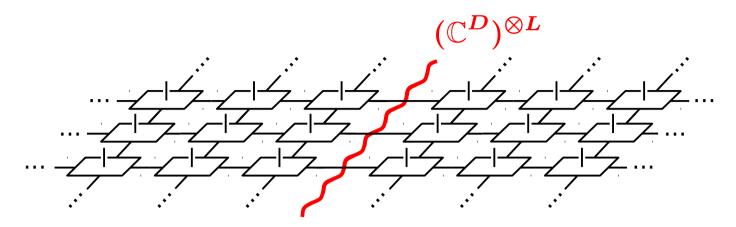
"Entanglement spectrum (ES)"  $E_i \equiv E_i(k)$  momentum k associated to 1D boundary  $\rightarrow$  spectrum of 1D "entanglement Hamiltonian"?

- FQHE: **Entanglement spectrum** resembles spectrum of anomalous edge theory (a conformal field theory)
  - → Entanglement spectrum can help to characterize topological phases



- Can we understand the relation between entanglement spectrum, edge physics, and topological order in the bulk?
- Can we understand why the **entanglement spectrum** relates to a **1D system**?

## **Bulk-edge correspondence in PEPS**



• Bipartition  $|\Phi_{AB}\rangle=\sum_i\sqrt{p_i}|\alpha_i\rangle|\beta_i\rangle$   $\to$  entanglement carried by

degrees of freedom  $i=(i_1,...,i_L)$  at boundary

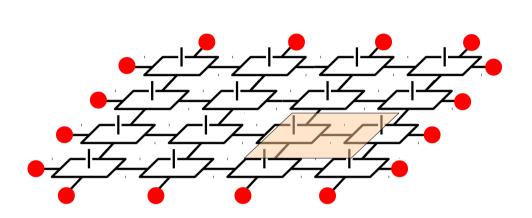
Allows for direct derivation of entanglement Hamiltonian

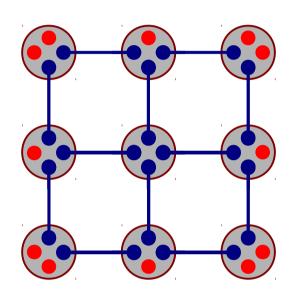
$$e^{-H_{
m ent}} = \sigma$$
 lives on entanglement degrees of freedom

- $\rightarrow H_{\rm ent}$  has natural 1D structure!
- ullet  $H_{
  m ent}$  inherits all symmetries from tensor

## **Edge physics**

• How to describe low-energy edge physics for parent Hamiltonian?





- Parametrized by choosing all possible boundary conditions
- Edge physics lives on the entanglement degrees of freedom

## Topological symmetries at the edge

Entanglement symmetry inherited by the edge:

$$\frac{Z}{Z} = Z - \frac{Z}{Z} = \frac{Z}{Z} - \frac{Z}{Z} -$$

- global constraint (here, parity) on entanglement degrees of freedom: Only states in even parity sector can appear at boundary!
  - → topological correction to entanglement entropy
  - → entanglement Hamiltonian has an anomalous term:

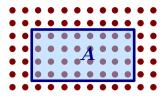
$$\rho = \Pi_{\text{even}} e^{-H} \Pi_{\text{even}} = e^{-H + \beta_{\text{topo}} \cdot H_{\text{topo}}}$$

- → edge physics constrained to even parity sector: anomalous!
- entanglement spectrum and edge physics exhibit the same anomaly, which originates in the topological order in the bulk

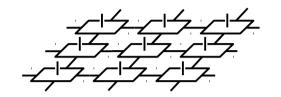
PEPS provide a natural one-dimensional Hilbert space which describes the edge physics and entanglement spectrum, and yield an explicit connection between edge physics, entanglement spectrum, and bulk topological order.

## **Summary**

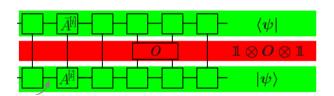
• Entanglement of quantum many-body systems: Area law



• Matrix Product States and PEPS: build entanglement locally

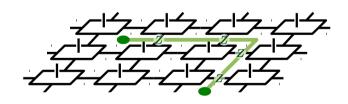


Efficient approximation: powerful numerical tool



• Framework to study structure of many-body systems

$$= V_g^{\dagger} V_g^{\dagger} V_g$$



Explicit 1D Hilbert space for entanglement

→ study of entanglement spectra & edge physics

