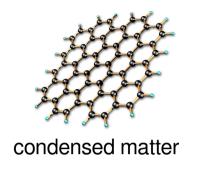
Matrix Product States and Tensor Network States

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Overview

Quantum many-body systems are all around!







quantum chemistry

high-energy physics

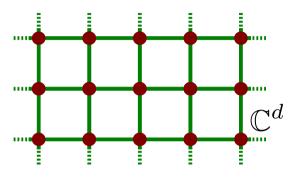
- Can exhibit complex quantum correlations (=multipartite entanglement)
 - → rich and unconventional physics, but difficult to understand!
- Quantum information and Entanglement Theory:
 Toolbox to characterize and utilize entanglement

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:

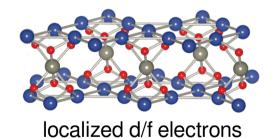


local interactions

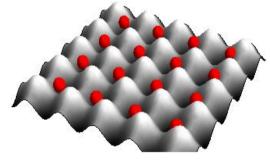
$$H = \sum_{\langle ij
angle} h_{ij}$$

... typically transl. invariant

• Realized in many systems:



half-filled band



quantum simulators, e.g. optical lattices

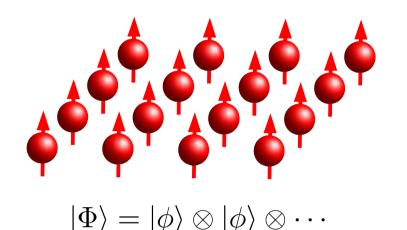
• Expecially interested in the **ground state** $|\Psi_0\rangle$,

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



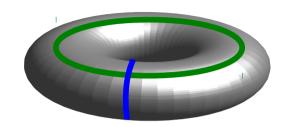
$$H = \sum_{\langle ij
angle} h_{ij}$$
 "mean field theory"

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

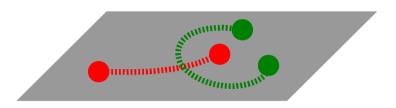
- Behavior fully characterized by a single spin $|\phi\rangle$ a local property (order parameter) → Landau theory of phases
- Behavior insensitive to boundary conditions, topology, ...

Exotic phases and topological order

Systems exist which cannot be described by mean field theory



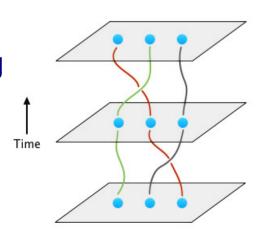
degeneracy depends on global properties



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:

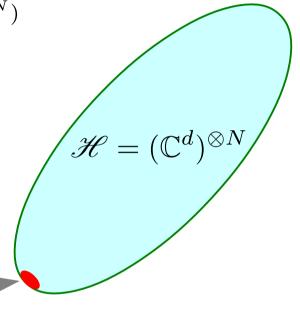
$$|\Psi_0\rangle = \sum_{i_1,\dots,i_N} c_{i_1\cdots i_N} |i_1,\dots,i_N\rangle \in (\mathbb{C}^d)^{\otimes N} = \mathbb{C}^{(d^N)}$$

exponentially large Hilbert space!

• but then again ...

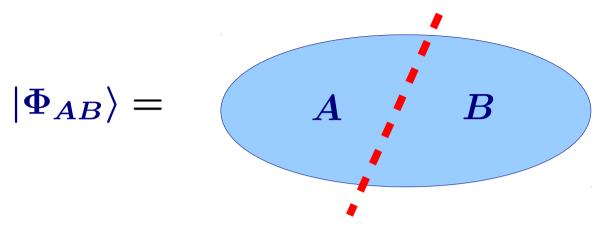
$$H = \sum_{\langle ij \rangle} h_{ij}$$
 has only $O(N)$ parameters

- \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



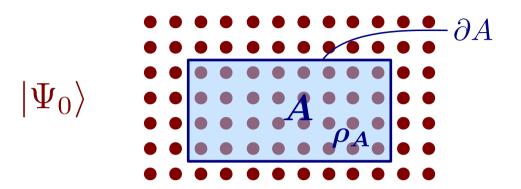
Schmidt decomposition
$$|\Phi_{AB}\rangle = \sum_{k} \sqrt{p_k} |\alpha_k\rangle_A |\beta_k\rangle_B \quad (|\alpha_k\rangle, |\beta_k\rangle \text{ ONB})$$

- 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?

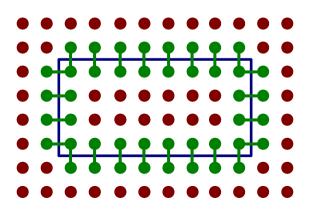


• entanglement entropy $S(\rho_A)$ of a region scales as boundary (vs. volume)

"area law" for entanglement

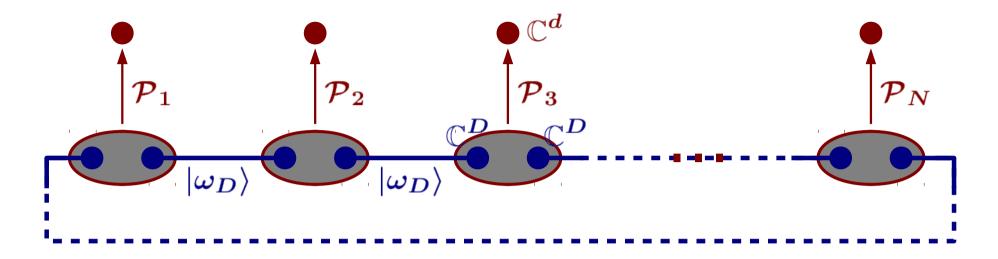
(for Hamiltonians with a **spectral gap**; but approx. true even without gap)

 Interpretation: entanglement is distributed locally



One dimension: Matrix Product States

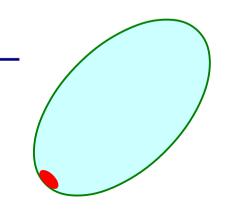
An ansatz for states with an area law



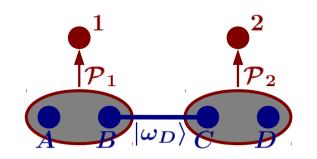
- each site composed of two **auxiliary particles** ("virtual particles") forming max. entangled **bonds** $|\omega_D\rangle := \sum_{i=1}^D |i,i\rangle$ (D: "bond dimension")
- apply linear map ("projector") $\mathcal{P}_k : \mathbb{C}^D \times \mathbb{C}^D \to \mathbb{C}^d$

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

- 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



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

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

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

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

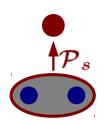
$$= \sum_{i,j,\alpha,\delta} (A^{[1],i}A^{[2],j})_{\alpha\delta}|i,j\rangle_{12}\langle\alpha,\delta|_{AD}$$

• 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



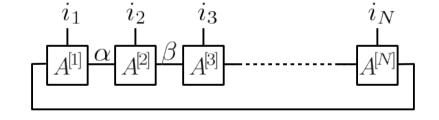
$$\mathcal{P}_s = \sum_{i,\alpha,\beta} A_{\alpha,\beta}^{[s],i} |i\rangle\langle\alpha,\beta|$$

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

Tensor Network notation:

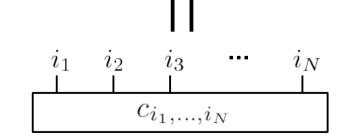
$$A^{i}_{\alpha\beta} \equiv \alpha - A - \beta \qquad \qquad \sum_{\beta} A^{i}_{\alpha\beta} B^{j}_{\beta\gamma} \equiv \alpha - A - B - \gamma$$

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



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

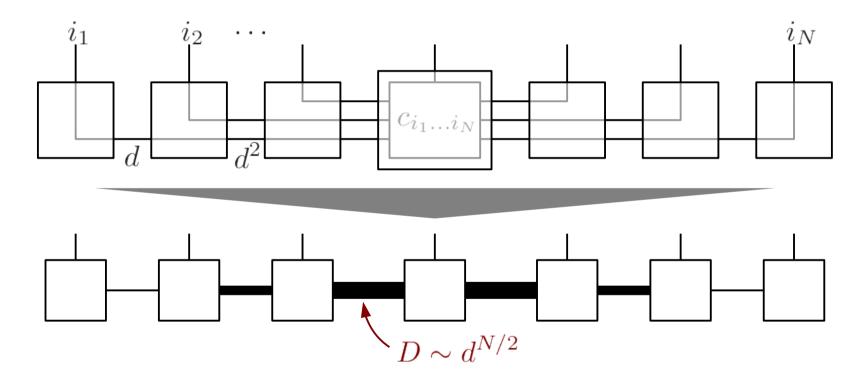


"Tensor Network States"

Completeness of MPS

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

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

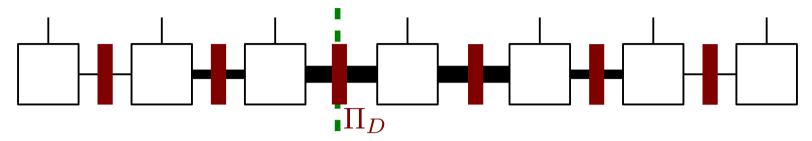


• Can be understood in terms of **teleporting** $|\psi\rangle$ using the entangled bonds



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 :

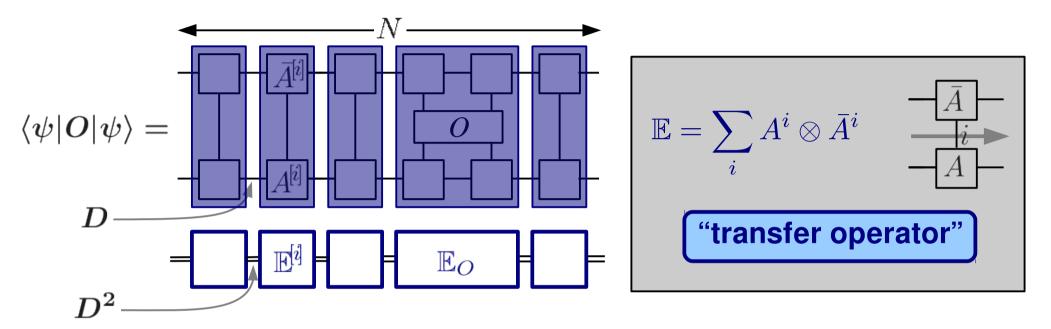
$$\rightarrow \operatorname{error} \ \epsilon(D) = \sum_{k>D} p_k$$

- 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?

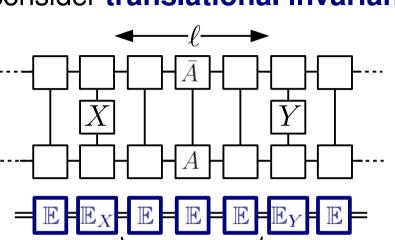


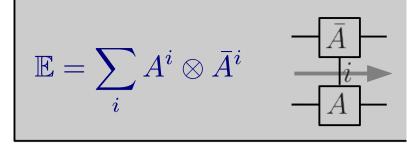
$$\langle \psi | O | \psi \rangle = [\mathbb{E}^{[1]} \mathbb{E}^{[2]} \cdots \mathbb{E}^{[k-1]} \mathbb{E}_O \mathbb{E}^{[k+2[} \cdots \mathbb{E}^{[N]}]$$

- 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:





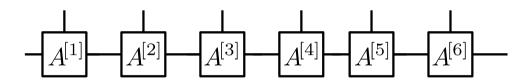
$$\mathbb{E} = \sum_{k} \lambda_k |r_k\rangle \langle l_k|$$

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

- 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

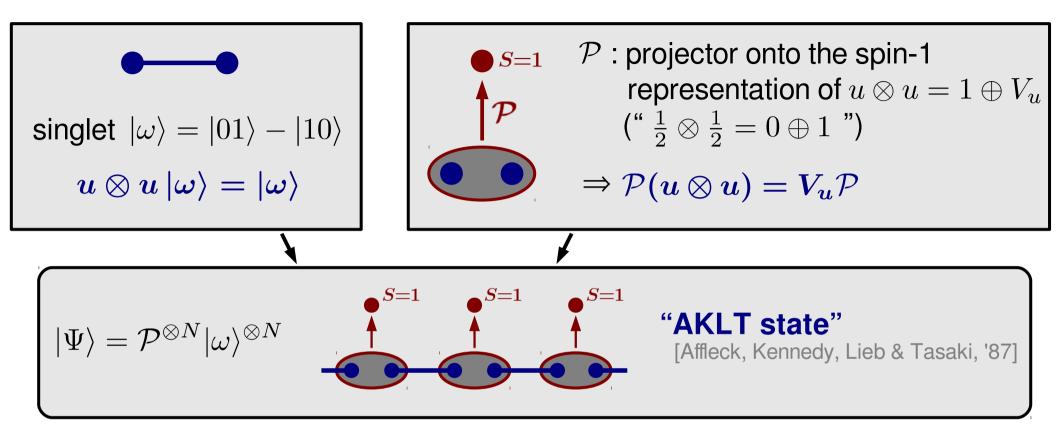
- MPS approximate ground states efficiently
- expectation values can be computed efficiently
- can we efficiently find the $|\psi\rangle$ which minimizes $\langle\psi|H|\psi\rangle$?



- 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:

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

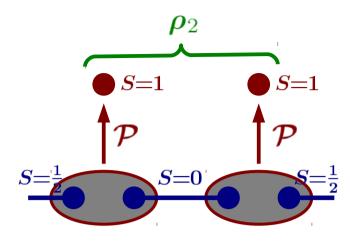
Can construct states w/ symmetries by encoding symmetries locally

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"

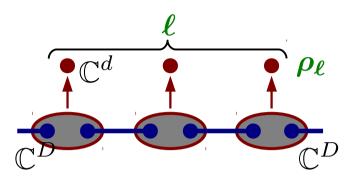
ullet *H* inherits spin-rotation symmetry of state by construction

(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_ℓ lives in d^ℓ -dimensional space

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

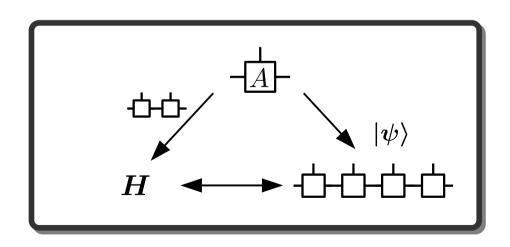
choose ℓ s.th. $d^{\ell} > D^2 \to \rho_{\ell}$ doesn't have full rank

- 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

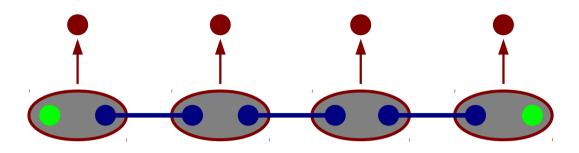
Symmetries in MPS can always be encoded locally

• Symmetries are inherited by the parent Hamiltonian!



Fractionalization

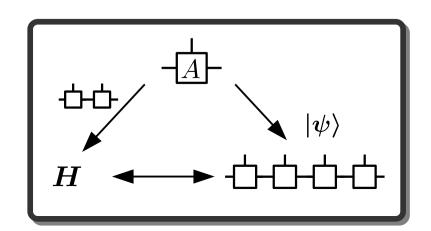
• Consider AKLT model on chain with open boundaries



- 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!

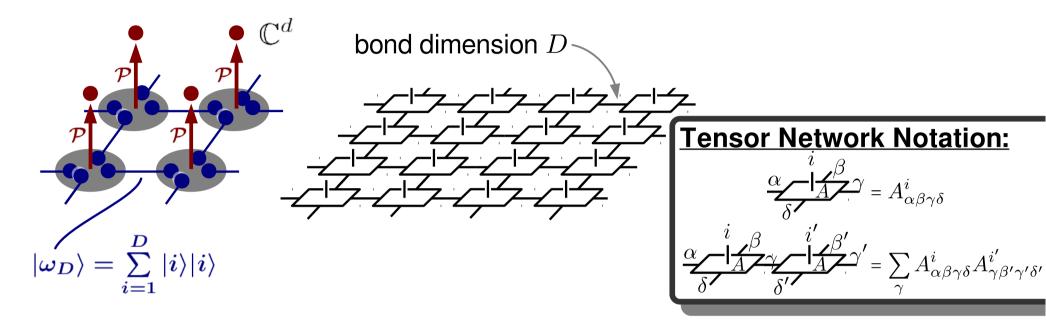


MPS encode physical symmetries locally, and can be used to model physical systems and study their different non-trivial phases.



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

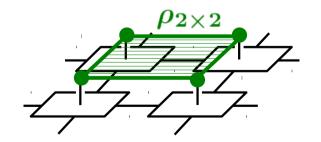
2D: Symmetries and parent Hamiltonians

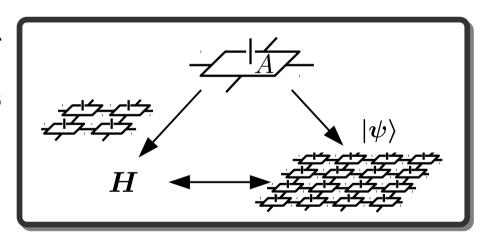
• **symmetries** can be encoded locally in **entanglement** degrees of freedom:

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

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

we can also define parent Hamiltonians

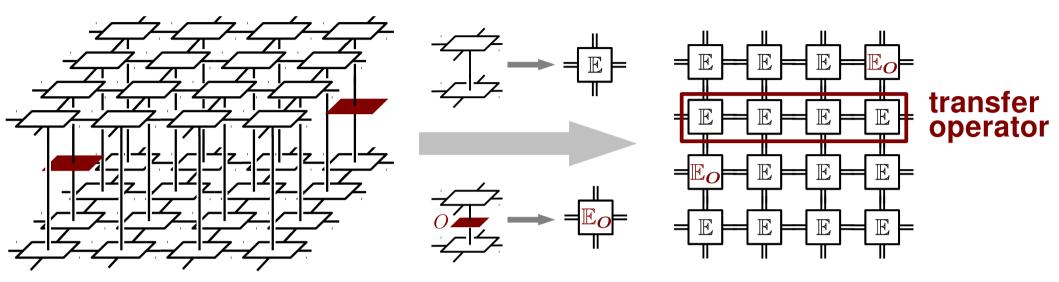




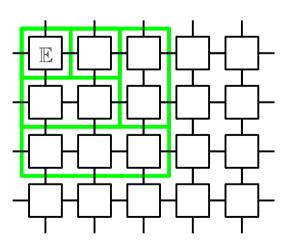
again, a full characterization of ground space and spectral gap is missing ...
 (and again, there are partial results)

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)

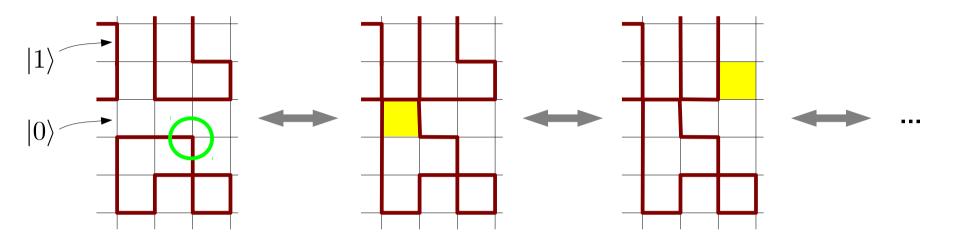
approximation methods necessary – e.g. by again using MPS

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.

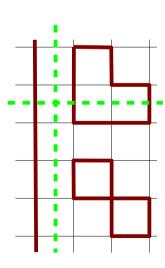


The Toric Code model

• 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):

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

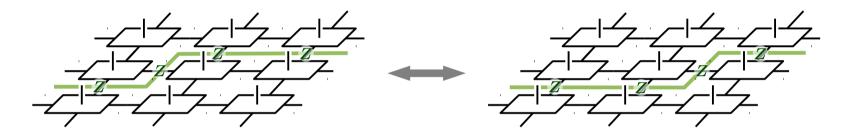
$$Z \xrightarrow{Z} Z$$

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

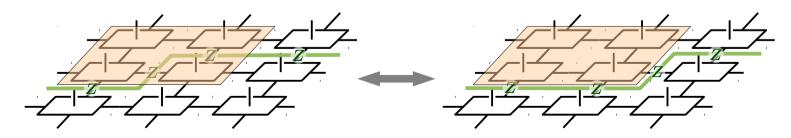
Entanglement symmetry and pulling through

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

pulling-through condition ⇒ Strings can be freely moved!



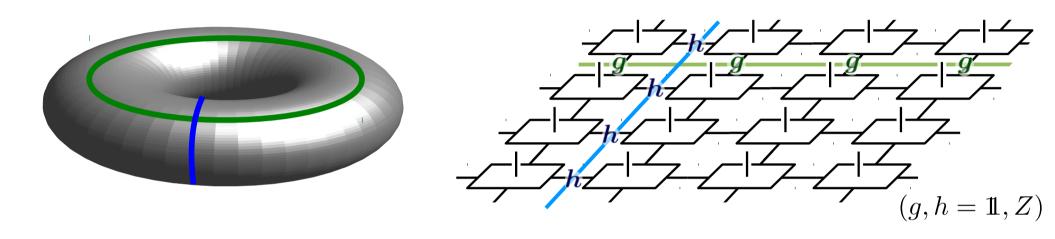
• Strings are invisible locally (e.g. to Hamiltonian)



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

Topological ground space manifold

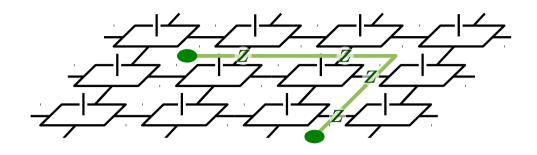
Torus: closed strings yield different ground states



- 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

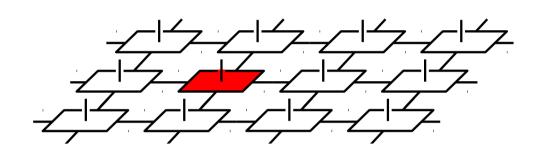
Symmetries and excitations

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

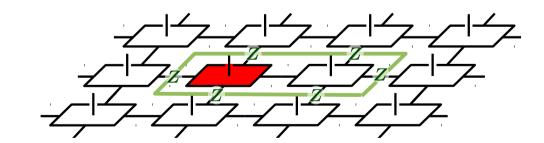


tensors with odd parity:

$$= - z = Z Z$$



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

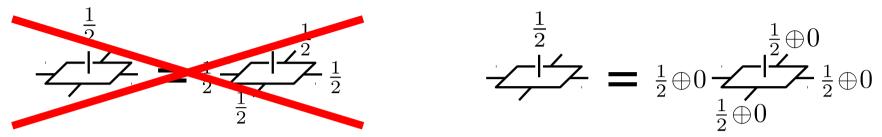


- modeling of anyonic excitations from local symmetries of tensor
- fully local description also at finite correlation length

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!

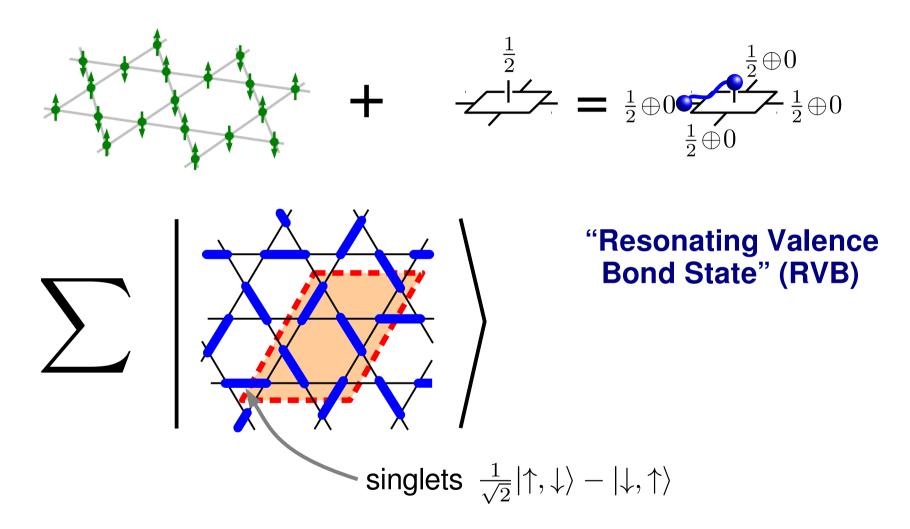
constraint: number of half-integer representations must be odd

$$Z = -Z Z Z Z Z Z Z = \begin{bmatrix} S = \frac{1}{2} \\ -1 \end{bmatrix}$$
 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

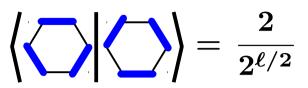
• SU(2) invariant PEPS on the kagome lattice:



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

RVB and dimer models

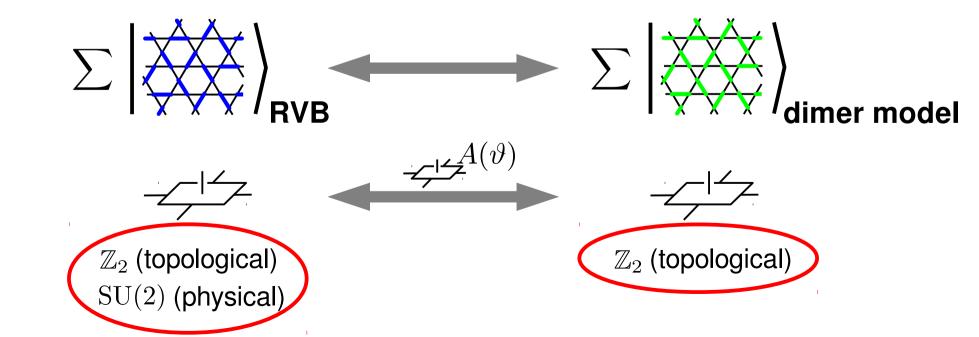
- RVB difficult to study:
 - configurations not orthogonal, negative signs
 - Topological? Magnetically ordered?



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

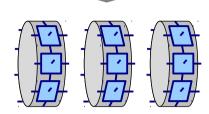
$$\left\langle \left\langle \right\rangle \right| \left\langle \right\rangle \right\rangle = 0$$

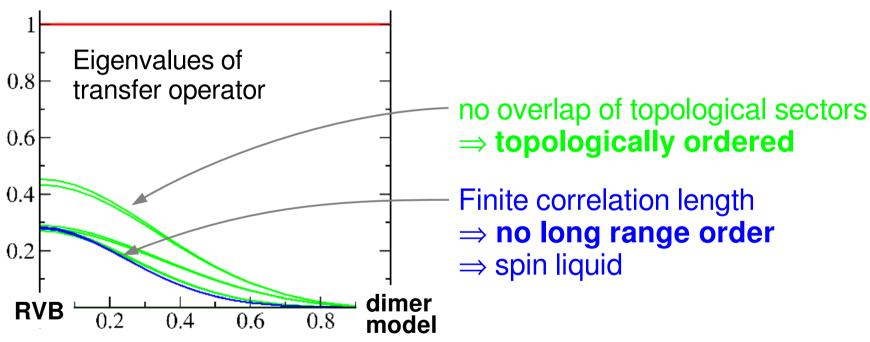
Interpolation in PEPS (w/ smooth Hamiltonian!):



Numerical study of the RVB state

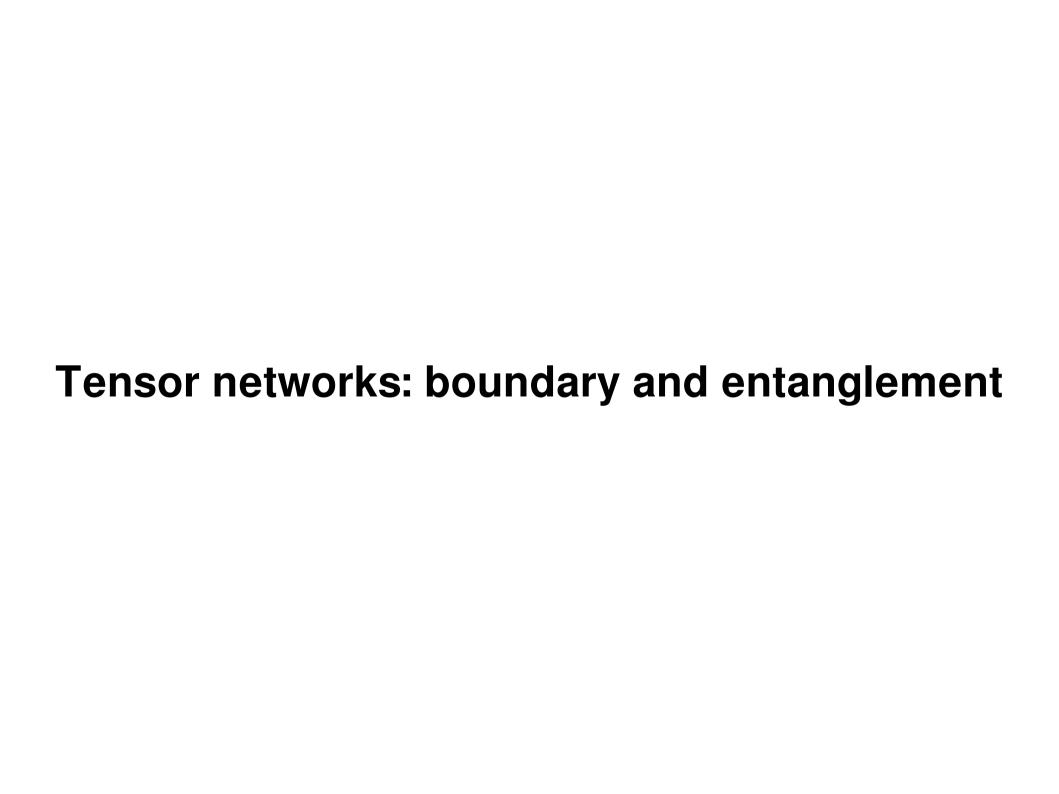
- numerical study of interpolation RVB ↔ dimer model
- "transfer operator": governs all correlation functions
 topological sector labeled by symmetry





- \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

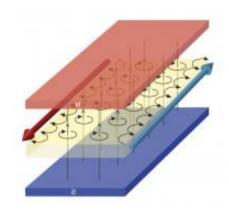
PEPS allow to study the interplay of physical and entanglement symmetries and to separately analyze their effect.



Edge physics of topological models

Fractional Quantum Hall effect (FQHE):

edge exhibits precisely quantized currents which are robust to any perturbation



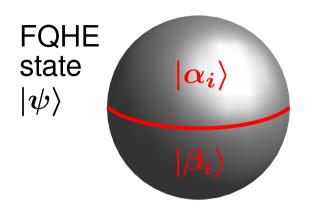
Such a behavior cannot occur in a truly one-dimensional system:

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

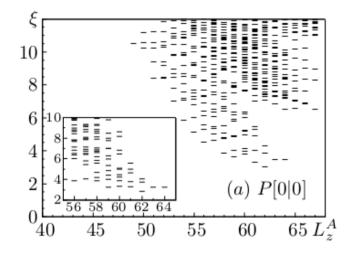
• Entanglement spectra: [Li & Haldane, PRL '08]



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

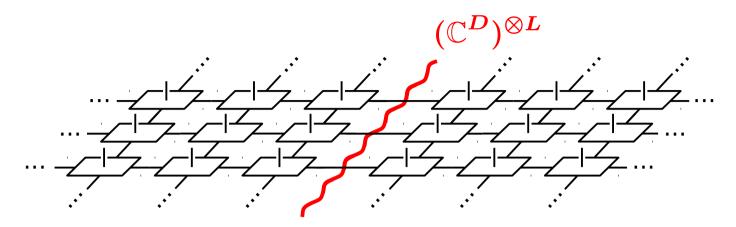
"Entanglement spectrum (ES)" $E_i \equiv E_i(k)$ momentum k associated to 1D boundary \rightarrow spectrum of 1D "entanglement Hamiltonian"?

- 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

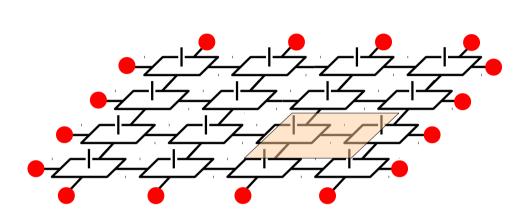
Allows for direct derivation of entanglement Hamiltonian

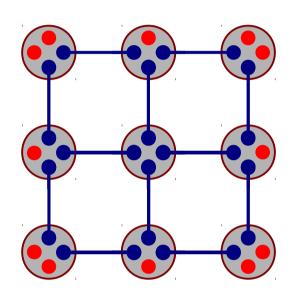
$$e^{-H_{
m ent}} = \sigma$$
 lives on entanglement degrees of freedom

- $\rightarrow H_{\rm ent}$ 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:

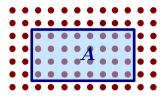
$$\rho = \Pi_{\text{even}} e^{-H} \Pi_{\text{even}} = e^{-H + \beta_{\text{topo}} \cdot H_{\text{topo}}}$$

- → 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

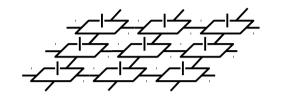
PEPS provide a natural one-dimensional Hilbert space which describes the edge physics and entanglement spectrum, and yield an explicit connection between edge physics, entanglement spectrum, and bulk topological order.

Summary

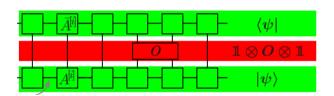
• Entanglement of quantum many-body systems: Area law



• Matrix Product States and PEPS: build entanglement locally

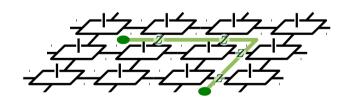


Efficient approximation: powerful numerical tool



• 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

