Efficient simulations of low-dimensional systems

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Efficient simulations of low-dimensional systems

Overview

(1) **Matrix-product states and probes for topological phases**

- Review: Entanglement and matrix-product states (MPS)
- MPS for infinite systems
- Extracting fingerprints of topological order

(2) **Efficient simulation of dynamical properties**

- Time-evolving block decimation (TEBD)
- Quench dynamics and entanglement growth
- MPO based time evolution

(3) **Tutorial: Hands on session**

(1) Matrix-product states and probes for topological phases

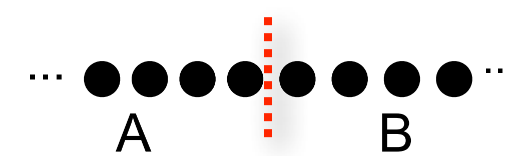
$$H|\psi\rangle = E|\psi\rangle$$

Entanglement

- A generic quantum state has a d^L dimensional Hilbert space

$$|\psi\rangle = \sum_{j_1, j_2, \ldots, j_L} \psi_{j_1, j_2, \ldots, j_L} |j_1\rangle |j_2\rangle \ldots |j_L\rangle \ , \ j_n = 1 \ldots d$$

- Decompose a state into a superposition of product states (Schmidt decomposition)



$$|\psi\rangle = \sum_{i,j} C_{i,j} |i\rangle_A \otimes |j\rangle_B = \sum_{\alpha} \Lambda_\alpha |\alpha\rangle_A \otimes |\alpha\rangle_B$$

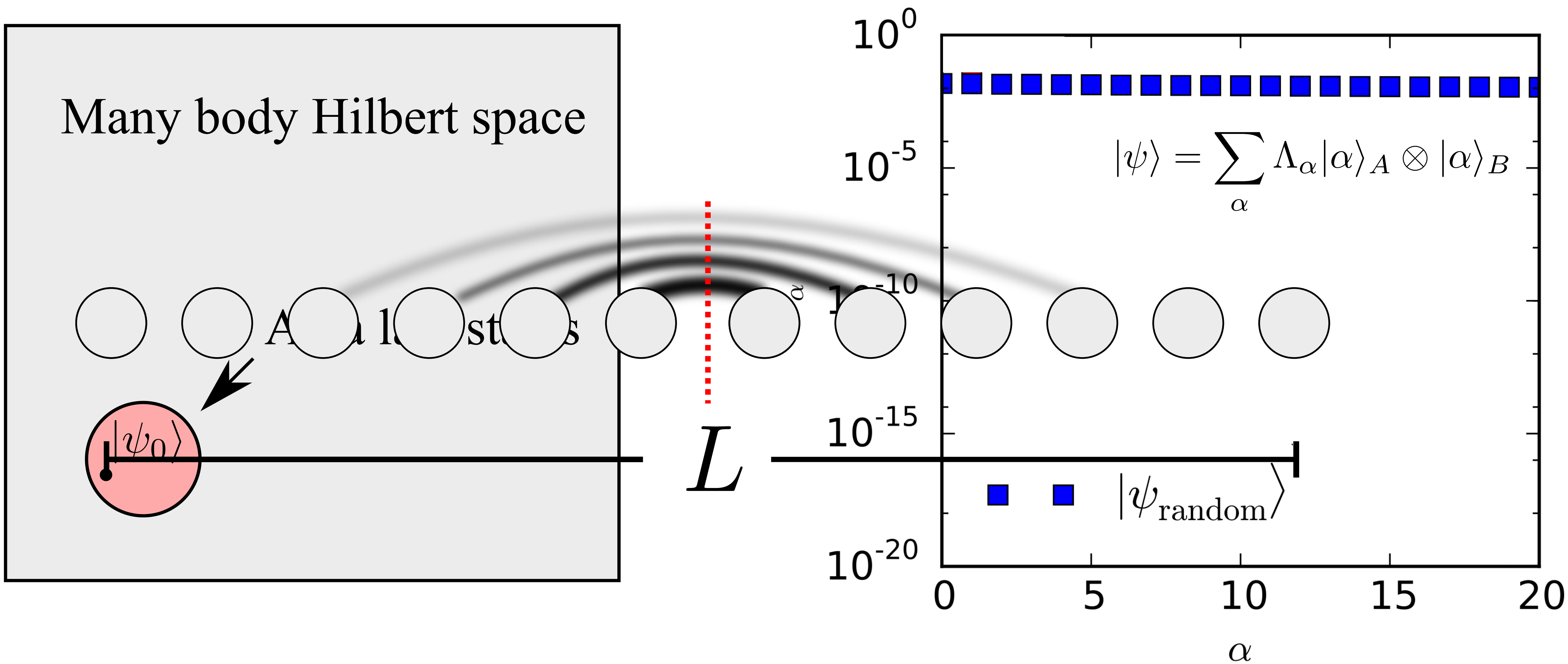
- Entanglement entropy as a measure for the amount of entanglement $S = -\sum_\alpha \Lambda_\alpha^2 \log \Lambda_\alpha^2$

- Equivalent to $S = -\mathrm{Tr} \rho_A \log \rho_A$ with $\rho_A = \mathrm{Tr}_B |\psi\rangle\langle\psi|$

Entanglement

Area law for ground states of local (gapped) Hamiltonians in one dimensional systems

$S(L) = \text{const.}$ [Srednicki '93, Hastings '07]



All ground states live in a tiny corner of the Hilbert space!

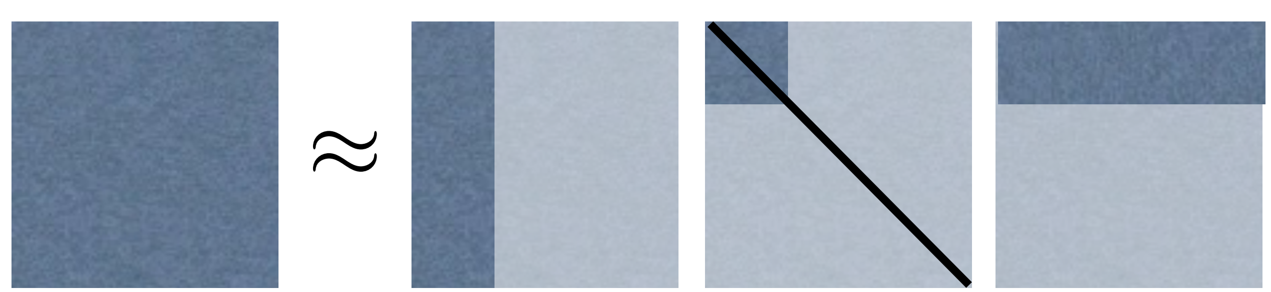
Compression of quantum states

- Example: $|\psi\rangle \quad = \quad \sum_{i=1}^{N_A} \sum_{j=1}^{N_B} C_{ij} |i\rangle_A |j\rangle_B = \sum_\gamma \lambda_\gamma |\phi_\gamma\rangle_A |\phi_\gamma\rangle_B$

- Matrix can represent an image (array of pixel)

$$C = \begin{pmatrix} 0.23 & \cdots & 0.56 \\ \vdots & \ddots & \vdots \\ 0.22 & \cdots & 0.34 \end{pmatrix} = \Bigg(\quad \Bigg)$$

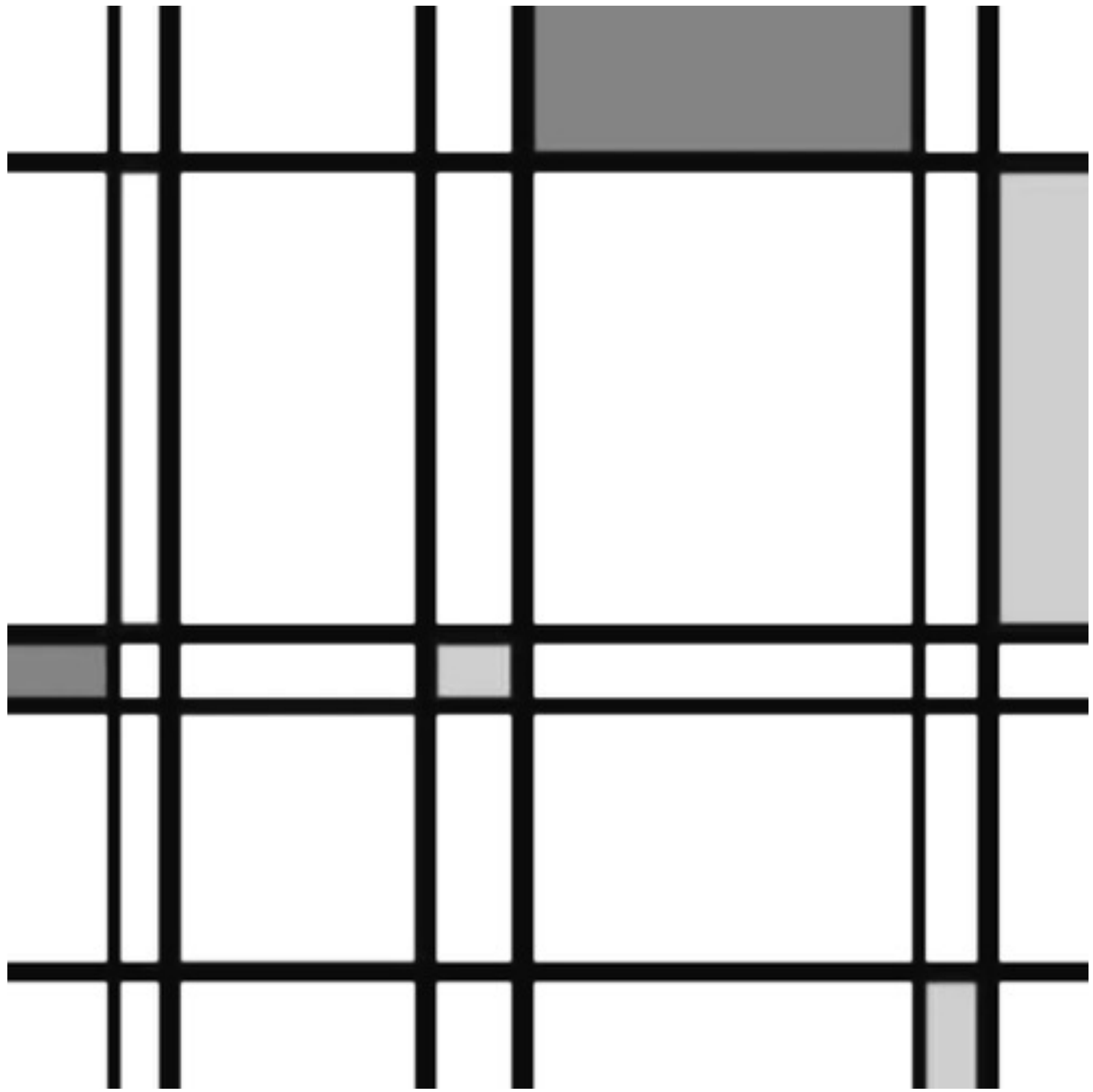
- Reconstruction of the matrix (image) from a small number of Schmidt states (SVD):



Compression of quantum states

Important features visible already for < 16 states!

Compression of quantum states

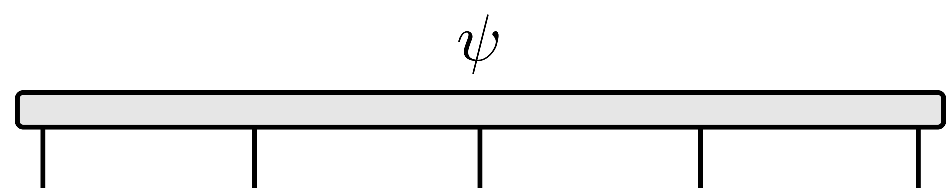


[Mondrian]

Compression of quantum states

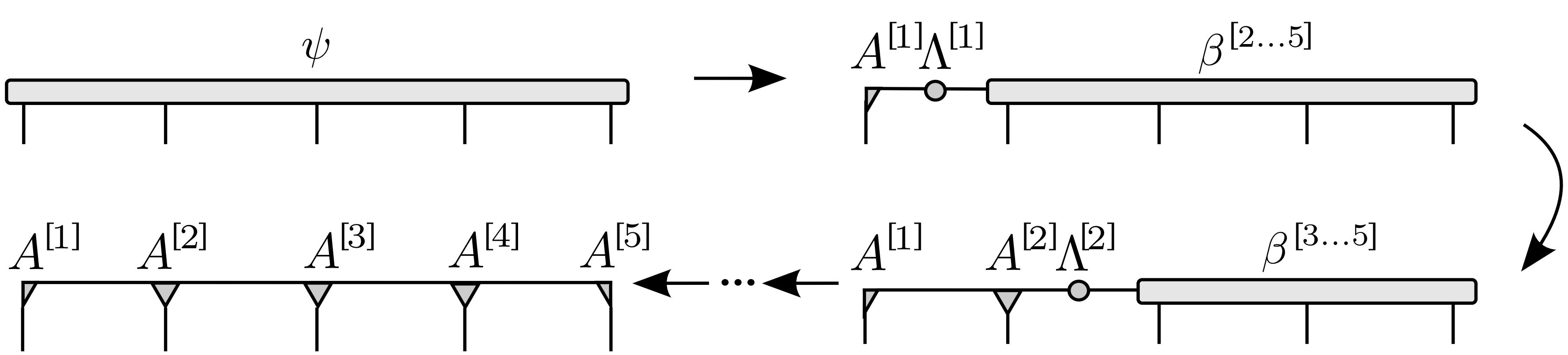
- Coefficients in the many-body wave function:
  Rank-L tensor: diagrammatic representation

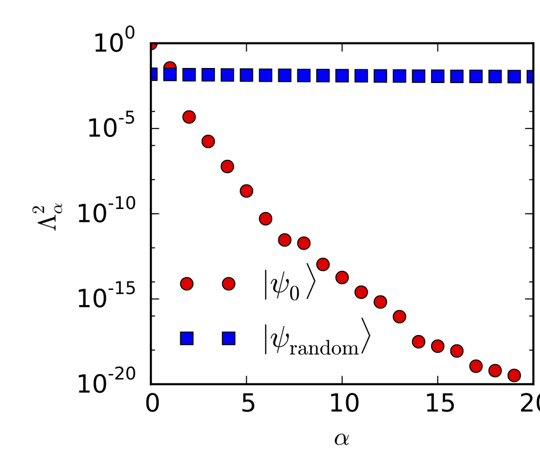
$$\psi_{j_1,j_2,j_3,j_4,j_5} =$$



- Successive Schmidt decompositions: **matrix-product states**

$$|\psi\rangle = \sum_{j_1=1}^{d} \sum_{\beta=1}^{d} A_{\beta}^{[1]j_1} \Lambda_{\beta}^{[1]} |j_1\rangle |\beta\rangle_{[2,\ldots N]}$$

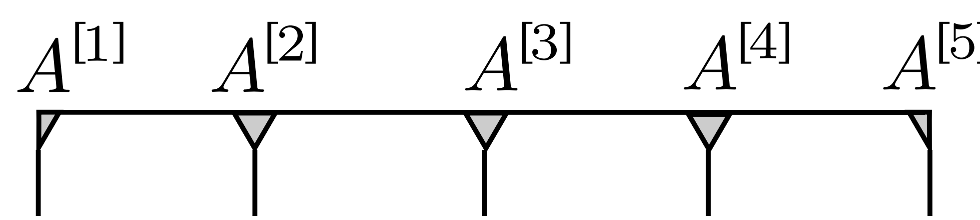




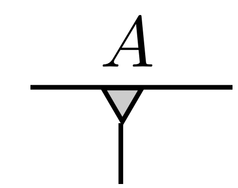
Matrix-Product States

- **Matrix-product states:** Reduction of variables:
  [M. Fannes et al. 92, Schuch et al '08]
  $2^L \to Ld\chi^2$

$$\psi_{j_1,j_2,j_3,j_4,j_5} \approx$$

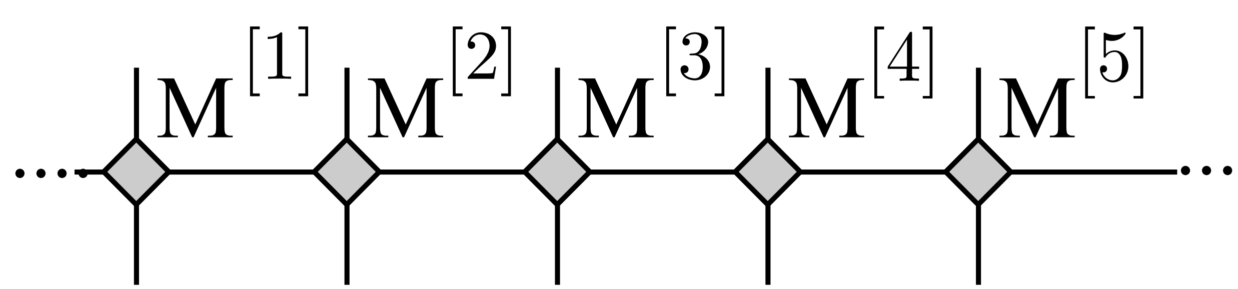


$$A^j_{\alpha\beta} =$$



- **Matrix-product operators** [Verstraete et al '04]

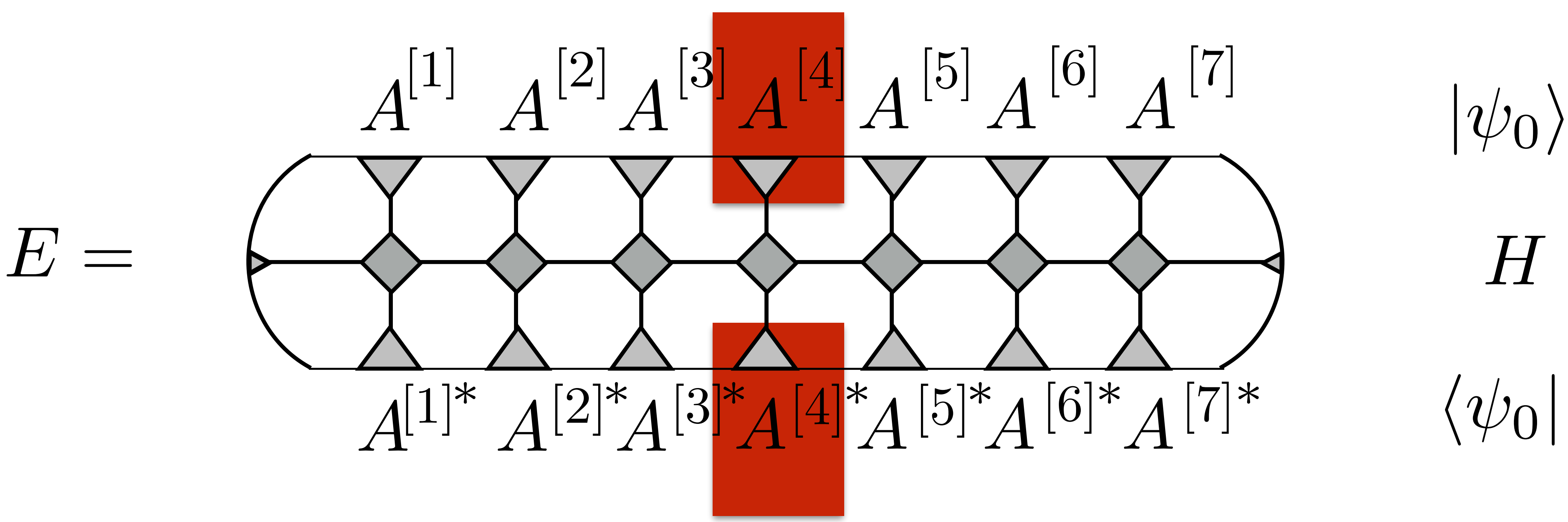
$$O^{j_1',j_2',j_3',j_4',j_5'}_{j_1,j_2,j_3,j_4,j_5} =$$



Matrix-Product States

- Efficient variational optimization of $\{A^{j}_{\alpha\beta}\}$:
  Density matrix renormalization group (DMRG)
  [White '92]

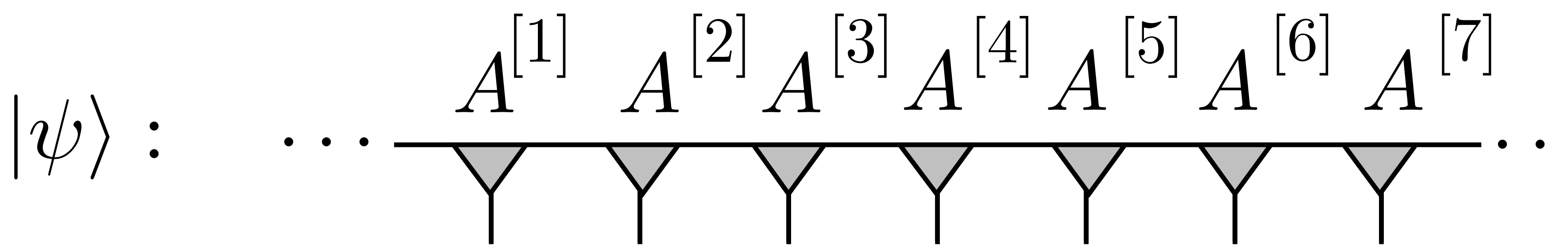
- Find the ground state iteratively



Infinite MPS and the canonical form

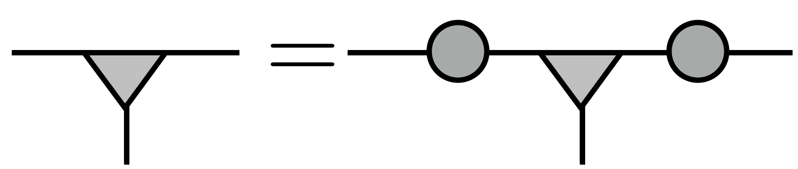
Infinite MPS and the canonical form

- Infinite and translationally invariant systems: $Ld\chi^2 \rightarrow d\chi^2$



- Choice of matrices is not unique

$$\tilde{A}^{i_n} \quad = \quad X A^{i_n} X^{-1}$$



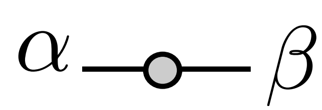
➡ $\tilde{A}^{i_n}$ describes the same state!

Infinite MPS and the canonical form

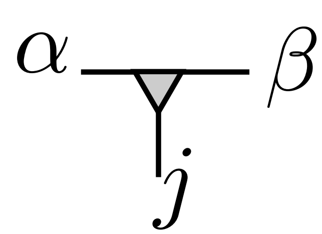
- Choose a convenient representation in **Canonical Form**: Bond index corresponds to Schmidt decomposition! [Vidal '03]

$$|\psi\rangle = \sum_{\alpha=1}^{\chi} \Lambda_\alpha |\alpha\rangle_L \otimes |\alpha\rangle_R \qquad \text{with} \qquad \langle\alpha|\alpha'\rangle = \delta_{\alpha\alpha'}$$

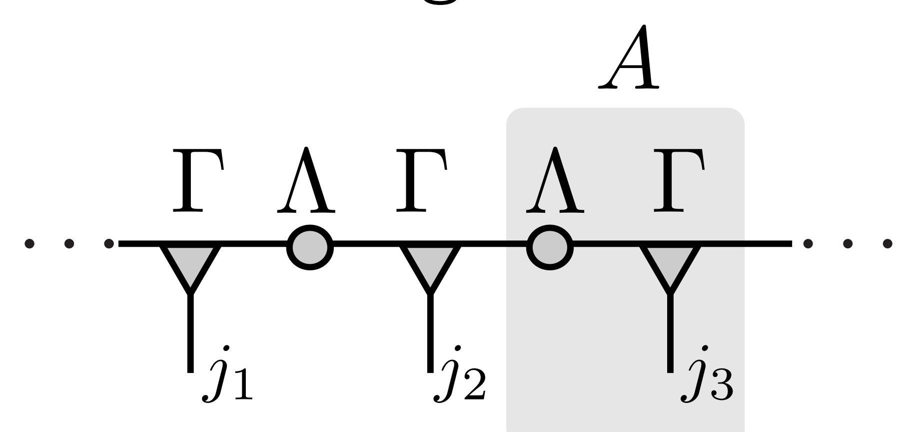
- w.l.o.g.: Write tensor $A^{i_n}_{\alpha\beta}$ as product of

$\Lambda_{\alpha\beta} =$ 

: Diagonal matrix with Schmidt values

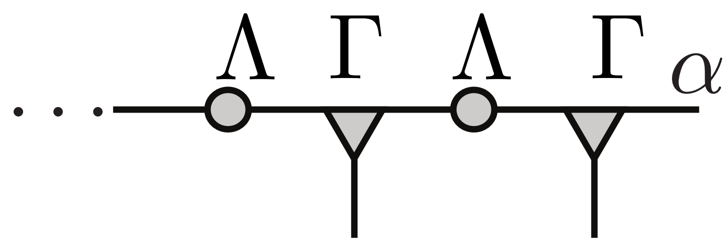
$\Gamma^{j}_{\alpha\beta} =$ 

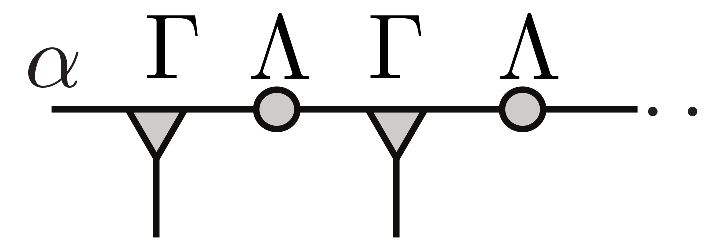
: Tensor relating to Schmidt basis

$\psi_{\ldots,\, j_1, j_2, j_3, \ldots} =$ 

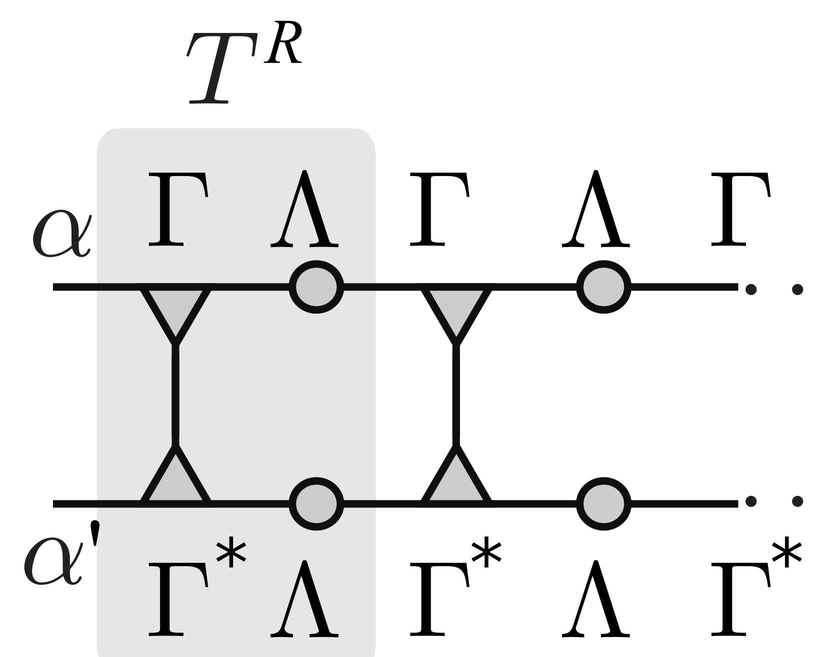
Infinite MPS and the canonical form

- Schmidt states in terms of the MPS:

$|\alpha\rangle_L =$ 

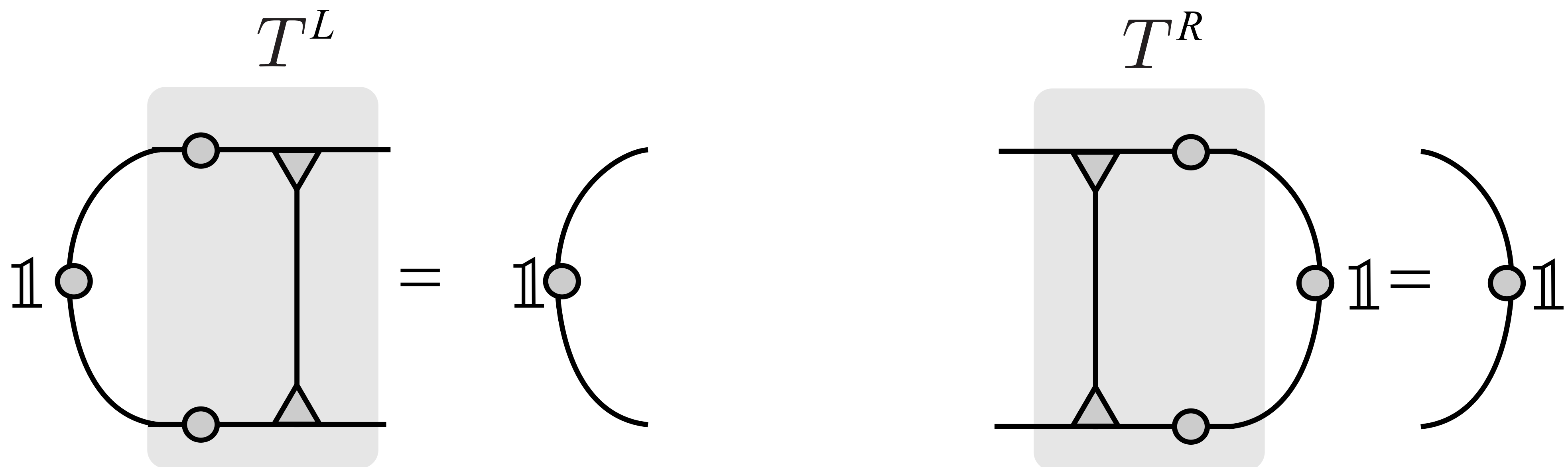
$|\alpha\rangle_R =$ 

- Orthogonality:

$\langle\alpha'|\alpha\rangle_R = \delta_{\alpha'\alpha} \equiv$ 

Infinite MPS and the canonical form

- Conditions for the canonical form:



- Left and right **transfer matrix** have dominant eigenvalue one and the corresponding eigenvector is the identity

$$T^L_{\alpha\alpha';\beta\beta'} = \sum_j \Lambda_\alpha \Lambda_{\alpha'} \, \Gamma^j_{\alpha\beta} \left(\Gamma^j_{\alpha'\beta'}\right)^*$$

Infinite MPS and the canonical form

- Example: **Ising ferromagnet** $|\ldots\uparrow\uparrow\uparrow\uparrow\ldots\rangle$

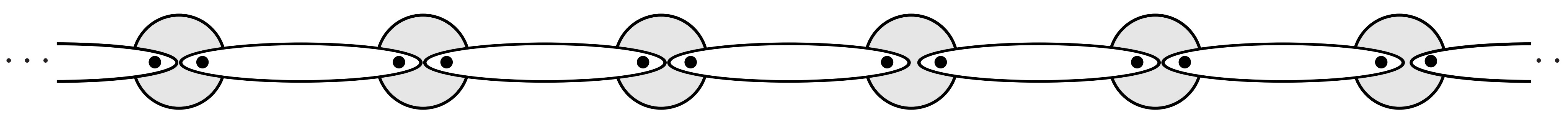
  $d = 2$ and $\chi = 1$ (product state)

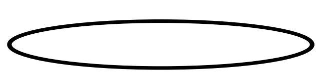
$$\Gamma^{\uparrow} = 1$$
$$\Gamma^{\downarrow} = 0$$
$$\Lambda = 1.$$

Infinite MPS and the canonical form

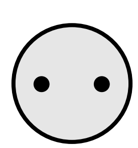
- Example: Affleck-Kennedy-Lieb-Tasaki (AKLT)
- Ground state the spin-1 Hamiltonian

$$H = \sum_j \vec{S}_j \vec{S}_{j+1} + \frac{1}{3}(\vec{S}_j \vec{S}_{j+1})^2,$$





$$= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$$



$$= |+1\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-1\rangle\langle\downarrow\downarrow|$$

Infinite MPS and the canonical form

- Example: Affleck-Kennedy-Lieb-Tasaki (AKLT)

$d = 3$ and $\chi = 2$

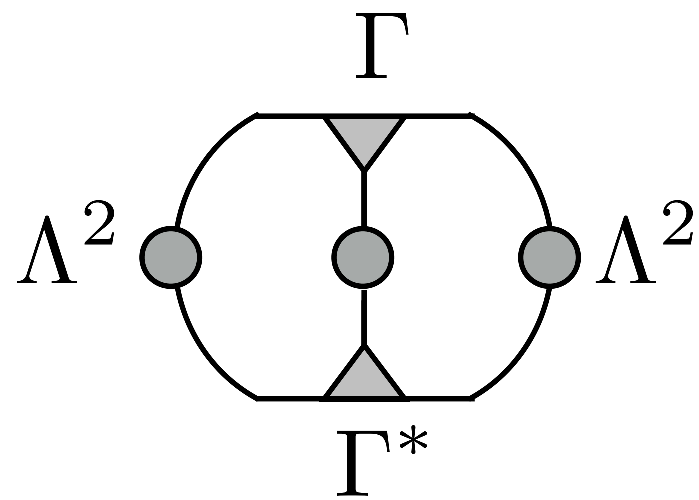
$$\begin{aligned} \Gamma^{-1} &= \sqrt{\frac{4}{3}}\sigma^{+},\ \Gamma^{0} = -\sqrt{\frac{2}{3}}\sigma^{z},\ \Gamma^{1} = -\sqrt{\frac{4}{3}}\sigma^{-} \\ \Lambda &= \sqrt{\frac{1}{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{aligned}$$

Show that the state is actually in canonical form!

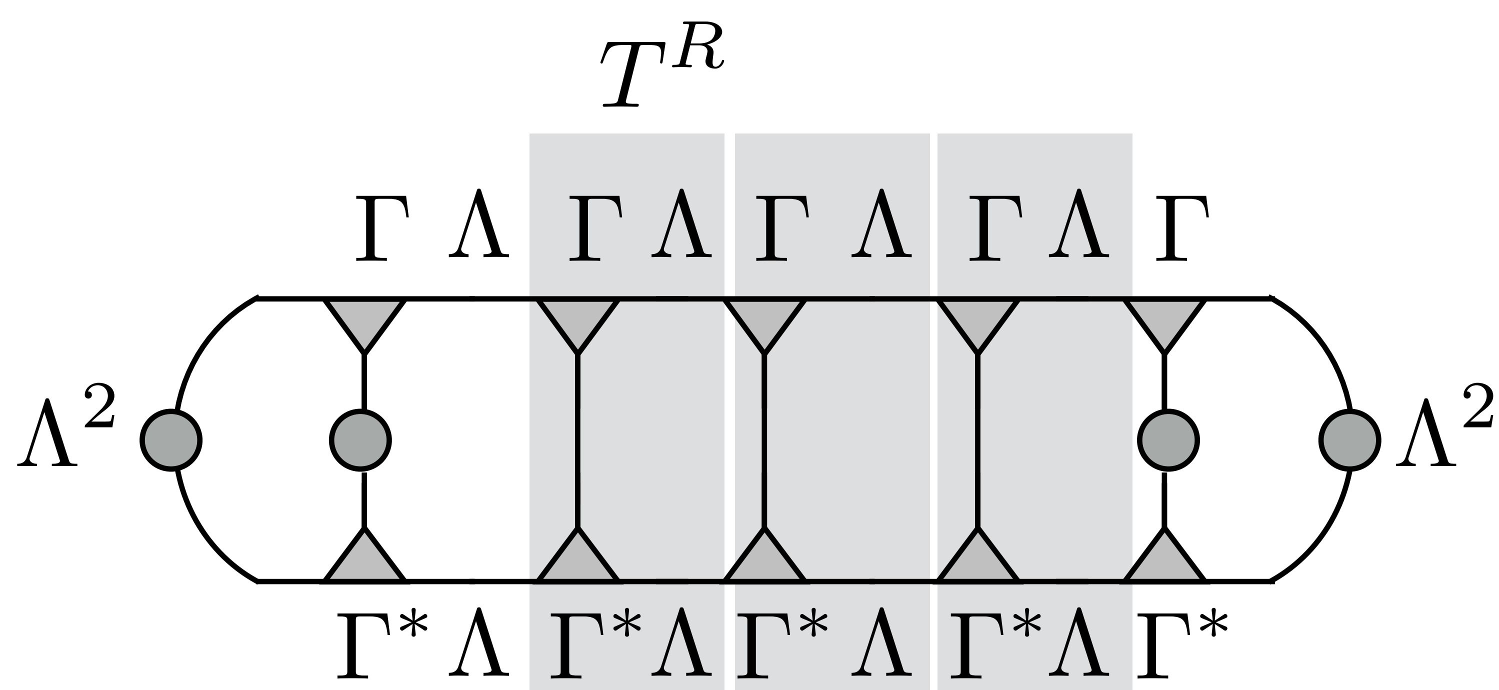
Infinite MPS and the canonical form

- Efficient evaluation of **expectation values**:

$$\langle \psi | O_n | \psi \rangle =$$



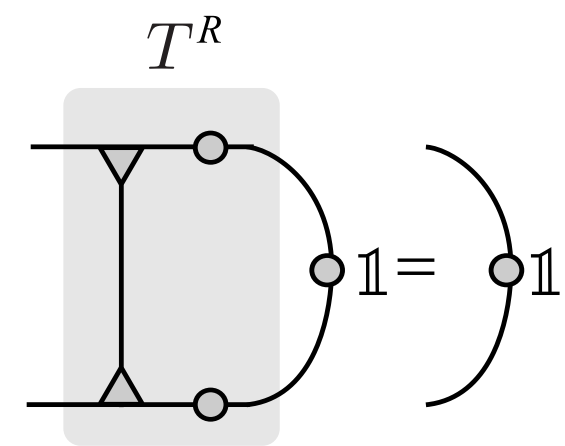
$$\langle \psi | O_m O_n | \psi \rangle =$$



Infinite MPS and the canonical form

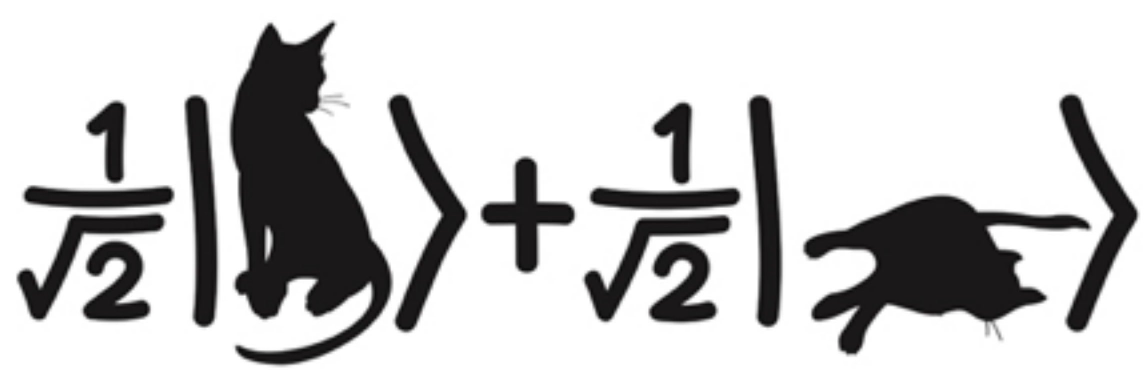
- **Correlation length** of an MPS:

$$\xi = -\frac{1}{\log|\epsilon_2|},$$

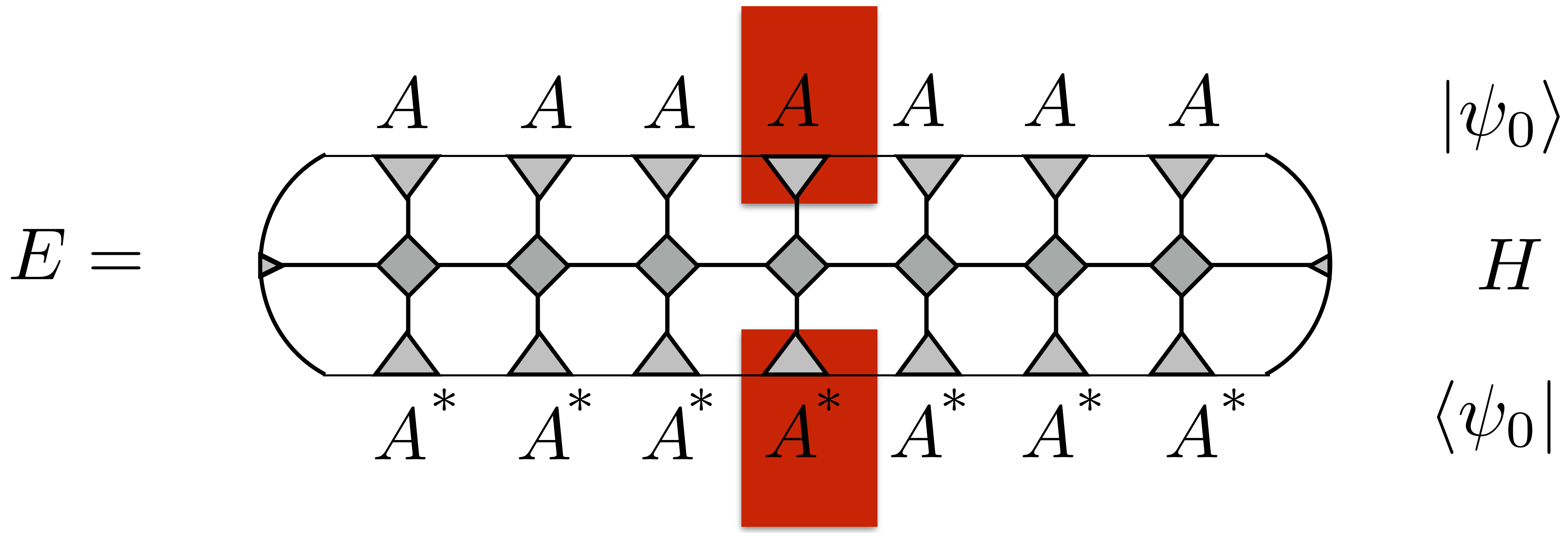


ϵ_2 is the second largest eigenvalue of the transfer matrix

- Degeneracy of largest eigenvalue (unity) shows that the MPS is a cat-state



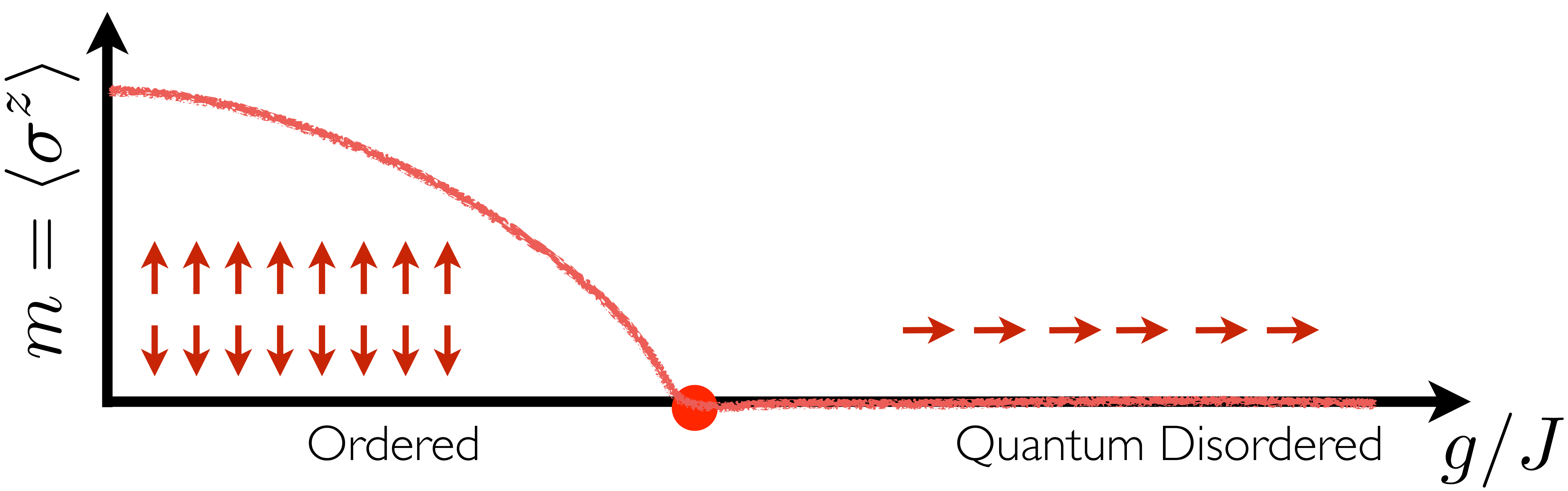
Simulations with infinite MPS



Infinite MPS and the canonical form

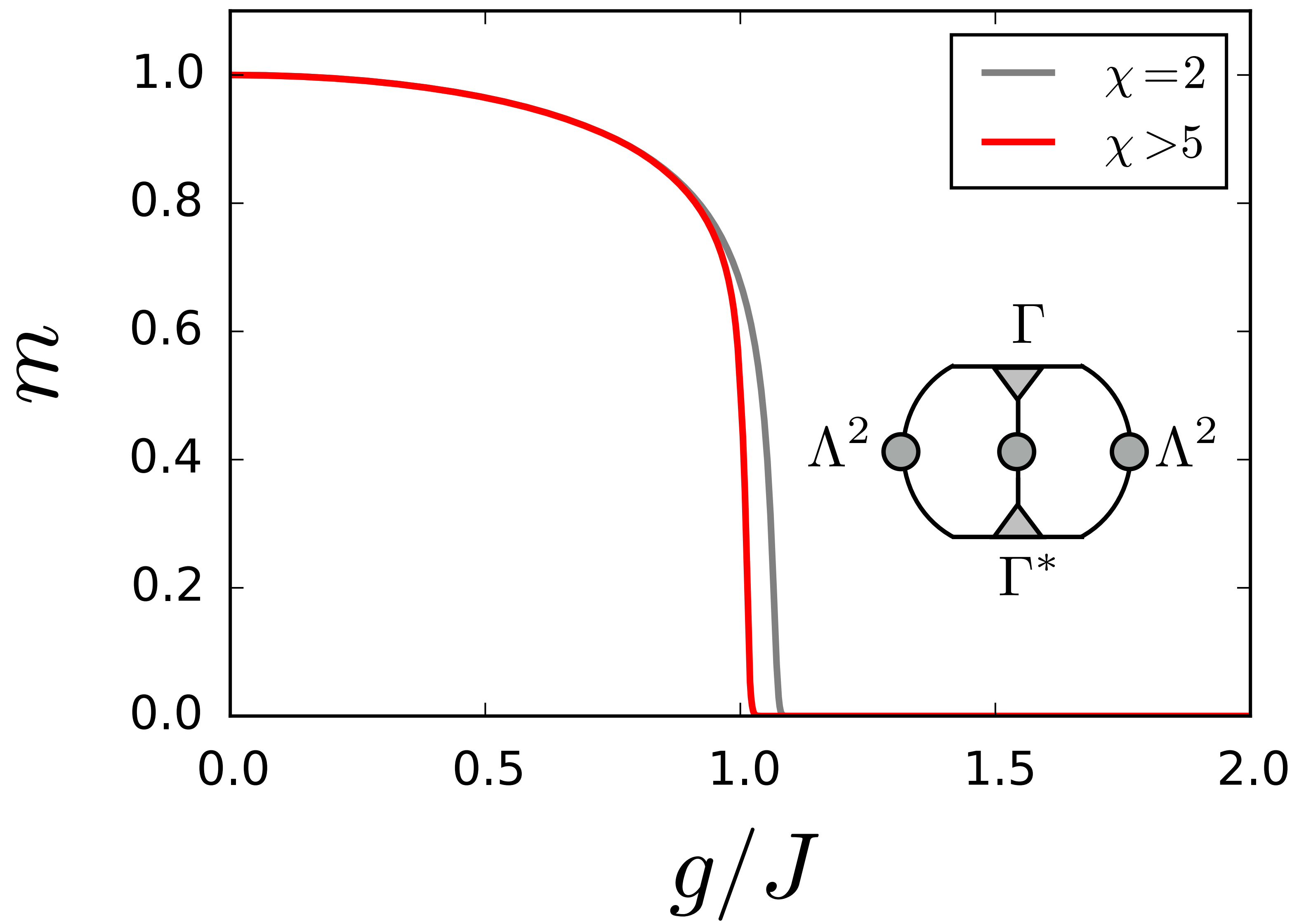
- Transverse field Ising model
  with $\mathbb{Z}_2$ symmetry [Elliott et al.'70]

$$H = -\sum_j (J\sigma_j^z \sigma_{j+1}^z + g\sigma_j^x)$$



Infinite MPS and the canonical form

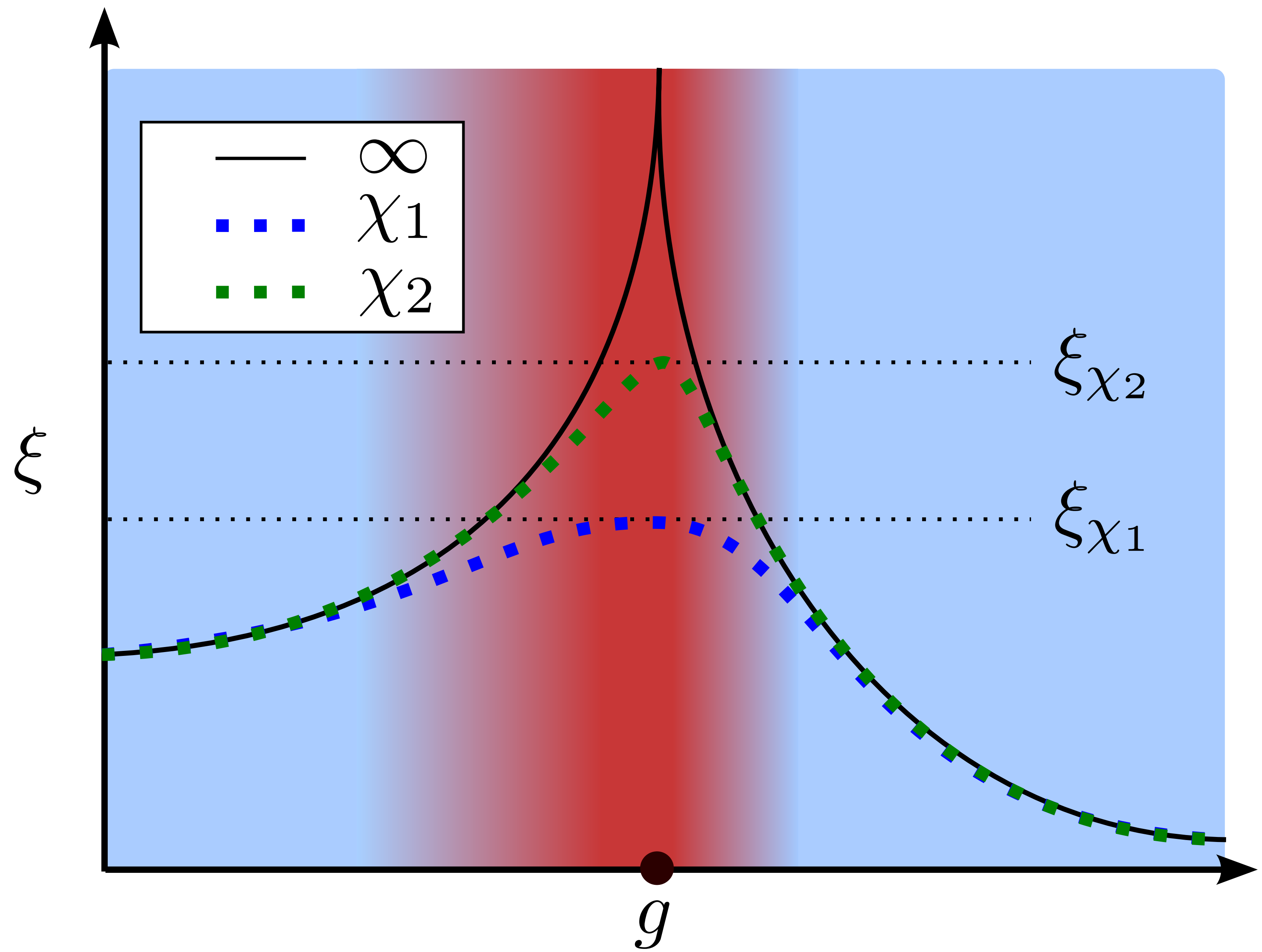
- Use DMRG to optimize an infinite MPS



Hands on session tomorrow!

Infinite MPS and the canonical form

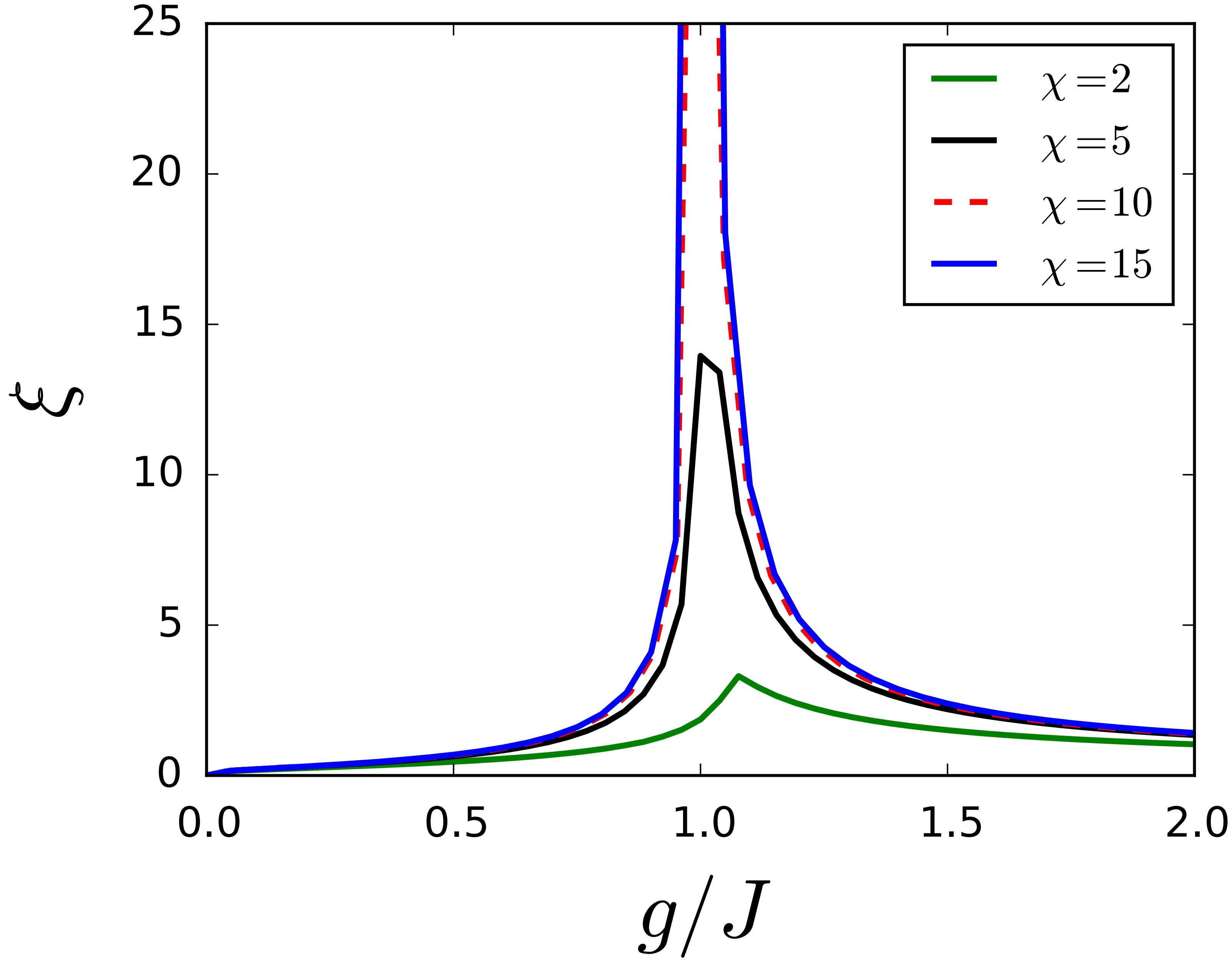
- **Finite entanglement scaling:** Entanglement and correlation length are always finite in an MPS



FP, S. Mukerjee, A.M. Turner, J. Moore Phys. Rev. Lett. **102**, 255701 (2009).

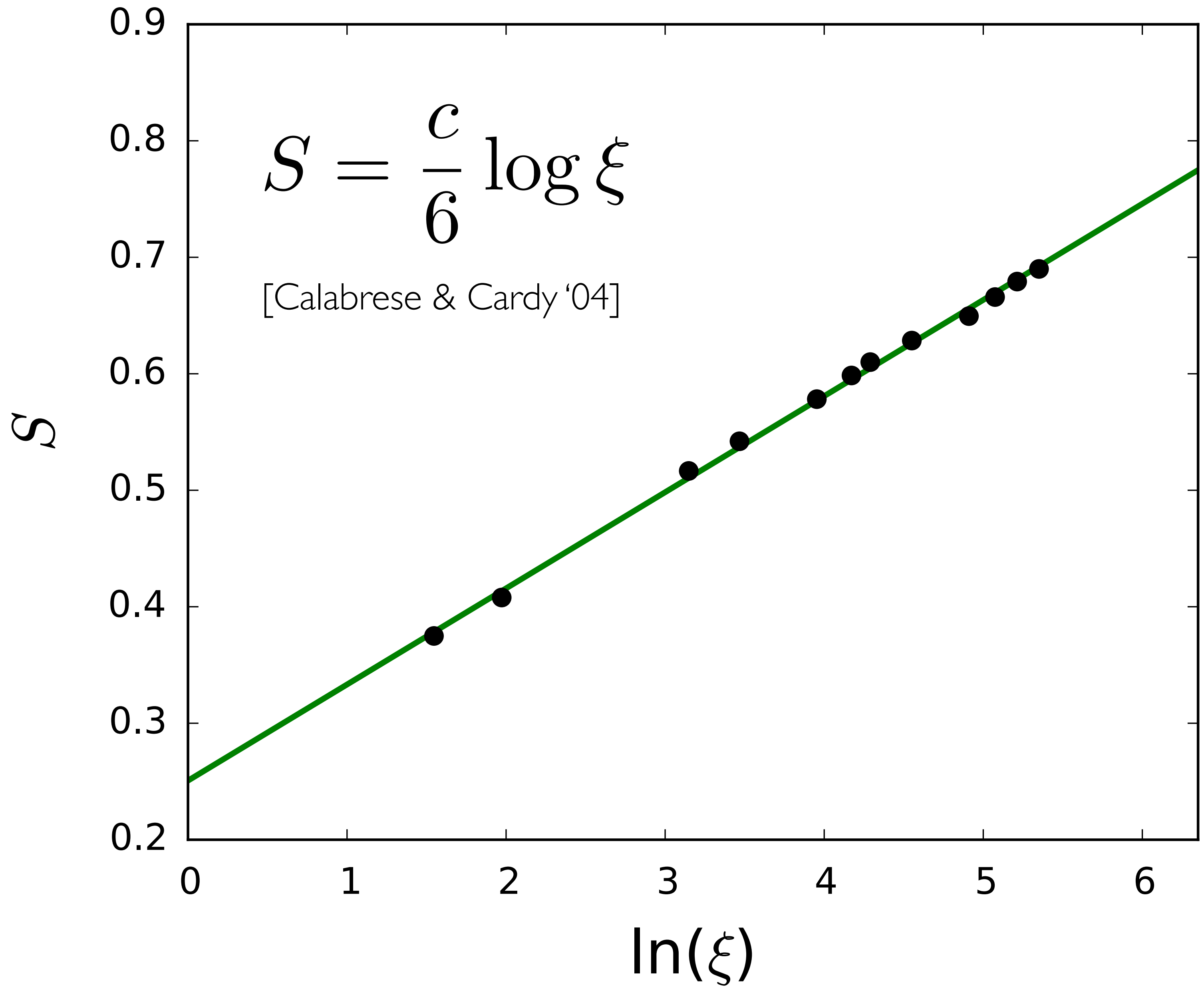
Infinite MPS and the canonical form

- **Finite entanglement scaling:** Entanglement and correlation length are always finite in an MPS



Infinite MPS and the canonical form

- **Finite entanglement scaling:** Extract central charge c

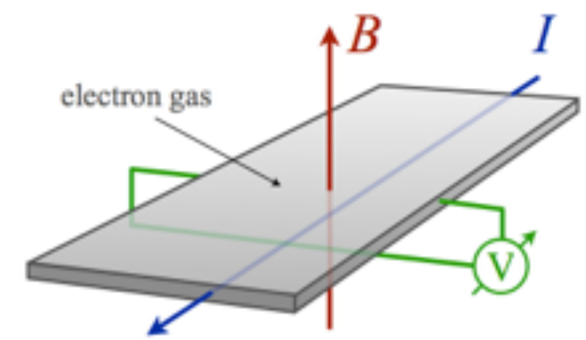


➡ Ising critical point: $c = 1/2$

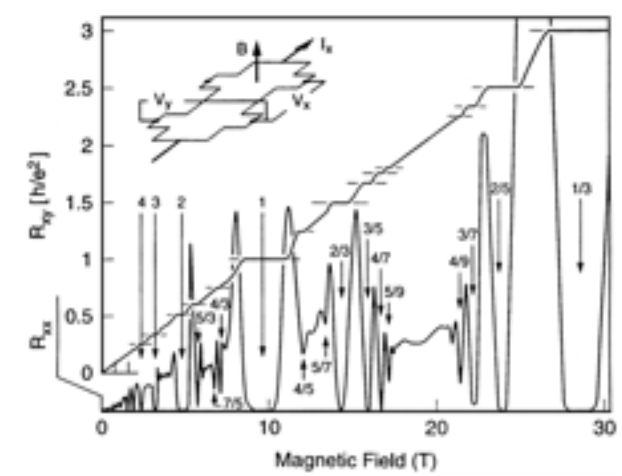
Extracting fingerprints of topological order

Topological phases of matter

- Topological phases cannot be described by symmetry breaking



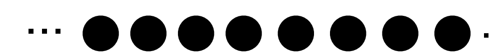
  - Quantum Hall effects [Klitzing '80, Tsui '82, Laughlin '83]
  - (gapped) spin-liquids [Anderson '73]

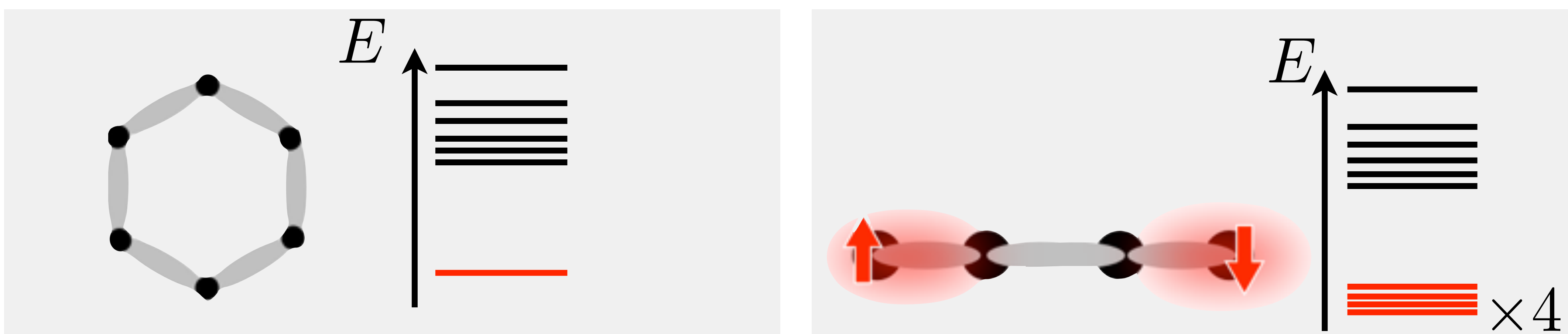


  - Topological insulators [Kane & Mele '05]
  - **Haldane spin chain** [Haldane '83]

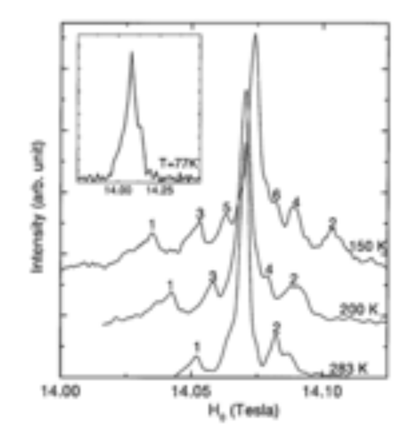
- Fascinating features: quantized conductance, fractionalization, protected edge states, …

Symmetry protected topological phases

- Spin-1 Heisenberg chain $H = \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$ 
  - Haldane phase: Gapped + no symmetry breaking
    [Haldane '83]
  - Spin-1/2 excitations at the edges: Protected by symmetry
    [Affleck et al '87]



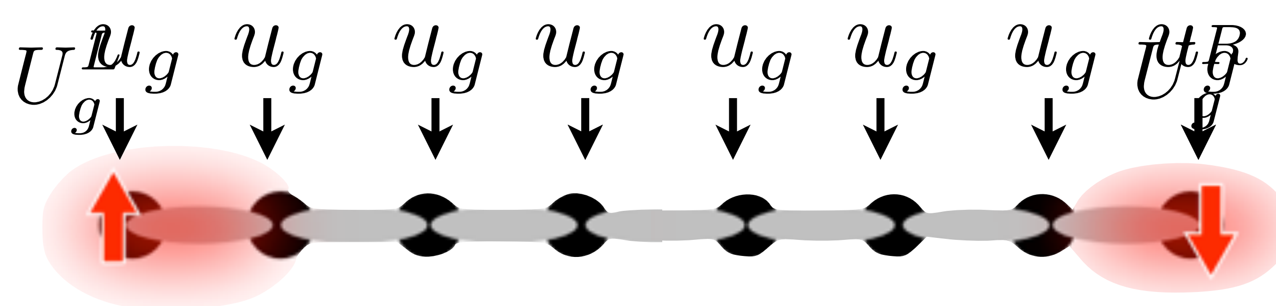
- Edge spins have been observed in the NMR profile close to the chain ends of Mg-doped Y_2BaNiO_5 [S.H. Glarum, et al., Tedoldi et al. '99]



Symmetry protected topological phases

- Hamiltonian and ground state $|\psi_0\rangle$ **symmetric under** $g, h \in G$

$|\psi_0\rangle$:



➡ **Bulk:** Linear on-site representation $u_g u_h = u_{gh}$
(e.g., spin-1)

➡ **Boundary: Projective representations** $U_g U_h = e^{i\phi(g,h)} U_{gh}$
(e.g., spin-1/2)

- Classified by the **second cohomology** group $H^2[G, U(1)]$
[Schur 1911]

➡ **Classification of Symmetry protected topological phases**
(…is complete [Chen et al. '11; Schuch et al '11])

FP, A.M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B **81**, 064439 (2010).

Symmetry protected topological phases

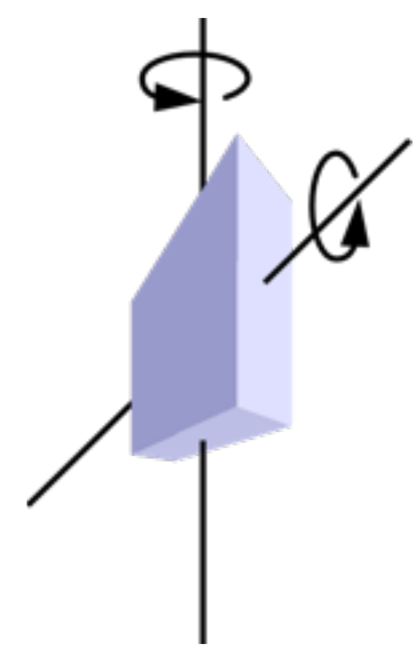
Which symmetries can stabilize topological phases?

- Example $\mathbb{Z}_n$: Rotation about single axis

$$R^n = \mathbb{1} \Rightarrow U_R^n = e^{i\phi}\mathbb{1}$$

  - Redefining $\tilde{U}_R = e^{-i\phi/n} U_R$ removes any phase

- Example $\mathbb{Z}_2 \times \mathbb{Z}_2$: Phase for pairs



$$R_x R_z = R_z R_x \Rightarrow U_x U_z = e^{i\phi_{xz}} U_z U_x$$

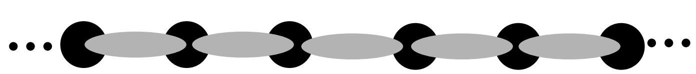
  - Phases $\phi_{xz} = 0, \pi$ cannot be gauged away: **Distinct topological phases**

FP, A.M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B 81, 064439 (2010).

1D symmetry protected topological phases

- Characteristic fingerprints of SPT's from DMRG

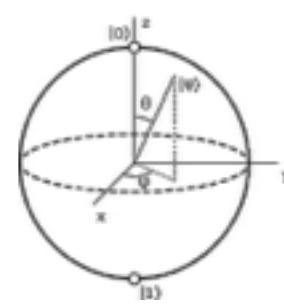
$|\psi\rangle \approx \sum_\alpha \lambda_\alpha |\phi^L_\alpha\rangle|\phi^R_\alpha\rangle$



$$[U_g]_{\alpha\alpha'} = \langle\phi^R_\alpha| \bigotimes_{j\in L} g_j |\phi^R_{\alpha'}\rangle$$

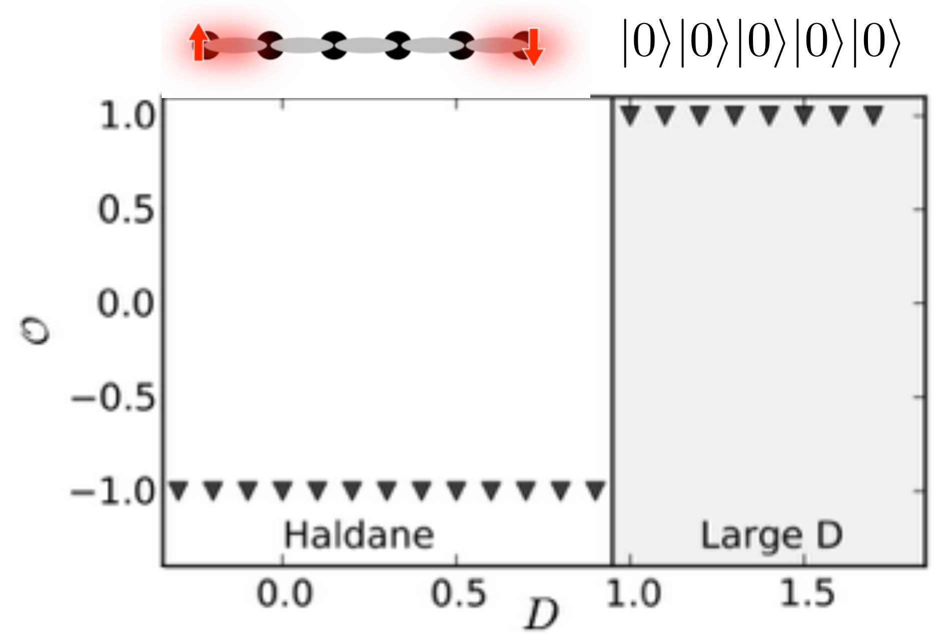
➡ Projective representations U_g can directly be extracted

- $\mathbb{Z}_2 \times \mathbb{Z}_2$ stabilizes the $S=1$ Haldane phase



$$\mathcal{O} \propto \mathrm{tr}(U_x U_z U_x^\dagger U_z^\dagger)$$

$$H = \sum_j \vec{S}_j \cdot \vec{S}_{j+1} + D \sum_j (S^z_j)^2$$



FP and A.M. Turner, Phys. Rev. B 86, 125441 (2012).

1D symmetry protected topological phases

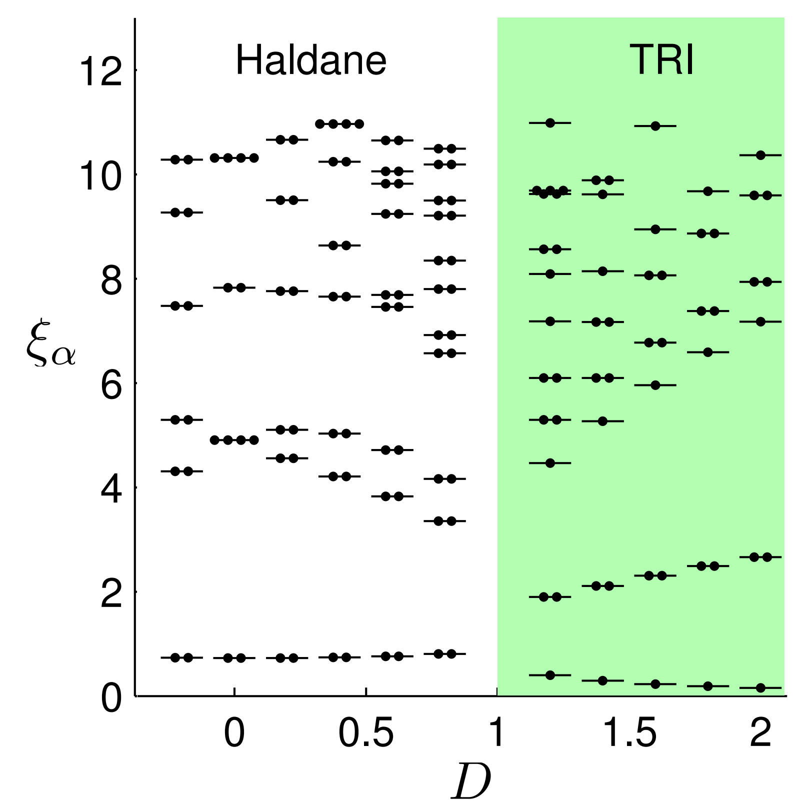
- Characteristic fingerprints of SPT's from DMRG

$|\psi\rangle \approx \sum_\alpha \lambda_\alpha |\phi_\alpha^L\rangle |\phi_\alpha^R\rangle$

➡ Entanglement spectrum:

[Li and Haldane '08]

$$\xi_\alpha = -\ln \lambda_\alpha^2$$



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