Entanglement In Many-Body Systems

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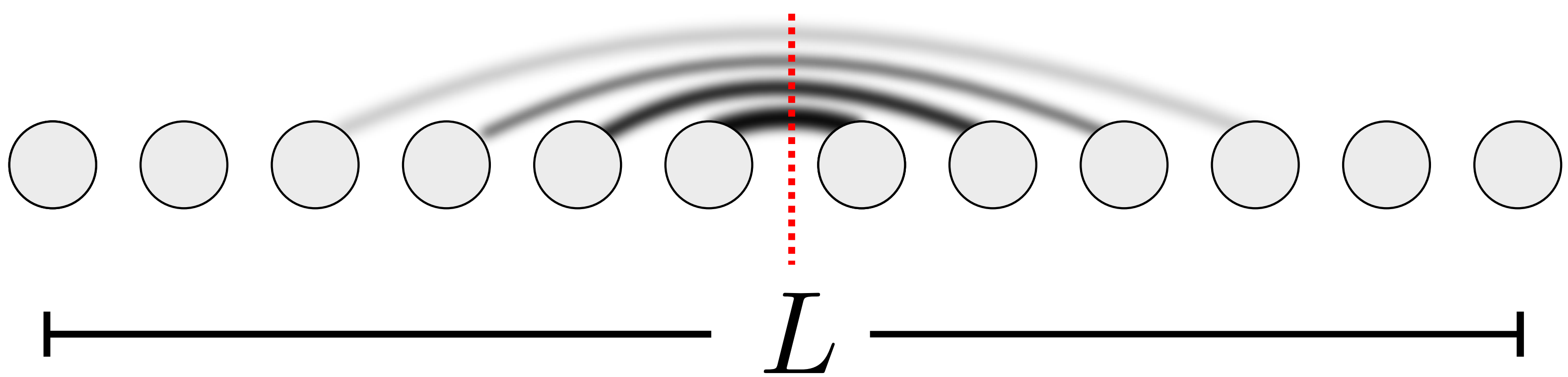


Autumn School on Correlated Electrons:
Topology, Entanglement, and Strong Correlations
21-25 September 2020, Forschungszentrum Jülich

Entanglement In Many-Body Systems

Why study quantum entanglement in many-body systems ?

- A **powerful theoretical probe** for quantum many-body systems: Characterization of universal properties (topological phases, critical points, many-body localization,…)

- Useful to construct **new algorithms** to efficiently simulate quantum many-body states in a computer (TEBD, DMRG, TNS, MERA,…)

- Core of **quantum information** processing

Efficient simulation of interacting topological matter

I) Introduction to many-body entanglement

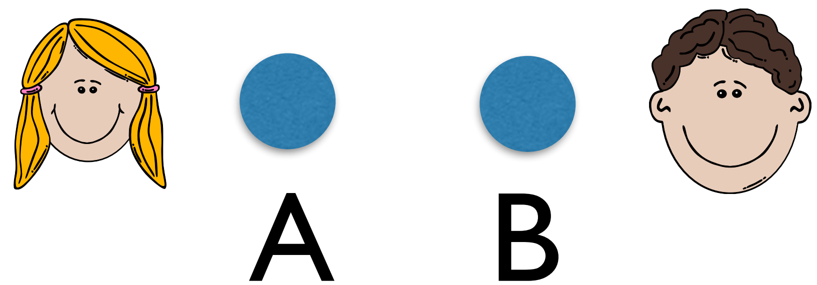
II) Matrix-Product States

III) Symmetry-protected topological (SPT) phases

IV) Universal entanglement scaling at critical points

V) Case study: Phase diagram of a spin-1 chain

Bipartite entanglement



Product state (=non-entangled):

$$|\psi\rangle = \frac{1}{2}\Big(|\uparrow\rangle_A + |\downarrow\rangle_A\Big)\Big(|\uparrow\rangle_B + |\downarrow\rangle_B\Big) \qquad \rightarrow S = 0$$

Entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\Big(|\uparrow\rangle_A|\downarrow\rangle_B + |\downarrow\rangle_A|\uparrow\rangle_B\Big) \qquad \rightarrow S = \log 2$$

Entanglement entropy as a measure for the amount of entanglement:

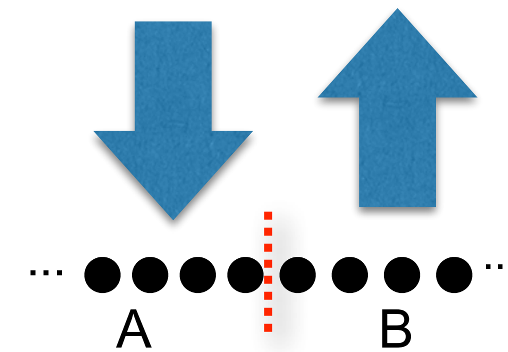
$S = -\mathrm{Tr}\rho_A \log \rho_A$ with $\rho_A = \mathrm{Tr}_B|\psi\rangle\langle\psi|$

Bipartite 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**)



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

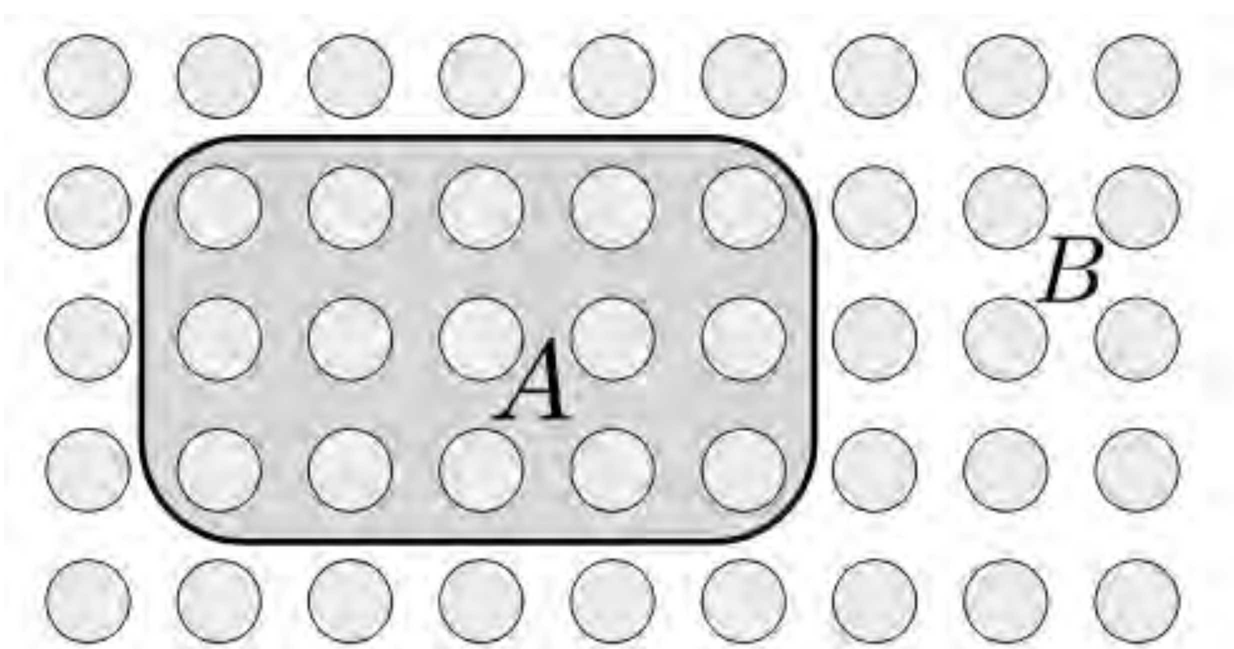
Entanglement entropy as a measure for the amount of entanglement $S = -\sum_\alpha \Lambda_\alpha^2 \log \Lambda_\alpha^2$

Bipartite entanglement

Area law for ground states of local (gapped) Hamiltonians

[Srednicki '93]

$$H|\psi_0\rangle = E_0|\psi_0\rangle$$

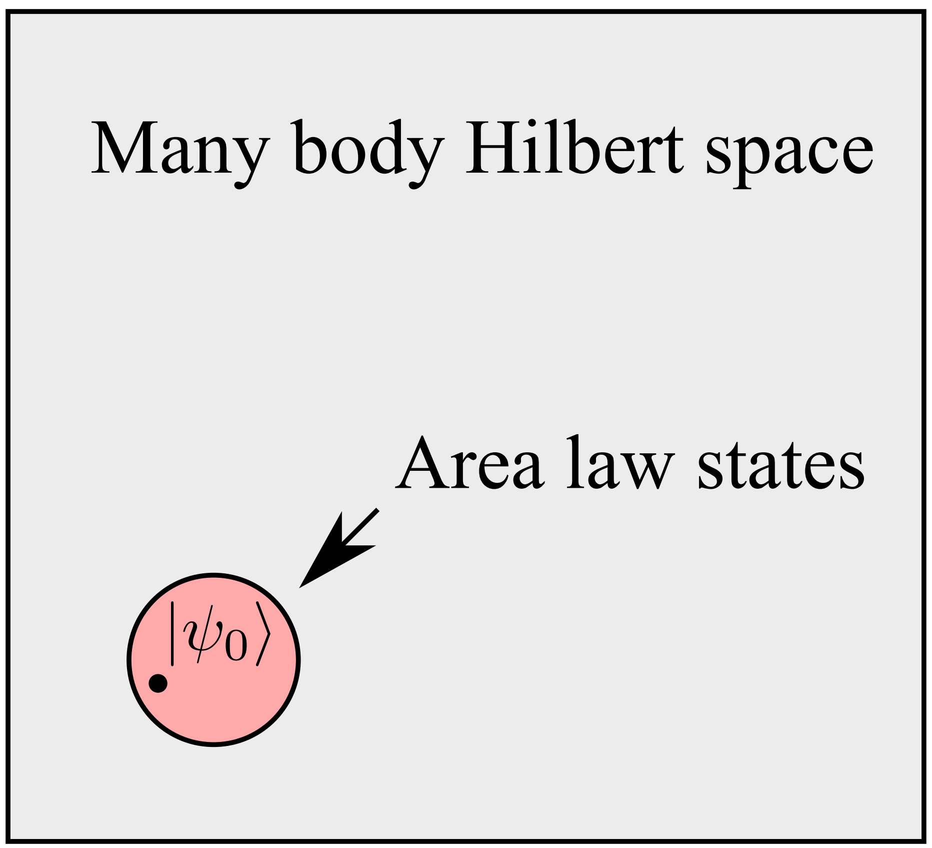


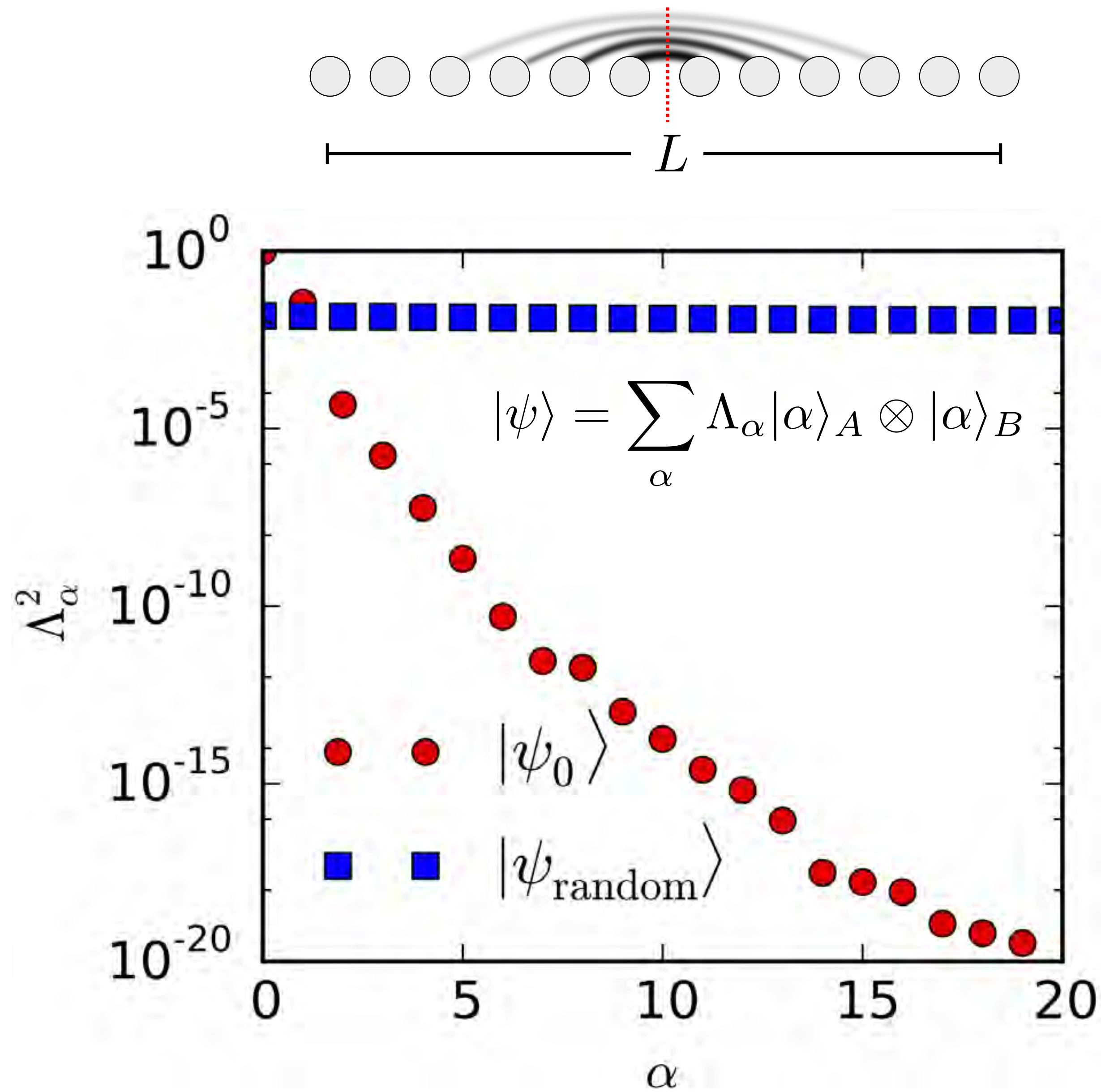
$$\rightarrow \quad S = \alpha|\partial A| + \ldots$$

Entanglement

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

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





- All ground states live in a tiny corner of the Hilbert space!
- Efficient compression by discarding small Schmidt values

Efficient simulation of interacting topological matter

I) Introduction to many-body entanglement ✓

II) Matrix-Product States

III) Symmetry-protected topological (SPT) phases

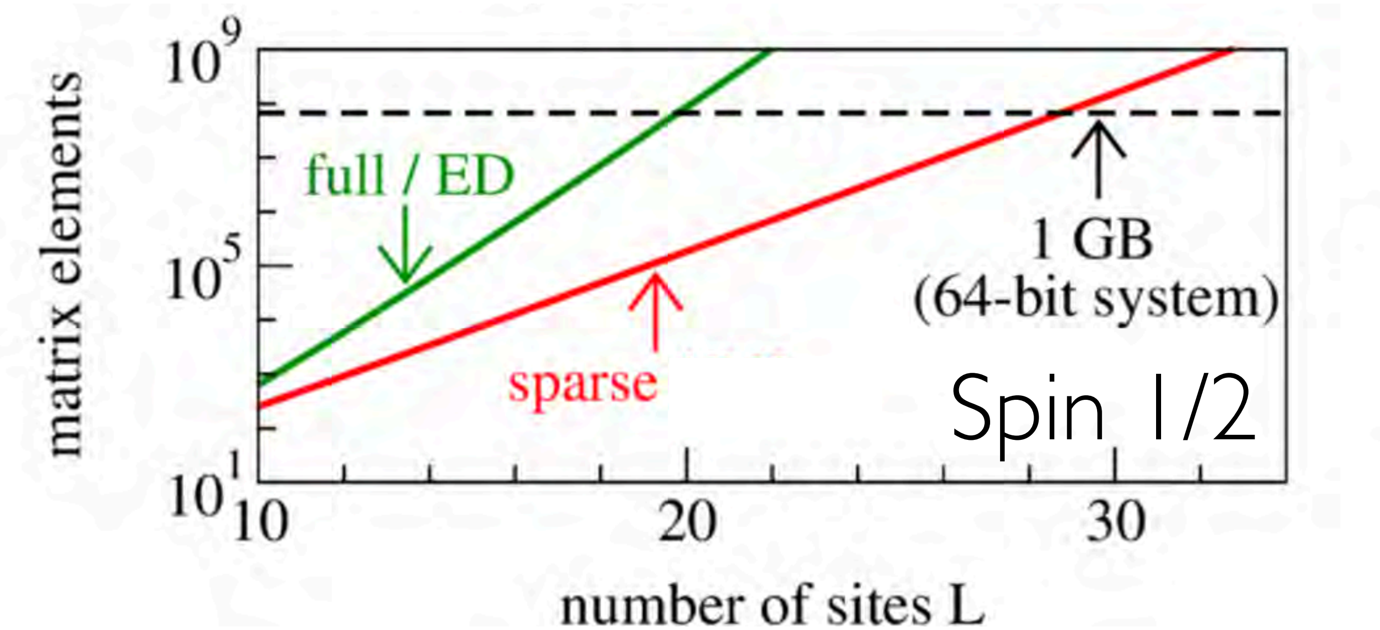
IV) Universal entanglement scaling at critical points

V) Case study: Phase diagram of a spin-1 chain

Complexity of a quantum many-body problem

Many-body Hilbert space

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



- Full diagonalization up to ~20 sites
- Sparse methods up to ~30 sites

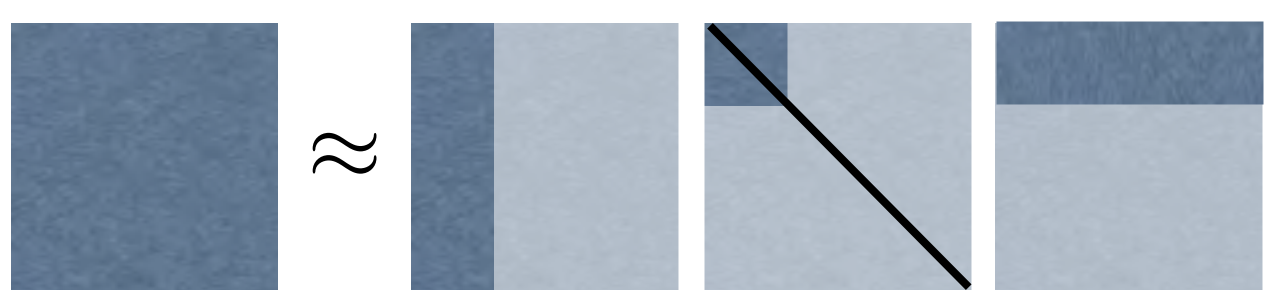
Compression of quantum states

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)

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

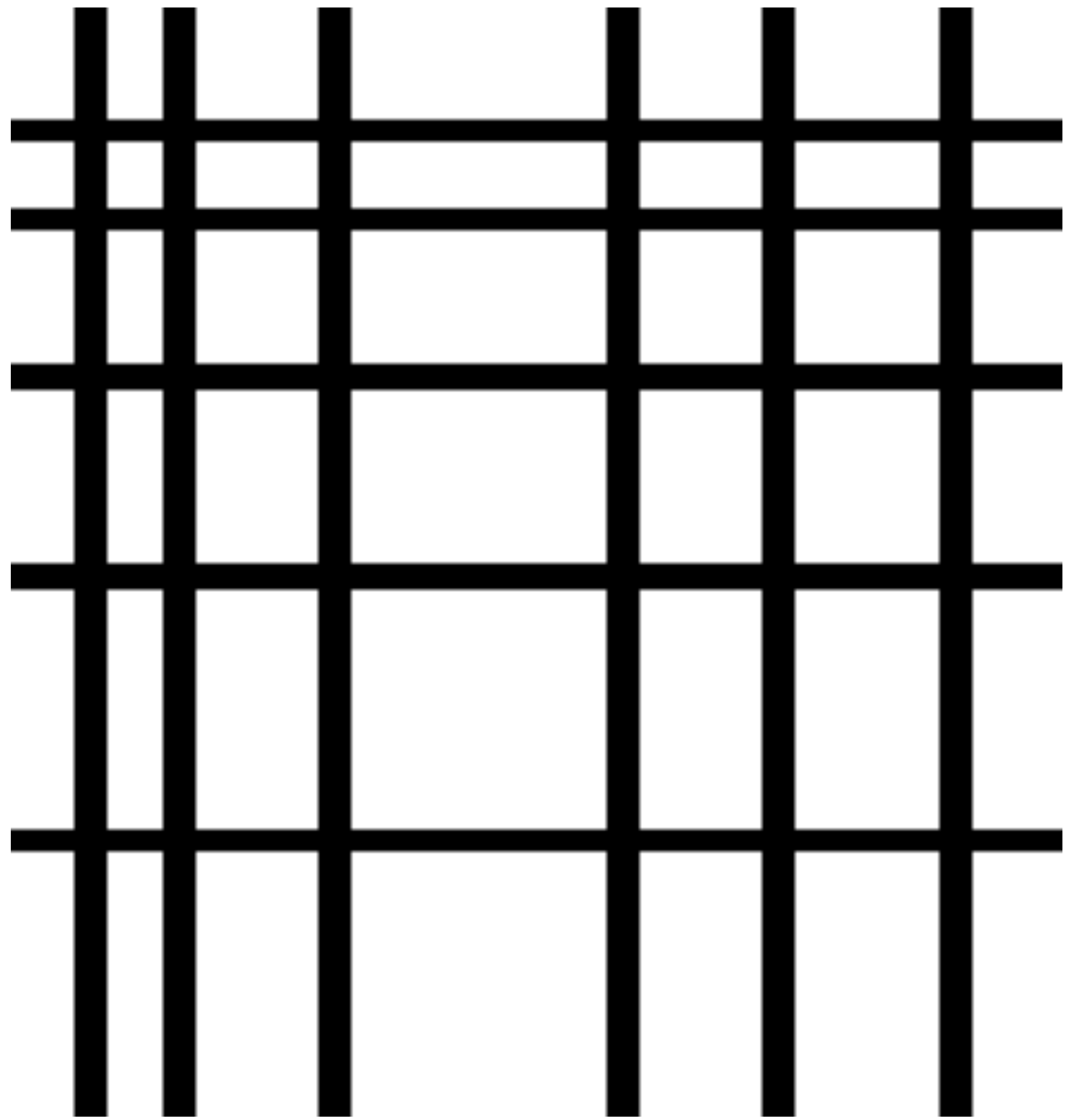
Reconstruction of the matrix (image) from a small number of Schmidt states (SVD):



Compression of quantum states

Important features visible already for < 16 states!

Compression of quantum states



[Mondrian]

Exact for $\chi = 1$ state!

https://colab.research.google.com/drive/1_4V66KqRXHMR-CQl18eqkQBu9EZqw2KM#scrollTo=hKqe82w-U-NM

Matrix-Product States

Many-body Hilbert space

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

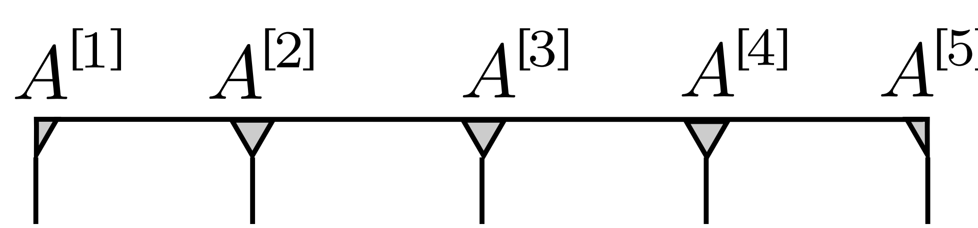
Matrix-Product States: Reduction of #variables $d^L \to L d \chi^2$

(subsequent SVDs on each bond)

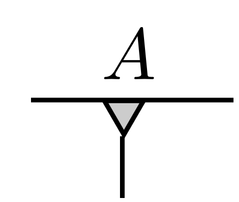
$$\psi_{j_1,j_2,\ldots,j_L} \approx \sum_{\alpha_1,\alpha_2,\ldots,\alpha_{L-1}} A^{j_1}_{\alpha_1} A^{j_2}_{\alpha_1,\alpha_2} \ldots A^{j_L}_{\alpha_{L-1}} \qquad \alpha_j = 1 \ldots \chi$$

Diagrammatic representation

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



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



Matrix-Product States

Simple examples of MPS…

Neel state $|\uparrow\downarrow\uparrow\downarrow\ldots\rangle$

$$M^{[2n-1]\uparrow} = M^{[2n]\downarrow} = \begin{pmatrix}1\end{pmatrix} \qquad M^{[2n-1]\downarrow} = M^{[2n]\uparrow} = \begin{pmatrix}0\end{pmatrix}$$

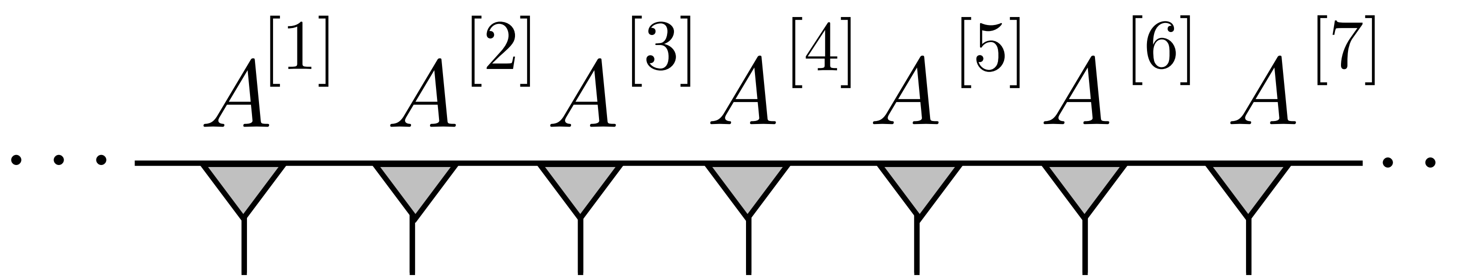
Dimerized state $\left(\frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle\right) \otimes \cdots \otimes \left(\frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle\right)$

$$M^{[2n-1]\uparrow} = \begin{pmatrix}\frac{1}{\sqrt{2}} & 0\end{pmatrix}, \quad M^{[2n-1]\downarrow} = \begin{pmatrix}0 & \frac{-1}{\sqrt{2}}\end{pmatrix}, \quad M^{[2n]\uparrow} = \begin{pmatrix}0\\1\end{pmatrix}, \quad M^{[2n]\downarrow} = \begin{pmatrix}1\\0\end{pmatrix}$$

MPS and the canonical form

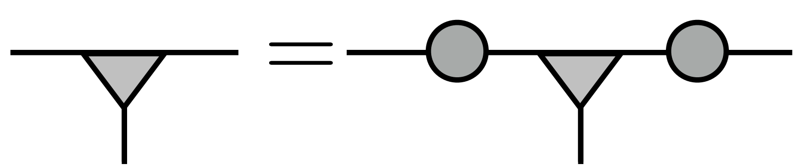
From now on: Leave out site indices!

$|\psi\rangle$:



MPS is not unique

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



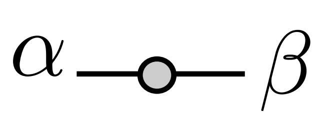
➡ $\tilde{A}^{i_n}$ describes the same state!

MPS and the canonical form

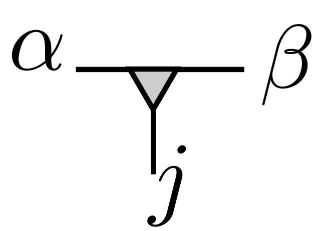
Choose a convenient representation in **Canonical Form**:
Bond index corresponds to Schmidt decomposition! [Vidal '03]

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

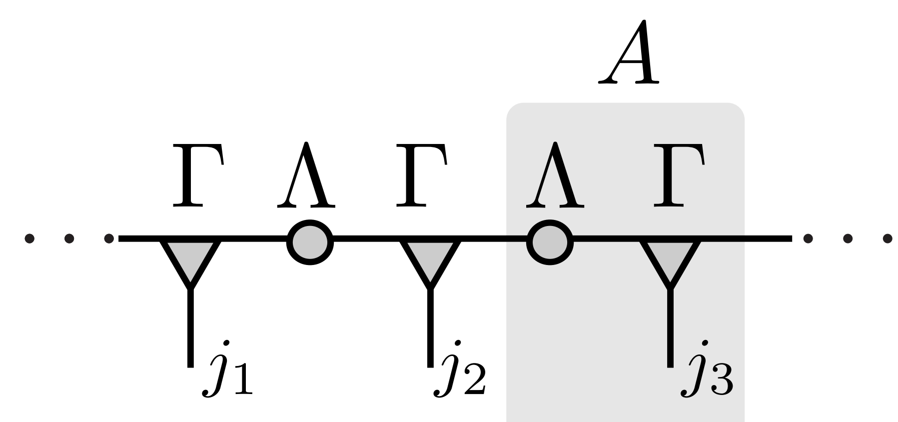
Write tensor $A^{i_n}_{\alpha\beta}$ as product of

$\Lambda_{\alpha\beta} =$ 

: Diagonal matrix with Schmidt values

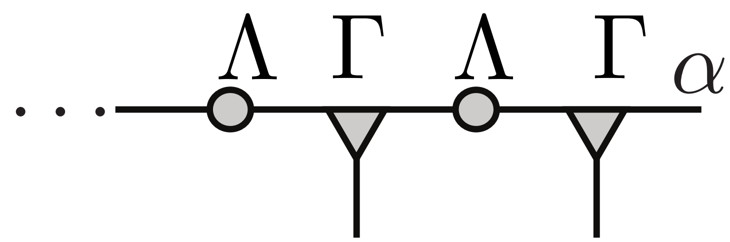
$\Gamma^{j}_{\alpha\beta} =$ 

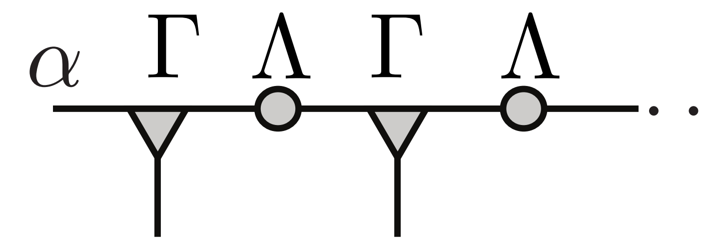
: Tensor relating to Schmidt basis

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

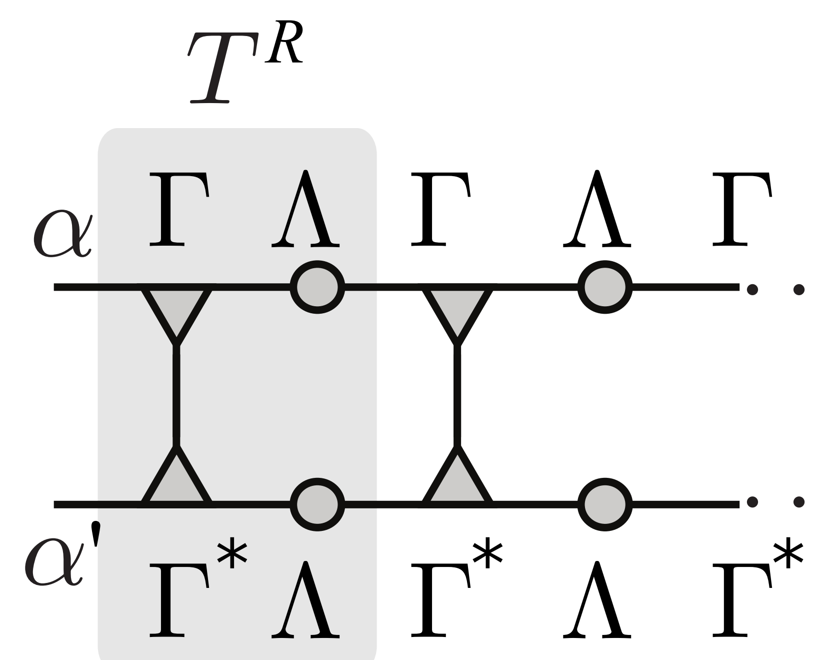
MPS and the canonical form

Schmidt states in terms of the MPS:

$|\alpha\rangle_L =$ 

$|\alpha\rangle_R =$ 

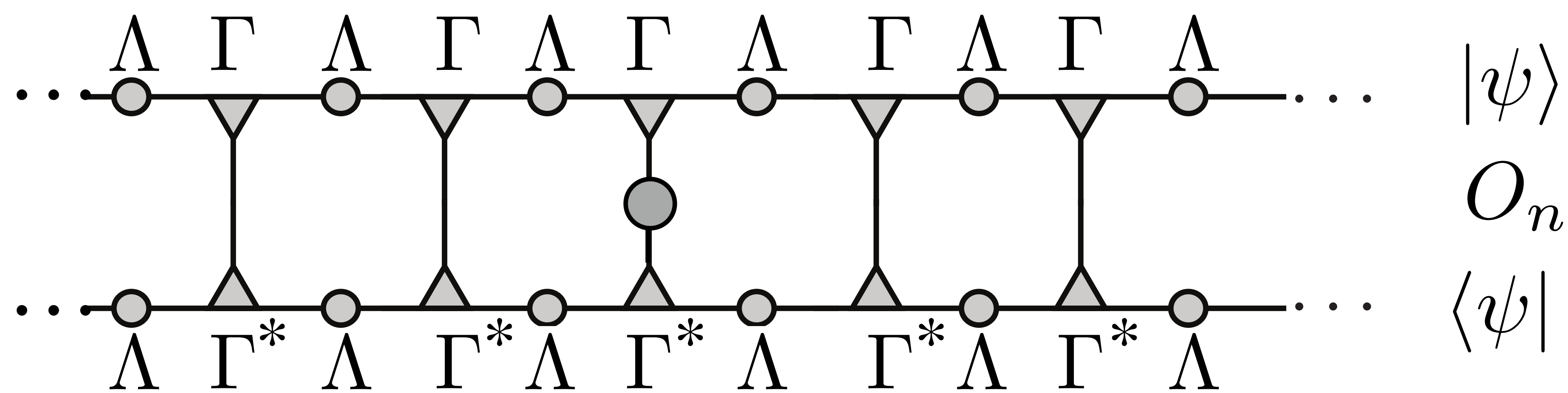
Orthogonality:

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

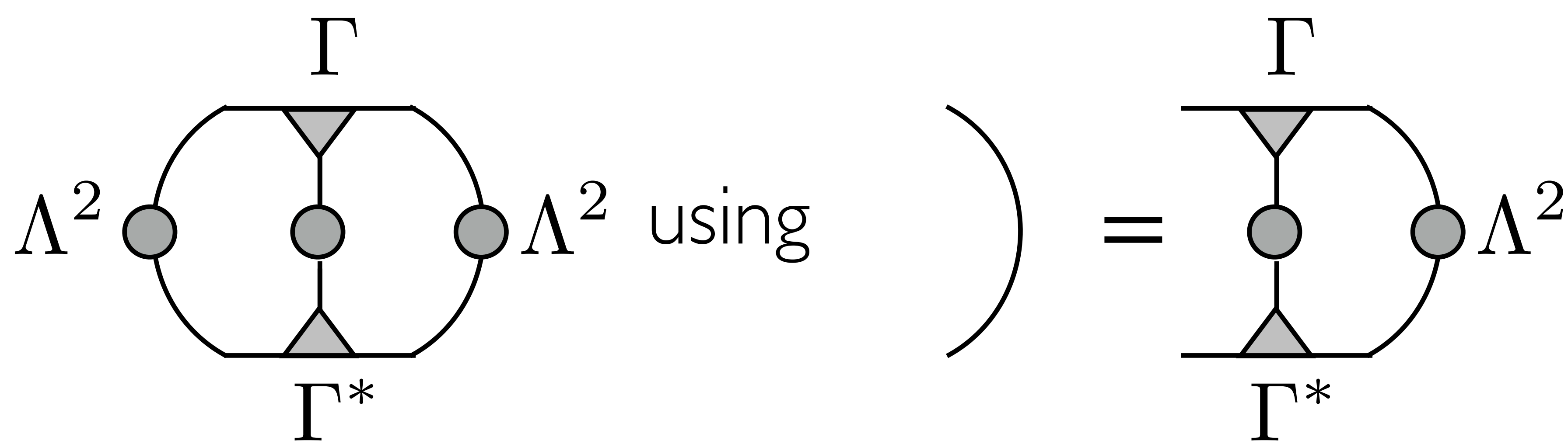
MPS and the canonical form

Efficient evaluation of **expectation values**:

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



$=$



Time evolving block decimation

Assume we have a Hamiltonian of the form

$$H = \sum_j h^{[j,j+1]}$$

Time evolution in real time

$$|\psi_t\rangle = \exp(-iHt)|\psi_{t=0}\rangle$$

Time evolution in imaginary time

$$|\psi_0\rangle = \lim_{\tau\to\infty} \frac{\exp(-H\tau)|\psi_i\rangle}{||\exp(-H\tau)|\psi_i\rangle||}$$

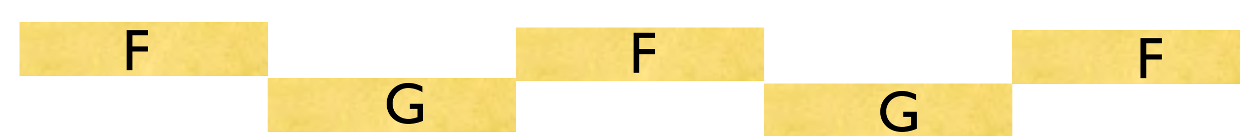
Time evolving block decimation

Consider a Hamiltonian $H = \sum_j h^{[j,j+1]}$ [Vidal '03]

Decompose the Hamiltonian as $\mathrm{H{=}F{+}G}$

$$F \equiv \sum_{\text{even } j} F^{[j]} \equiv \sum_{\text{even } j} h^{[j,j+1]}$$

$$G \equiv \sum_{\text{odd } j} G^{[j]} \equiv \sum_{\text{odd } j} h^{[j,j+1]}$$



We observe $[F^{[r]}, F^{[r']}] = 0$ $([G^{[r]}, G^{[r']}] = 0)$
but $[G, F] \neq 0$

Time evolving block decimation

Apply Suzuki-Trotter decomposition of order p

$$\exp\left(-i(F+G)\delta t\right) \approx f_p\left[\exp(-F\delta t), \exp(-G\delta t)\right]$$

with $f_1(x,y) = xy$, $f_2(x,y) = x^{1/2} y x^{1/2}$, etc.

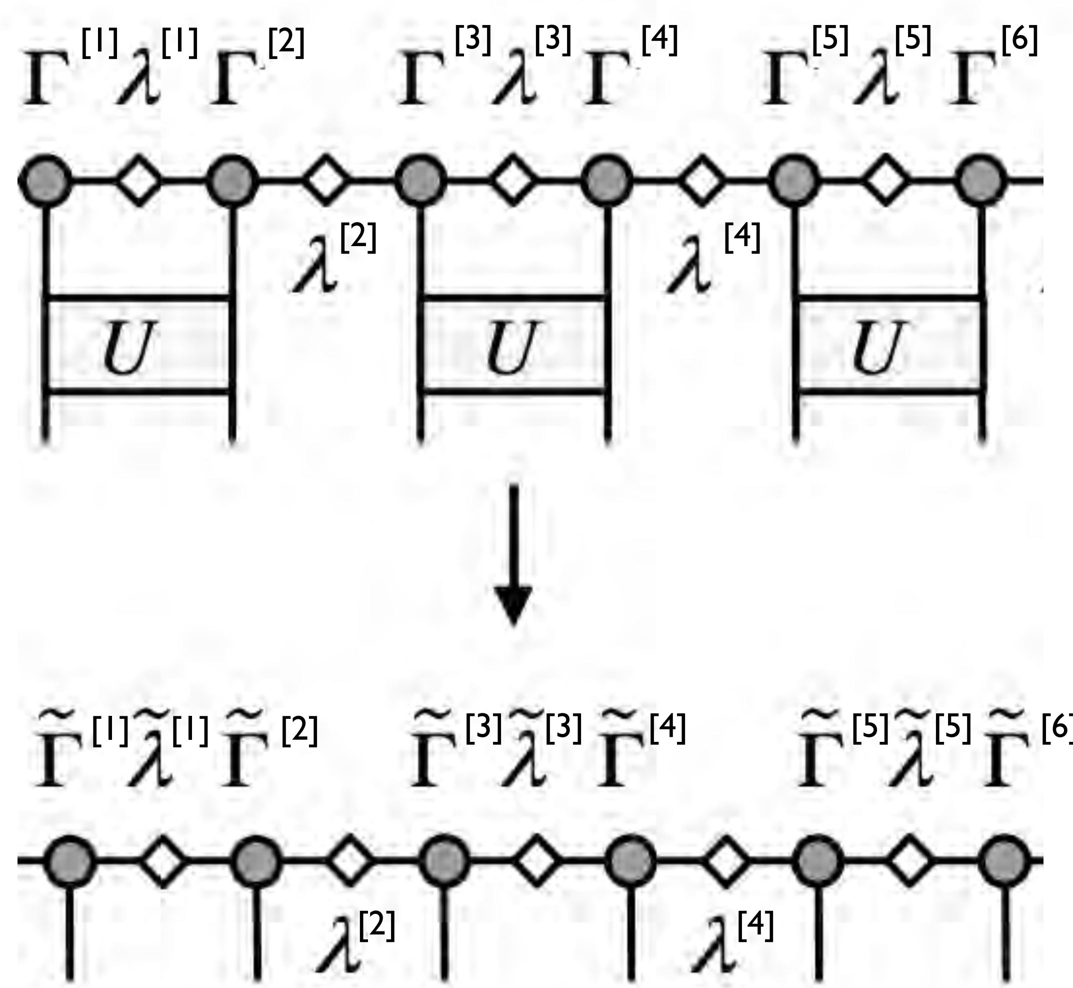
Two chains of two-site gates

$$\begin{aligned} U_F &= \prod_{\text{even } r} \exp(-iF^{[r]}\delta t) \\ U_G &= \prod_{\text{odd } r} \exp(-iG^{[r]}\delta t) \end{aligned}$$

Each gate affects the state only locally

Time evolving block decimation

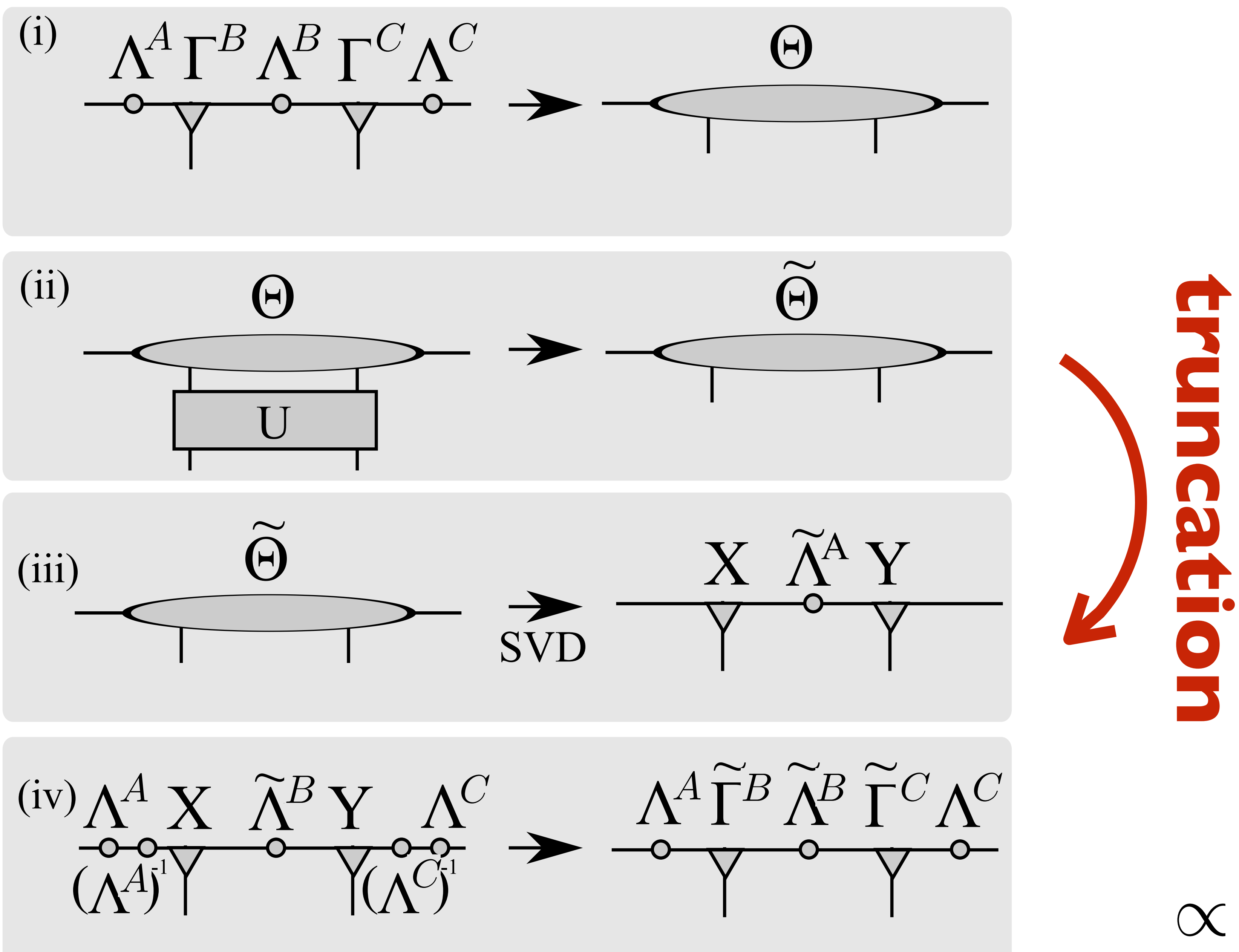
Time Evolving Block Decimation algorithm (TEBD)



How do we get the original form back?

Time evolving block decimation

Time Evolving Block Decimation (TEBD) algorithm [Vidal '03]



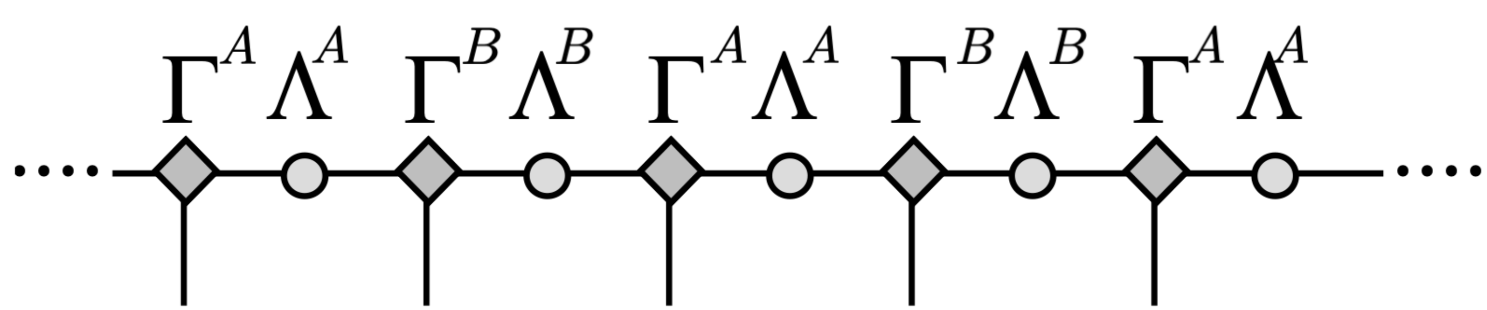
$\propto d^3\chi^3$

Translationally invariant, infinite systems!

Assume that $|\psi\rangle$ is translational invariant and $L = \infty$:
infinite TEBD (**iTEBD**)

Partially break translational symmetry to simulate the action of the gates

$$\Gamma^{[2r]} = \Gamma^A,\ \lambda^{[2r]} = \lambda^A,\ \Gamma^{[2r+1]} = \Gamma^B,\ \lambda^{[2r+1]} = \lambda^B$$



iTEBD toy code:

https://colab.research.google.com/drive/1G_8r4lfiCYKHLmhrFKH4NT4Q2ZWdTNRT

Efficient simulation of interacting topological matter

I) Introduction to many-body entanglement ✓

II) Matrix-Product States ✓

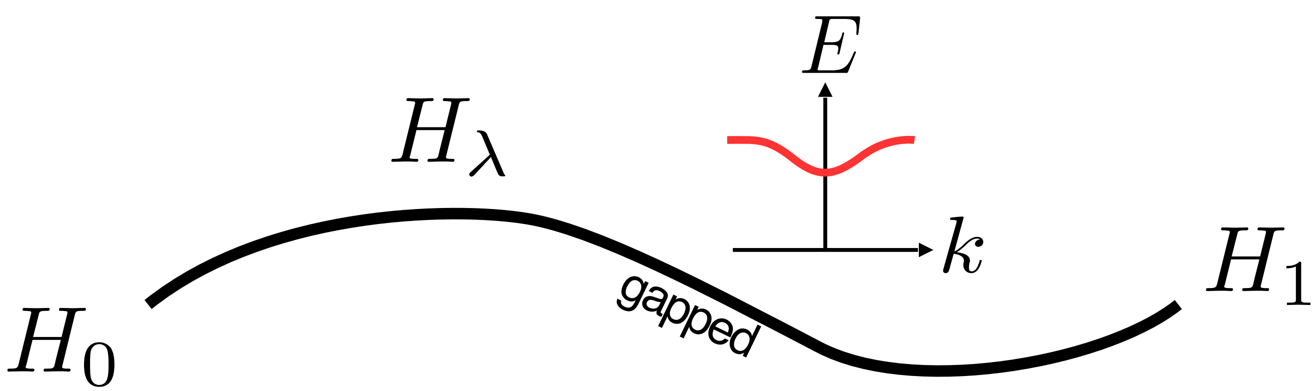
III) Symmetry-protected topological (SPT) phases

IV) Universal entanglement scaling at critical points

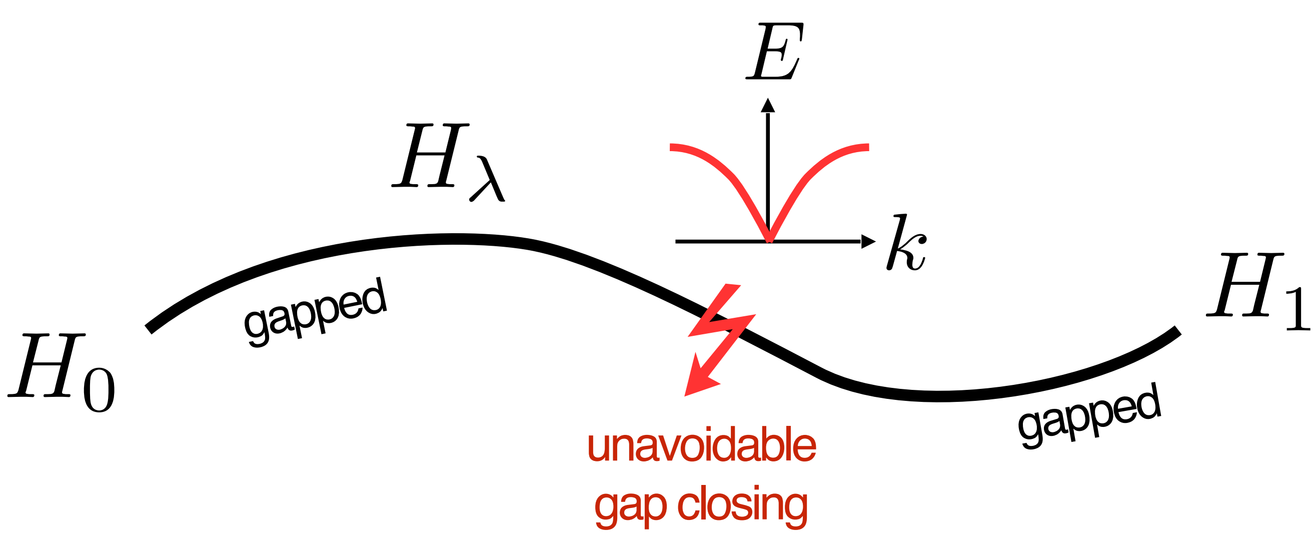
V) Case study: Phase diagram of a spin-1 chain

Matter occurs in different phases

Gapped quantum phases $(T = 0)$: Two Hamiltonians are in the same phase if a path of gapped Hamiltonians connects them



Same phase



Different phases

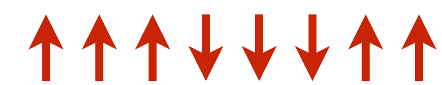
Gapped phases completely classified in 1D

[Chen et al. '12]

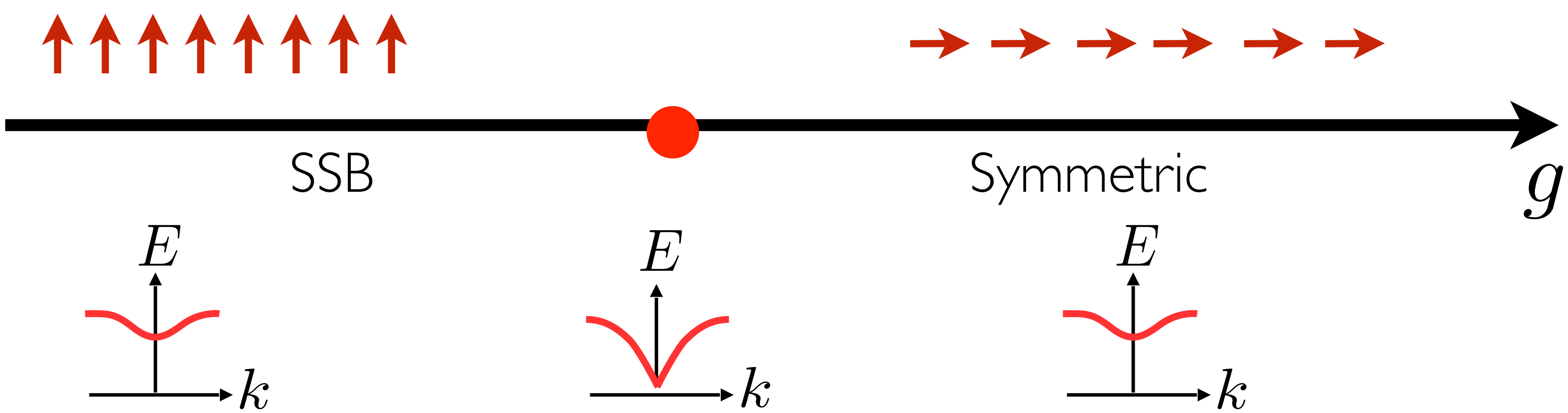
Spontaneous symmetry breaking (SSB)

Transverse field Ising model: $\mathbb{Z}_2$ symmetry

$$H = -\sum_j S_j^z S_{j+1}^z - g \sum_j S_j^x$$



$m \neq 0$ $\qquad$ $m = 0$

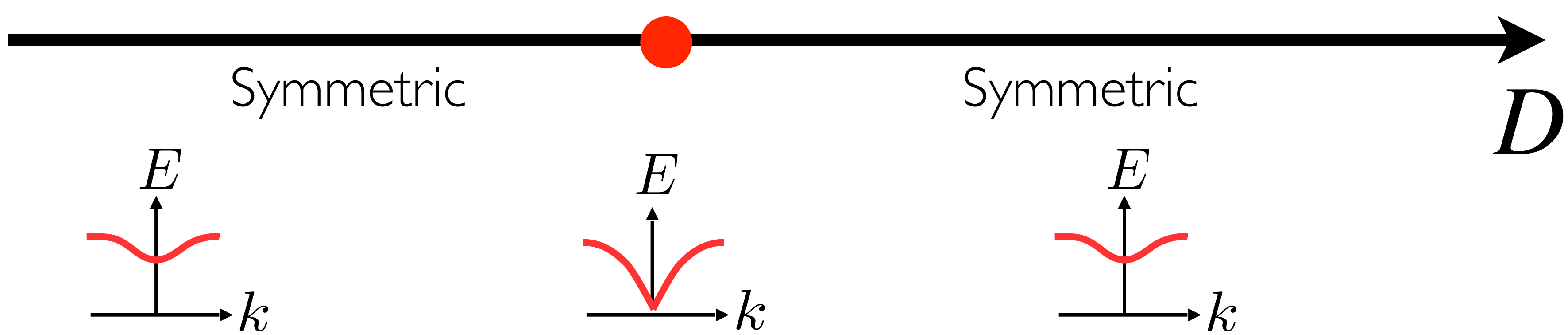


Local order parameter in SSB Phase:
Landau theory of phase transitions

Symmetry-protected topological (SPT)

Haldane phase in a spin-1 chain: $\mathbb{Z}_2 \times \mathbb{Z}_2$, time reversal, ...

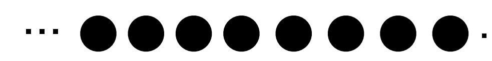
$$H = \sum_j \vec{S}_j \cdot \vec{S}_{j+1} + D \sum_j (S_j^z)^2$$



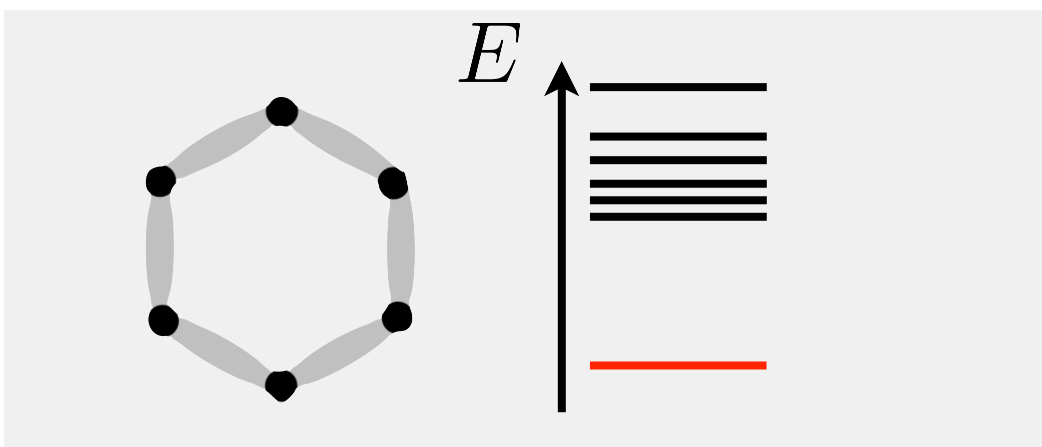
Classified by "Symmetry fractionalization"

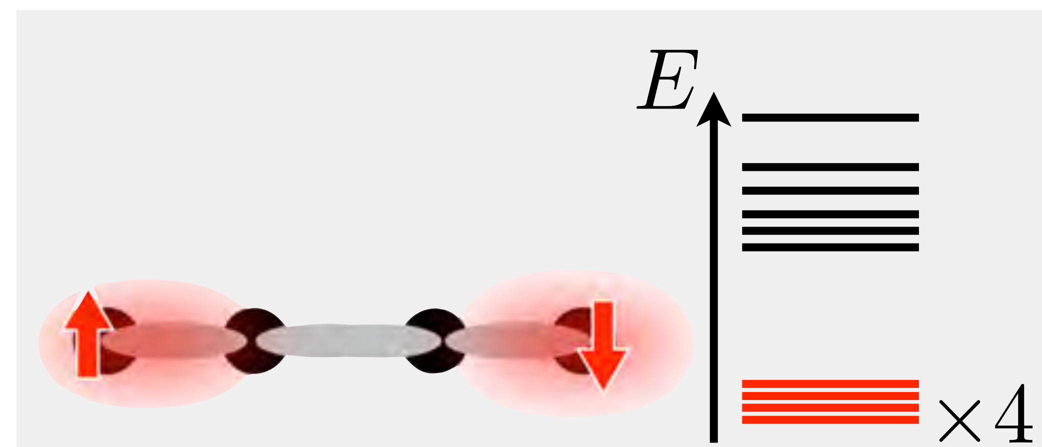
[FP, Turner, Berg, Oshikawa '10, Chen et al. '11; Schuch et al '11]

Symmetry fractionalization

Spin-1 Heisenberg chain $H = \sum_j \vec{S}_j \cdot \vec{S}_{j+1}$ 

- **Haldane phase:** Gapped and no symmetry breaking [Haldane '83]
- **Spin-1/2** excitations at the edges [Affleck et al. '88]





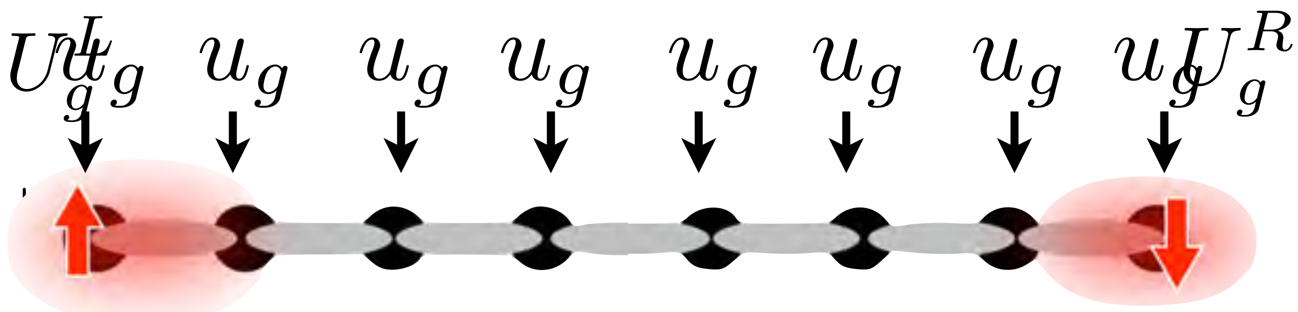
Haldane phase protected by…

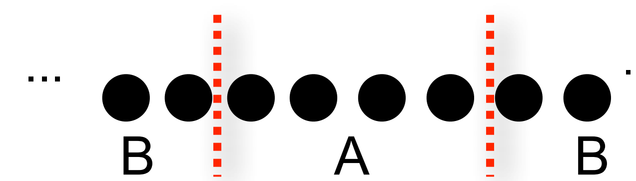
Spin rotation ($\mathbb{Z}_2 \times \mathbb{Z}_2$), Time reversal, Inversion symmetry

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

Symmetry protected topological phases

Local Hamiltonian and gapped ground state $|\psi_0\rangle$:
Symmetric under $g, h \in G$





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** $H^2[G, U(1)]$ [Schur 1911]

➡ Classification of **symmetry protected topological phases**
[see also 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

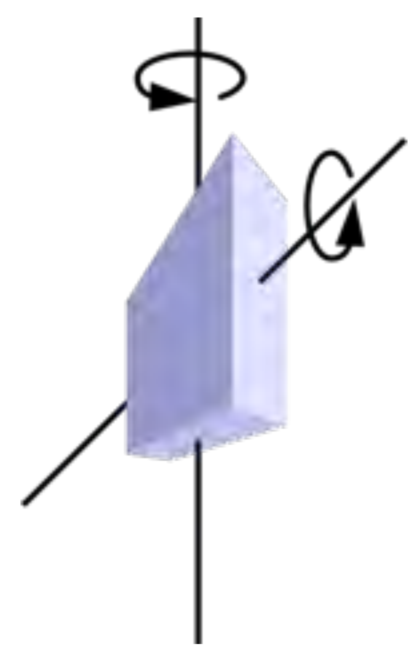
  $$R^n = \mathbb{1} \Rightarrow U_R^n = e^{i\phi}\mathbb{1}$$

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

- Example $\mathbb{Z}_2 \times \mathbb{Z}_2$: Rotation about two axes

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

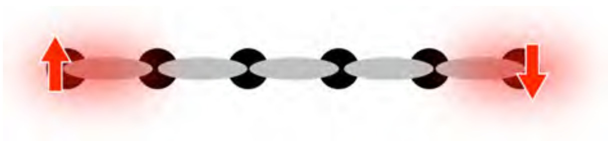
  - Phases $\phi_{xz} = 0, \pi$ cannot be gauged away: Distinct topological phases



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

Symmetry protected topological phases

$\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry protects the Haldane phase

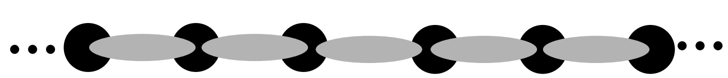


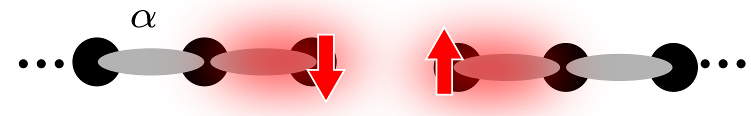
$$|0\rangle|0\rangle|0\rangle|0\rangle|0\rangle$$

Schmidt states have 'artificial edges'

$$|\psi\rangle \approx \sum_\alpha \Lambda_\alpha |\alpha\rangle_A \otimes |\alpha\rangle_B$$

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





- Projective representations U_g can be directly extracted

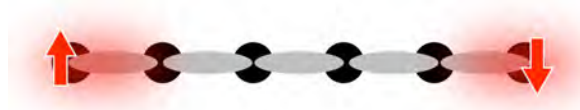
FP, A.M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B **81**, 064439 (2010).
FP and A.M. Turner, Phys. Rev. B **86**, 125441 (2012).

Symmetry protected topological phases

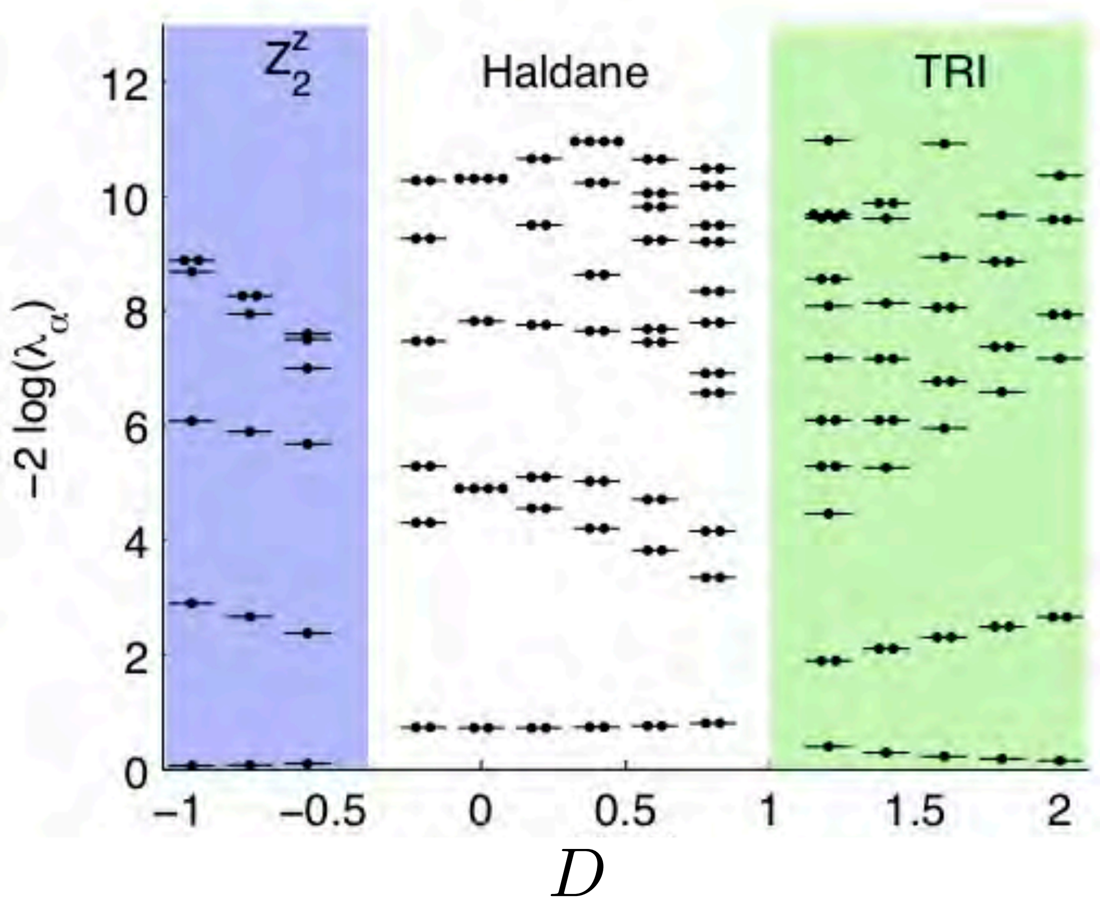
$\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry protects the Haldane phase

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

Entanglement spectrum $\epsilon_\alpha = -\log \Lambda_\alpha^2$



$|0\rangle|0\rangle|0\rangle|0\rangle|0\rangle$



$$|\psi\rangle = \sum_\alpha \Lambda_\alpha |\alpha\rangle_A \otimes |\alpha\rangle_B$$

➡ **Even fold degeneracy in the Haldane phase!**

(similar to Kramer DG)

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

$$\phi_{xz} = 0, \pi$$

FP, A.M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B **81**, 064439 (2010).
FP and A.M. Turner, Phys. Rev. B **86**, 125441 (2012).

Efficient simulation of interacting topological matter

I) Introduction to many-body entanglement ✓

II) Matrix-Product States ✓

III) Symmetry-protected topological (SPT) phases ✓

IV) Universal entanglement scaling at critical points

V) Case study: Phase diagram of a spin-1 chain

Critical Systems with Conformal Invariance

Critical points with **conformal invariance**: mapping onto field theories in 1+1 dimensions [di Francesco et al. 1997]

- Invariance under infinite dimensional symmetry group (all holomorphic functions)
- Linearly dispersing excitation with velocity u

Invariance under such a large class of functions places a lot of constraints on properties

- Free energy density [Affleck '86]

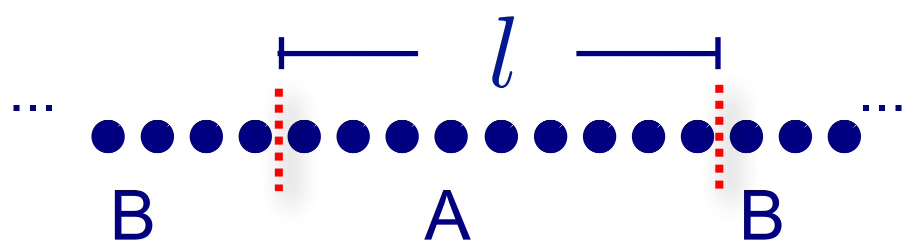
$$F(T) = E_0 - \frac{\pi c T^2}{6u}$$

c is the number of critical excitations

Critical Systems with Conformal Invariance

Scaling relation for the block entropy in critical systems with conformal invariance [Holzhey et al. '94]

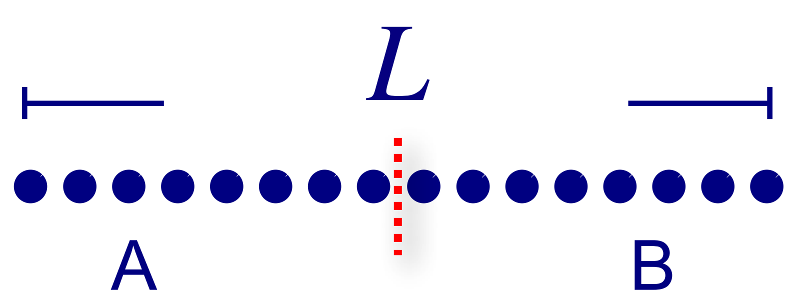
$$S = \frac{c}{3} \log \ell + \text{const} \,.$$



- Entanglement entropy diverges logarithmically as $\ell \to \infty$

Half chain entropy is

$$S = \frac{c}{6} \log L + \text{const} \,.$$



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Case study: Phase diagram of a spin-1 chain

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

- Python 3 library for simulations
  https://github.com/tenpy/tenpy

```
from tenpy.networks.mps import MPS
from tenpy.models.spins import SpinModel
from tenpy.algorithms import dmrg

M = SpinModel({"S":1,"L": 16,"bc_MPS": "finite",
                "Jx": 0,"Jy": 0,"Jz": 0,"D":2})
psi = MPS.from_product_state(M.lat.mps_sites(), [1]*16, "finite")
dmrg_params = {"trunc_params": {"chi_max": 30, "svd_min": 1.e-10}}
info = dmrg.run(psi, M, dmrg_params)
print("S[j] =", psi.entanglement_entropy())
```

Case study: Phase diagram of a spin-1 chain

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