

Tensor Networks and the Many-Body Problem

Frank Pollmann (TUM)

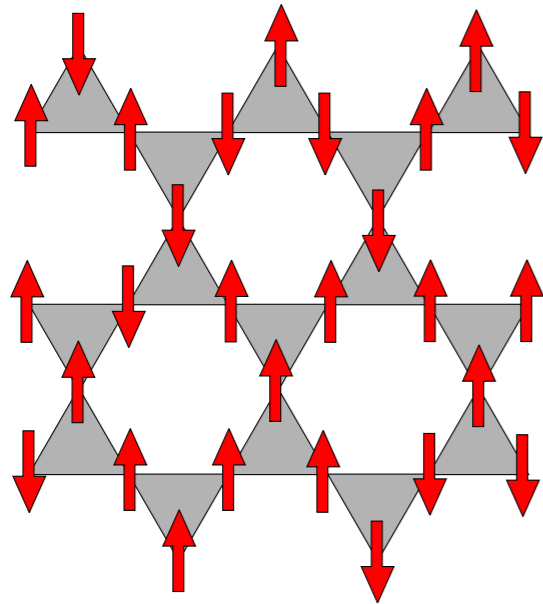


Slides & Tutorials:

<http://go.tum.de/475840>

Quantum Dynamics: From Electrons to Qbits
ICTP, August 2022

Efficient Simulation of Quantum Many-Body Systems



$$H = \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$



What is the nature of the many body ground state $|\psi_0\rangle$?

Efficient Simulation of Quantum Many-Body Systems

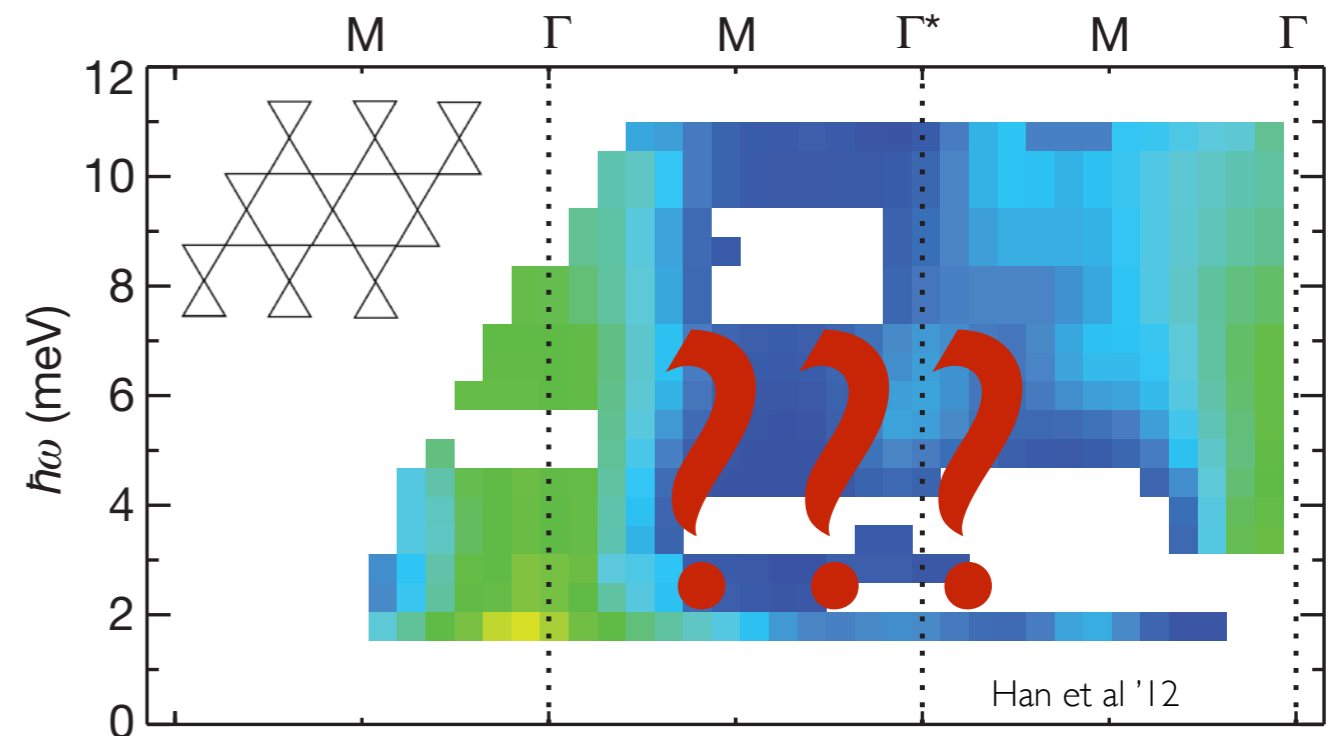
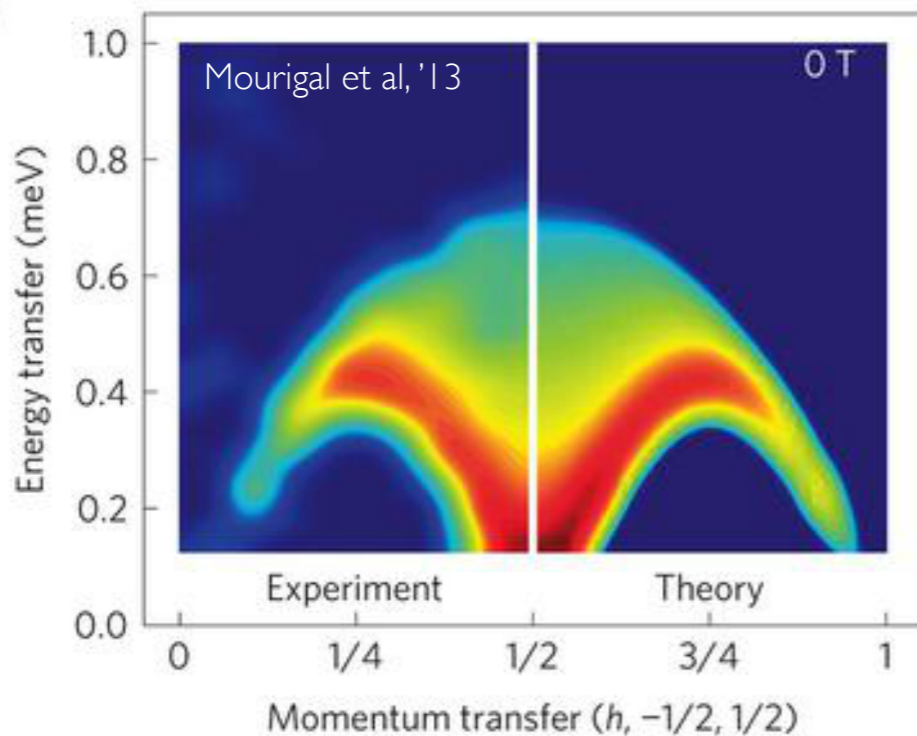
1D quantum spin liquid: Fractional **spinon excitations** in the antiferromagnetic $S=1/2$ Heisenberg chain



Copper Sulphate

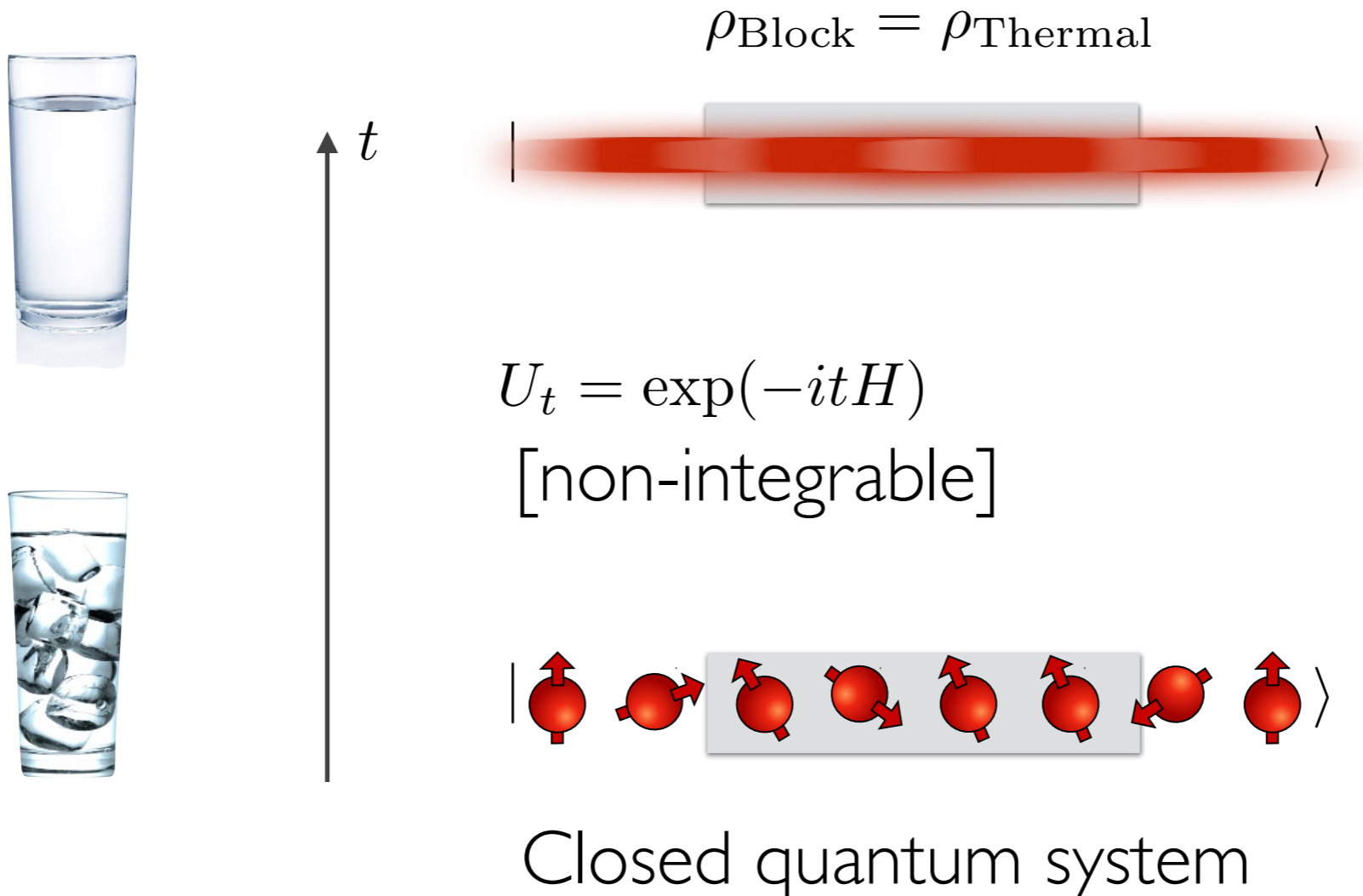


Dynamical structure factor:

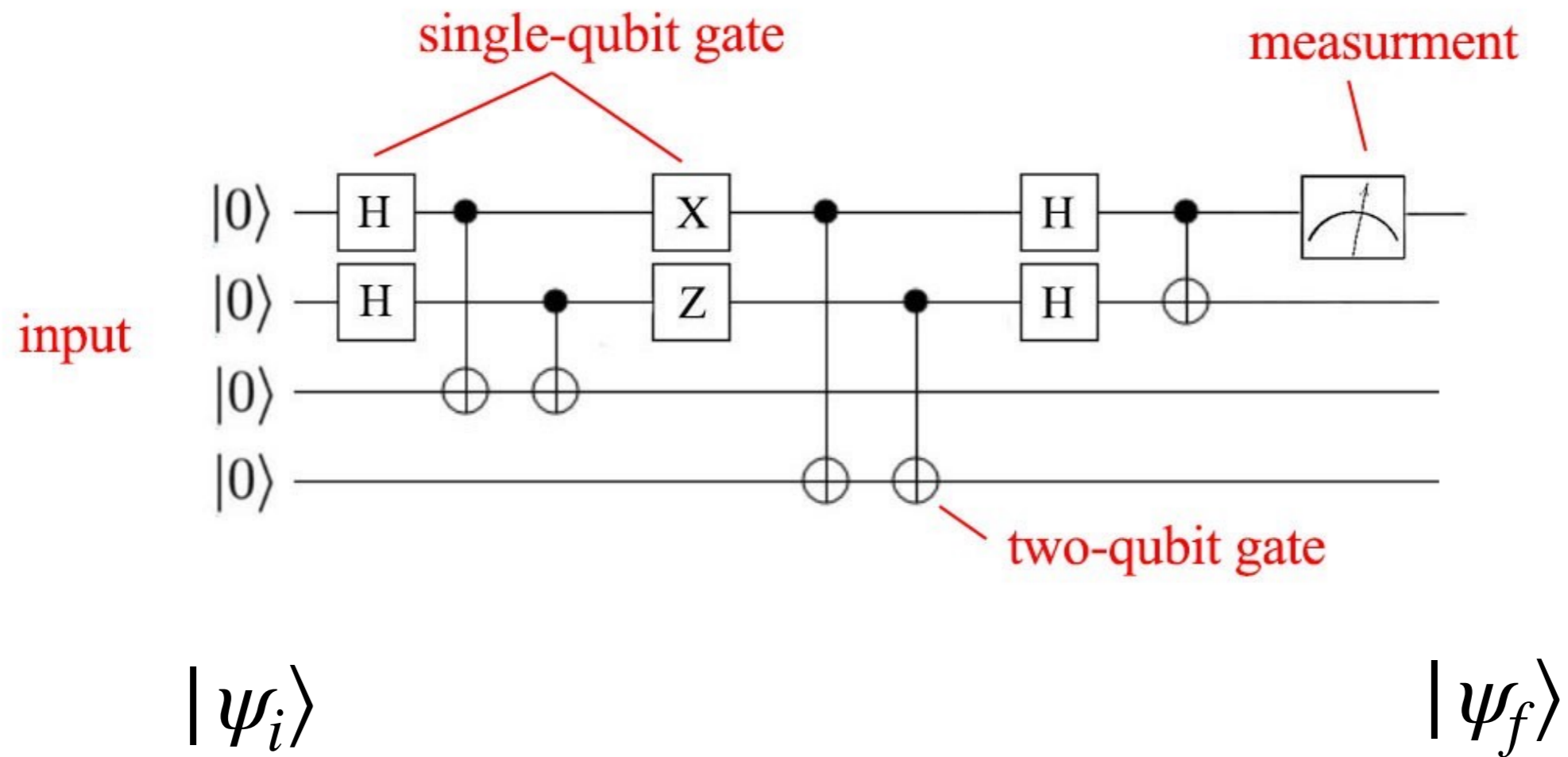


Simulating Quantum Thermalization

Investigate whether/how closed quantum many-body systems thermalize:



Simulating a Quantum Computer



Quantum Many-Body Systems

The Hilbert space of a quantum many body system grows exponentially!

$$|\psi\rangle = \sum_{j_1, j_2, \dots, j_L} \psi_{j_1, j_2, \dots, j_L} |j_1\rangle |j_2\rangle \dots |j_L\rangle$$

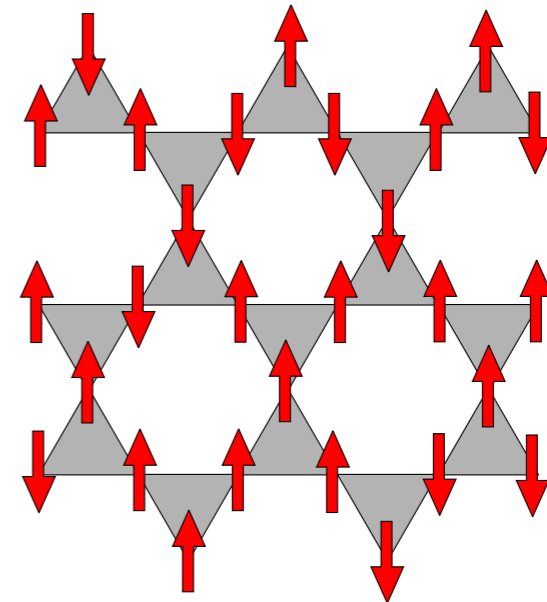
For N spin-1/2 particles: **2^N states**

10 spins dim=1'024

20 spins dim=1'048'576

30 spins dim=1'073'741'824

40 spins dim=1'099'511'627'776



Matrix-Product States

Many-body Hilbert space


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

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

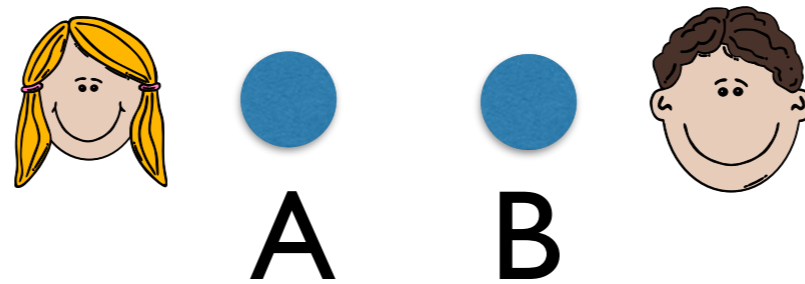
$$\psi_{j_1, j_2, \dots, j_L} \approx \sum_{\alpha_1, \alpha_2, \dots, \alpha_{L-1}} A_{\alpha_1}^{j_1} A_{\alpha_1, \alpha_2}^{j_2} \cdots A_{\alpha_{L-1}}^{j_L} \quad \alpha_j = 1 \dots \chi$$

Once we have an MPS representation, we can calculate (almost) everything exactly!

Tensor Networks and the Many-Body Problem

- I) Entanglement and Matrix-Product States 
- II) Time Evolving Block Decimation
- III) Density-Matrix Renormalization Group
- IV) Extracting topological invariants
- V) (isometric Tensor-Network States)

Bipartite Entanglement

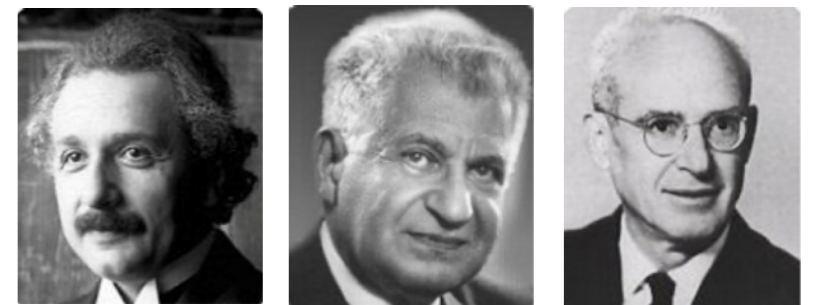


Product state (=non-entangled):

$$|\psi\rangle = \frac{1}{2} \left(|\uparrow\rangle_A + |\downarrow\rangle_A \right) \left(|\uparrow\rangle_B + |\downarrow\rangle_B \right)$$

Entangled state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_A |\downarrow\rangle_B + |\downarrow\rangle_A |\uparrow\rangle_B \right)$$



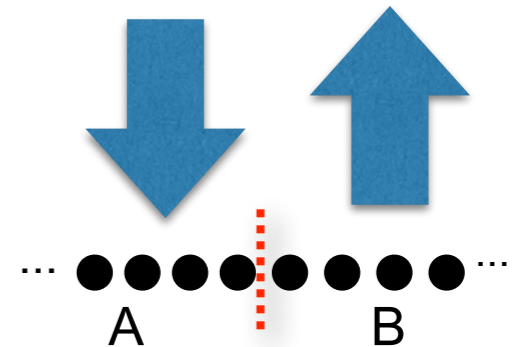
[Einstein, Rosen, Podolsky '35]

Bipartite Entanglement

Quantum state in d^L dimensional Hilbert space

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

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



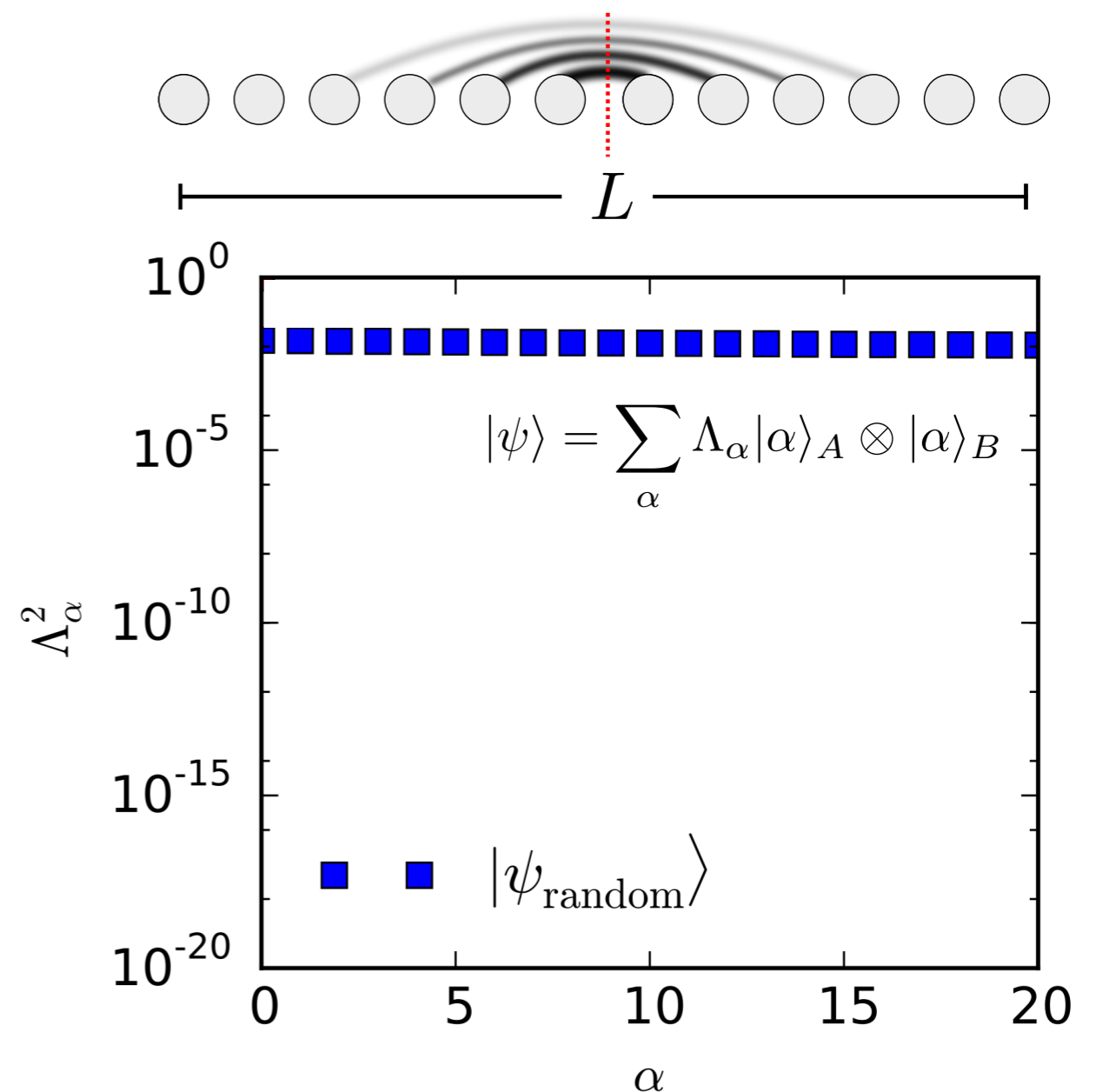
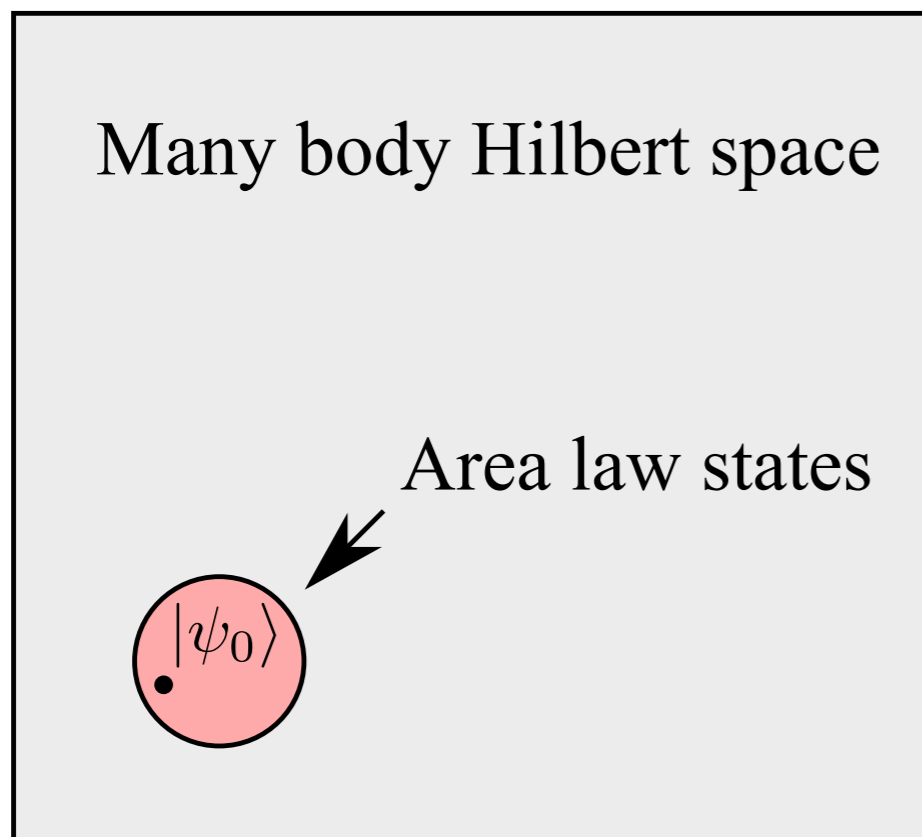
$$|\psi\rangle = \sum_{i,j} C_{i,j} |i\rangle_A \otimes |j\rangle_B = \sum_{\alpha} \Lambda_{\alpha} |\alpha\rangle_A \otimes |\alpha\rangle_B, \quad \langle \alpha | \alpha' \rangle = \delta_{\alpha \alpha'}$$

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 in one dimensional systems

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



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

Tutorial: (A) SVD Compression

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

Matrix can represent an image (array of pixel)

$$C = \begin{pmatrix} 0.23 & \cdots & 0.56 \\ \vdots & \ddots & \vdots \\ 0.22 & \cdots & 0.34 \end{pmatrix} = \left(\text{Image of Golden Gate Bridge} \right)_{\chi = 1200}$$

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



Tutorial: (A) SVD Compression

<http://go.tum.de/475840>

- I) Analyse the Schmidt spectra of the images and how much they can be compressed
- II) How does the number of singular values needed to represent the image on its size?
- III) How does a product state look like as an image?

Matrix-Product States

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

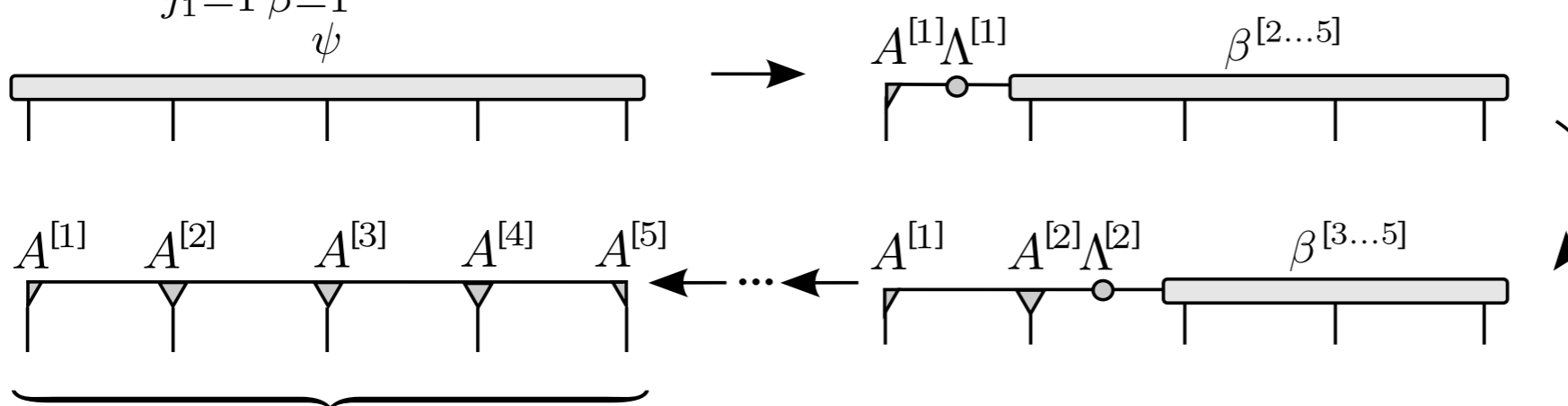
$$\psi_{j_1, j_2, j_3, j_4, j_5} = \text{---} \overline{\text{---}} \text{---} \psi$$

$$A_{i,j} = \text{---} \square \text{---}$$

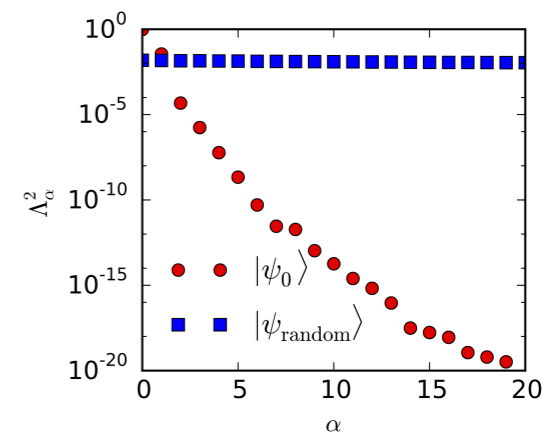
$$\sum_k A_{i,k} B_{k,j} = \text{---} \square \text{---} \square \text{---}$$

Successive Schmidt decompositions

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



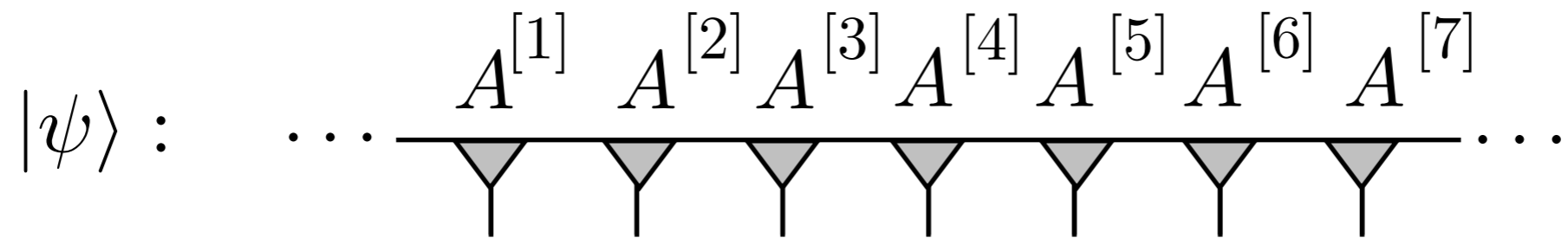
$$\sum_{\alpha_1, \alpha_2, \dots, \alpha_{L-1}} A_{\alpha_1}^{j_1} A_{\alpha_1, \alpha_2}^{j_2} \dots A_{\alpha_{L-1}}^{j_L}$$



MPS are tailored to describe 1D systems with an area law!

MPS and the Canonical Form

From now on: Leave out site indices!



MPS is not unique

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

Diagram illustrating the equivalence between a single tensor and a tensor with two auxiliary sites. On the left, a single downward-pointing triangle is connected to a horizontal line. On the right, two gray circles (auxiliary sites) are connected to the horizontal line, with a downward-pointing triangle between them. An equals sign is between the two diagrams.

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

MPS and the Canonical Form

Choose a convenient representation in **Canonical Form**:

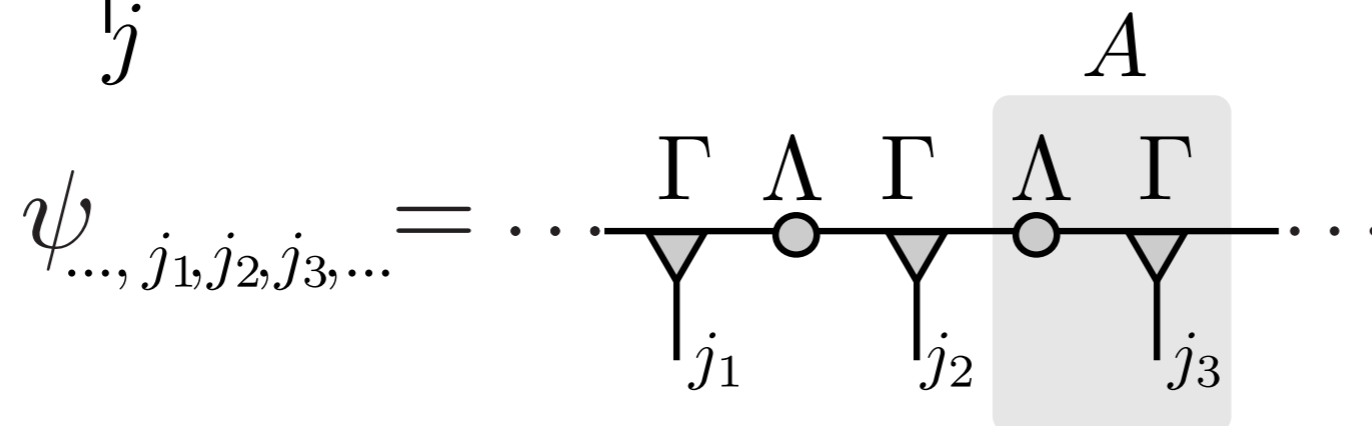
Bond index corresponds to Schmidt decomposition! [Vidal '03]

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

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

$\Lambda_{\alpha\beta} = \alpha \text{---} \circ \text{---} \beta$: Diagonal matrix with Schmidt values

$\Gamma_{\alpha\beta}^j = \alpha \text{---} \nabla_j \text{---} \beta$: Tensor relating to Schmidt basis



MPS and the Canonical Form

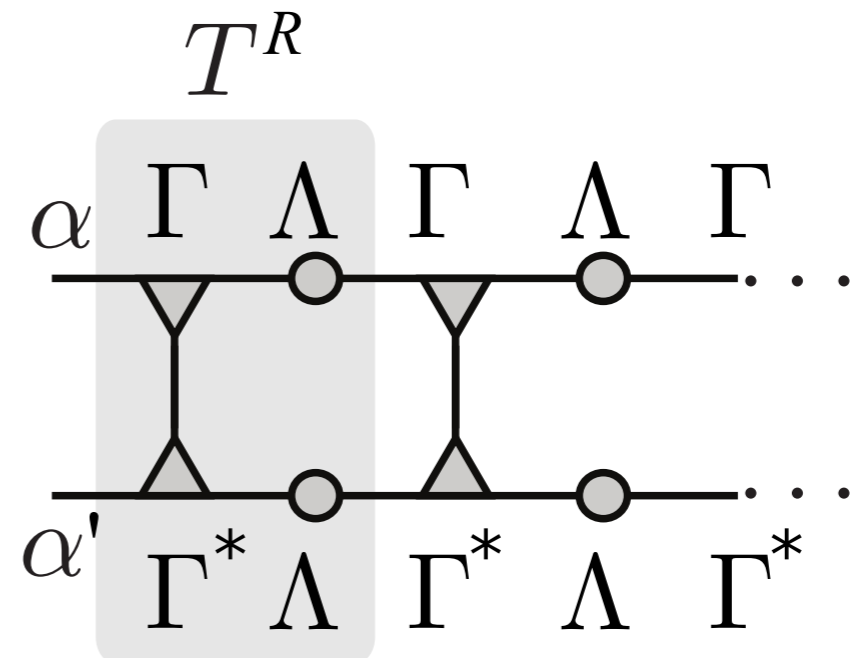
Schmidt states in terms of the MPS:

$$|\alpha\rangle_L = \dots \text{---} \overset{\Lambda}{\circ} \text{---} \overset{\Gamma}{\nabla} \text{---} \overset{\Lambda}{\circ} \text{---} \overset{\Gamma}{\nabla} \text{---} \alpha$$

$$|\alpha\rangle_R = \alpha \text{---} \overset{\Gamma}{\nabla} \text{---} \overset{\Lambda}{\circ} \text{---} \overset{\Gamma}{\nabla} \text{---} \overset{\Lambda}{\circ} \text{---} \dots$$

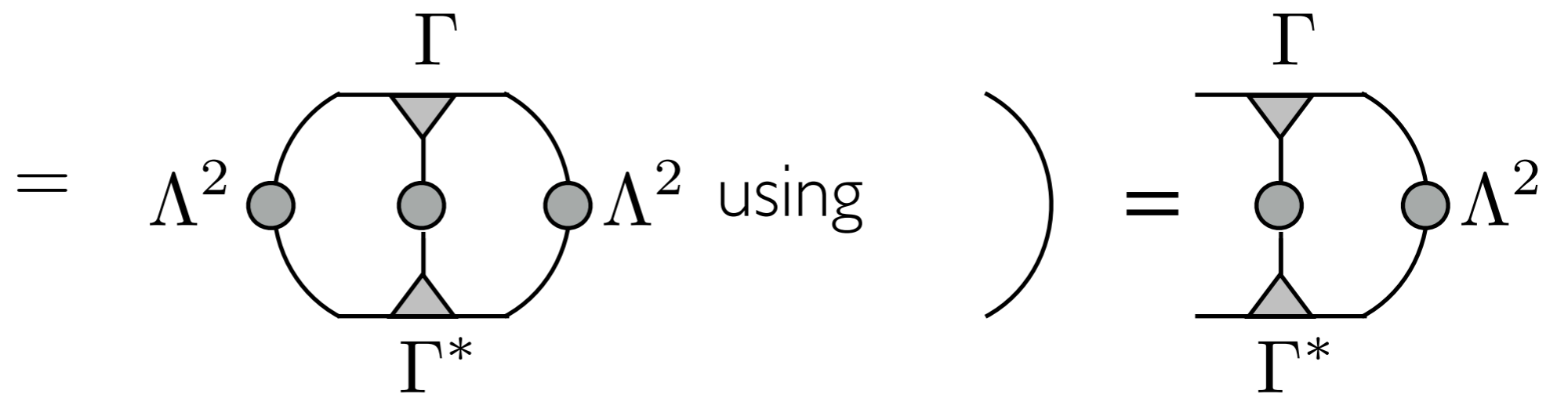
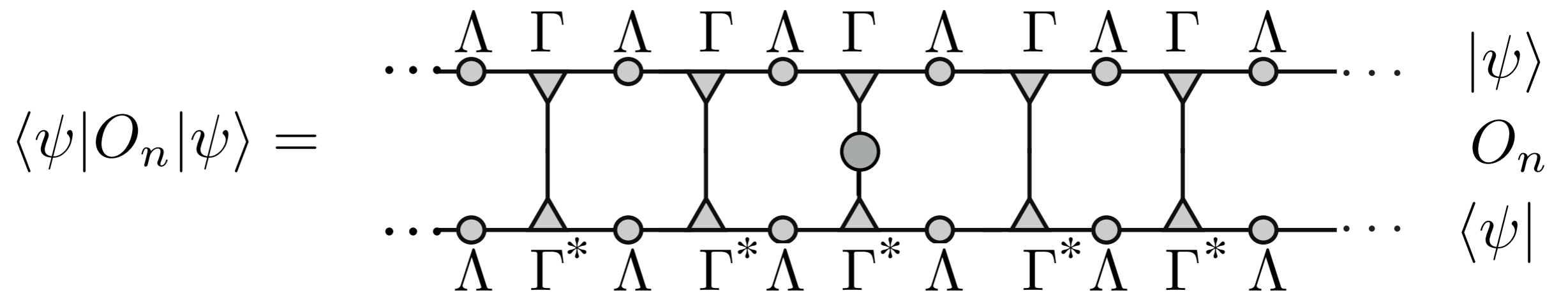
Orthogonality:

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



MPS and the Canonical Form

Efficient evaluation of **expectation values**:



MPS and the Canonical Form

Efficient evaluation of **correlation functions**:

$$\langle \psi | O_m O_n | \psi \rangle = \Lambda^2 \text{ (Diagram) } \Lambda^2$$

The diagram illustrates the contraction of a Matrix Product State (MPS) tensor network for a correlation function. The chain consists of tensors arranged in two rows. The top row tensors are labeled Γ and Λ , and the bottom row tensors are labeled Γ^* and Λ . The chain is connected at both ends by arcs labeled Λ^2 . A shaded region labeled T^R covers three tensors in the middle of the chain, representing the operators O_m and O_n .

Tensor Networks and the Many-Body Problem

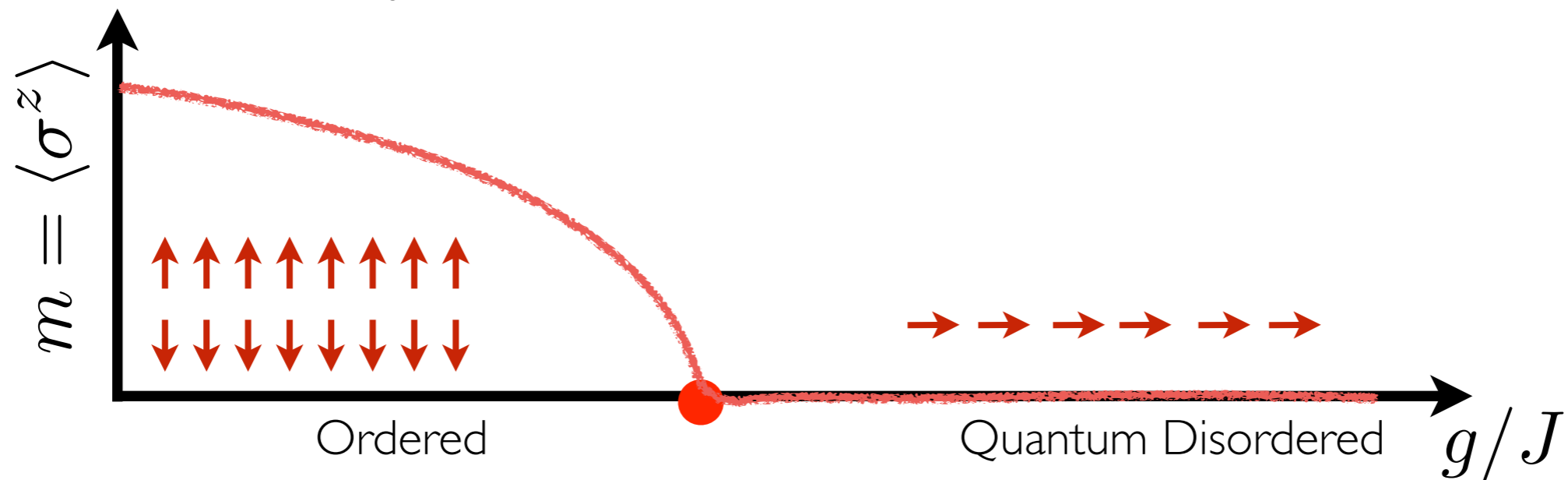
- I) Entanglement and Matrix-Product States
- II) Time Evolving Block Decimation
- III) Density-Matrix Renormalization Group
- IV) Extracting topological invariants
- V) (isometric Tensor-Network States)



Transverse Field Ising Model

Quantum phases at $T = 0$: Transverse field Ising model
with \mathbb{Z}_2 symmetry [Elliott et al. '70]

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



Entanglement of the ground state depends on g/J .

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

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

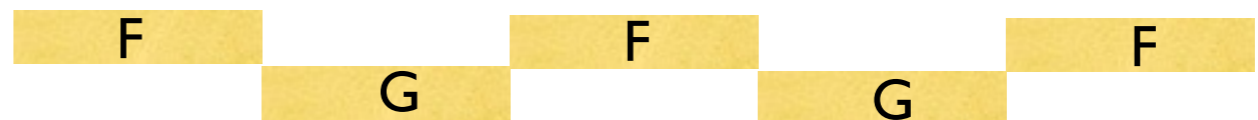
Time Evolving Block Decimation

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

Decompose the Hamiltonian as $H=F+G$

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

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



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

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

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

Two chains of two-site gates

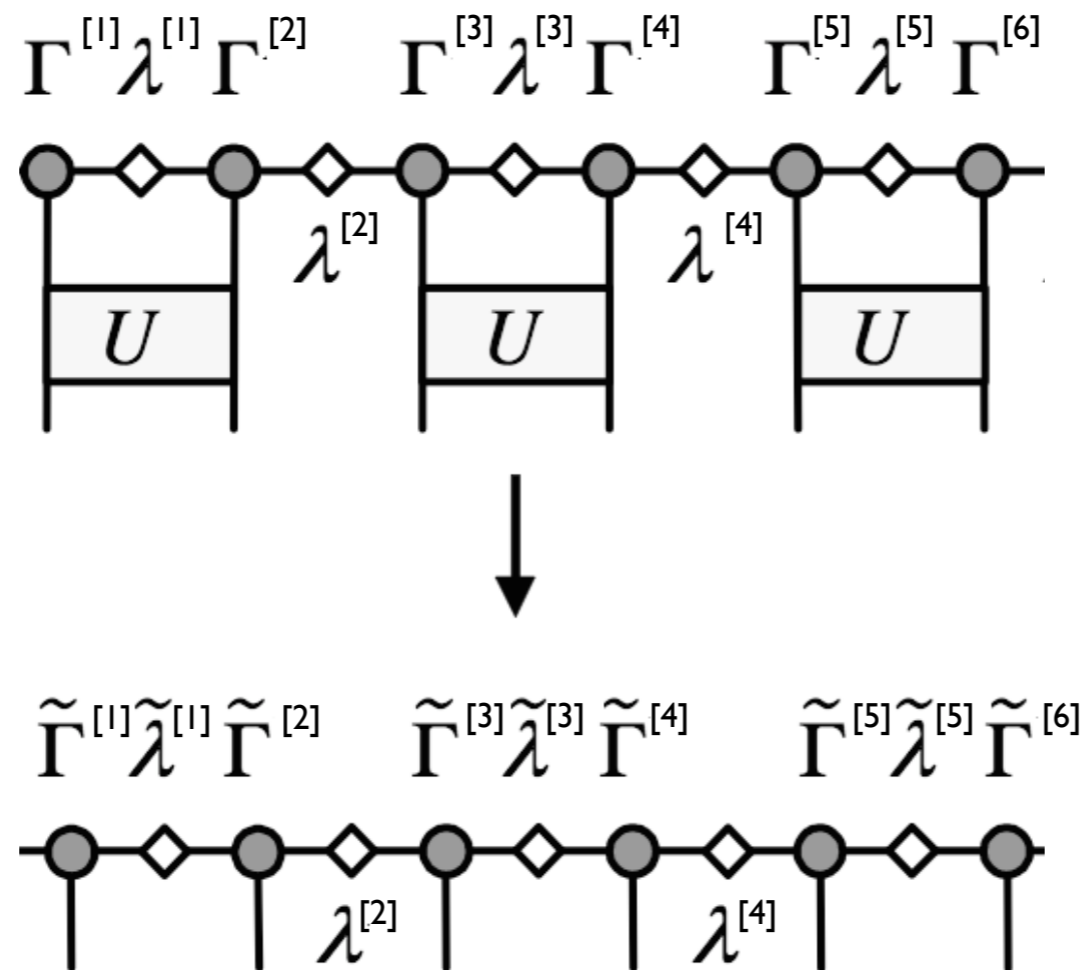
$$U_F = \prod_{\text{even } r} \exp(-iF^{[r]}\delta t)$$

$$U_G = \prod_{\text{odd } r} \exp(-iG^{[r]}\delta t)$$

Each gate affects the state only locally

Time Evolving Block Decimation

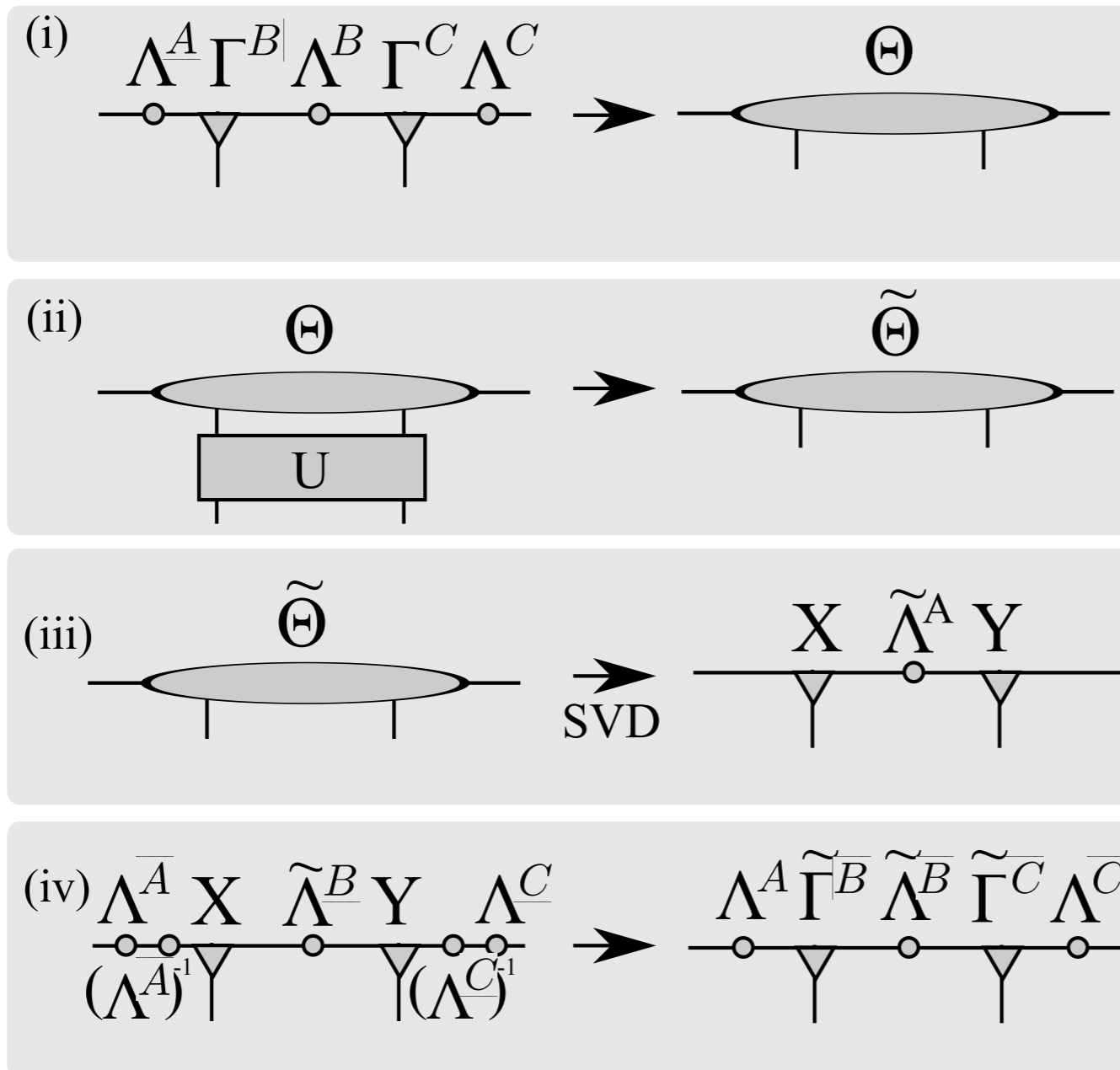
Time Evolving Block Decimation algorithm (TEBD)



How do we get the original form back?

Time Evolving Block Decimation

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



truncation

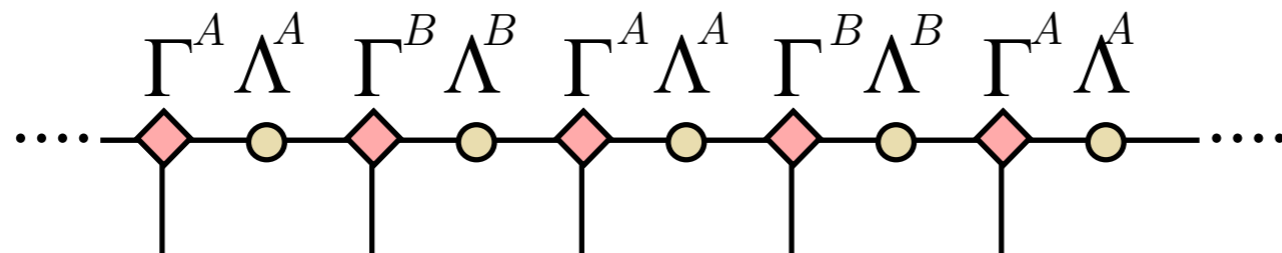
$$\propto d^3 \chi^3$$

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

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



Tutorial: (B) TEBD

<http://go.tum.de/475840>

- I) Check the convergence of the code for different parameters (number of iterations, χ , $d\tau$).
- II) Evaluate the phase diagram of the transverse field Ising model by plotting the magnetization, correlation length)
- III) Check the stability of the transition by adding new terms to the Hamiltonian: $\sum_i \sigma_i^x \sigma_{i+1}^x$ and $\sum_i \sigma_i^z$
- IV) Plot the entanglement growth following a global quench.

Tensor Networks and the Many-Body Problem

I) Entanglement and Matrix-Product States

II) Time Evolving Block Decimation

III) Density-Matrix Renormalization Group



IV) Extracting topological invariants

V) (isometric Tensor-Network States)

Density Matrix Renormalization Group (DMRG)

DMRG: Find the MPS representation of the ground state of a given Hamiltonian variationally

[White '92]

- ▶ Much faster convergence than TEBD
- ▶ Long range interactions can be easily implemented
- ▶ Similarly to TEBD, it allows to work directly in the thermodynamic limit

Density Matrix Renormalization Group (DMRG)

Matrix-Product Operators (MPO): Generalization of MPS

$$\mathcal{O}_{i_1 i_2 \dots i_L, i'_1 i'_2 \dots i'_L} =$$

The diagram illustrates the MPO operator $\mathcal{O}_{i_1 i_2 \dots i_L, i'_1 i'_2 \dots i'_L}$ as a product of three layers of tensors. Each layer consists of four diamond-shaped tensors labeled 'M' connected horizontally. The top layer has vertical lines extending downwards from each diamond. The middle layer has vertical lines extending upwards from each diamond, connecting to a horizontal line with four circles and four downward-pointing triangles. The bottom layer has vertical lines extending upwards from each diamond, connecting to a horizontal line with four circles and four downward-pointing triangles, and a horizontal line below it with four upward-pointing triangles and four circles. The labels Γ , Λ , and Γ^* are placed above and below the horizontal lines to indicate the indices of the tensors.

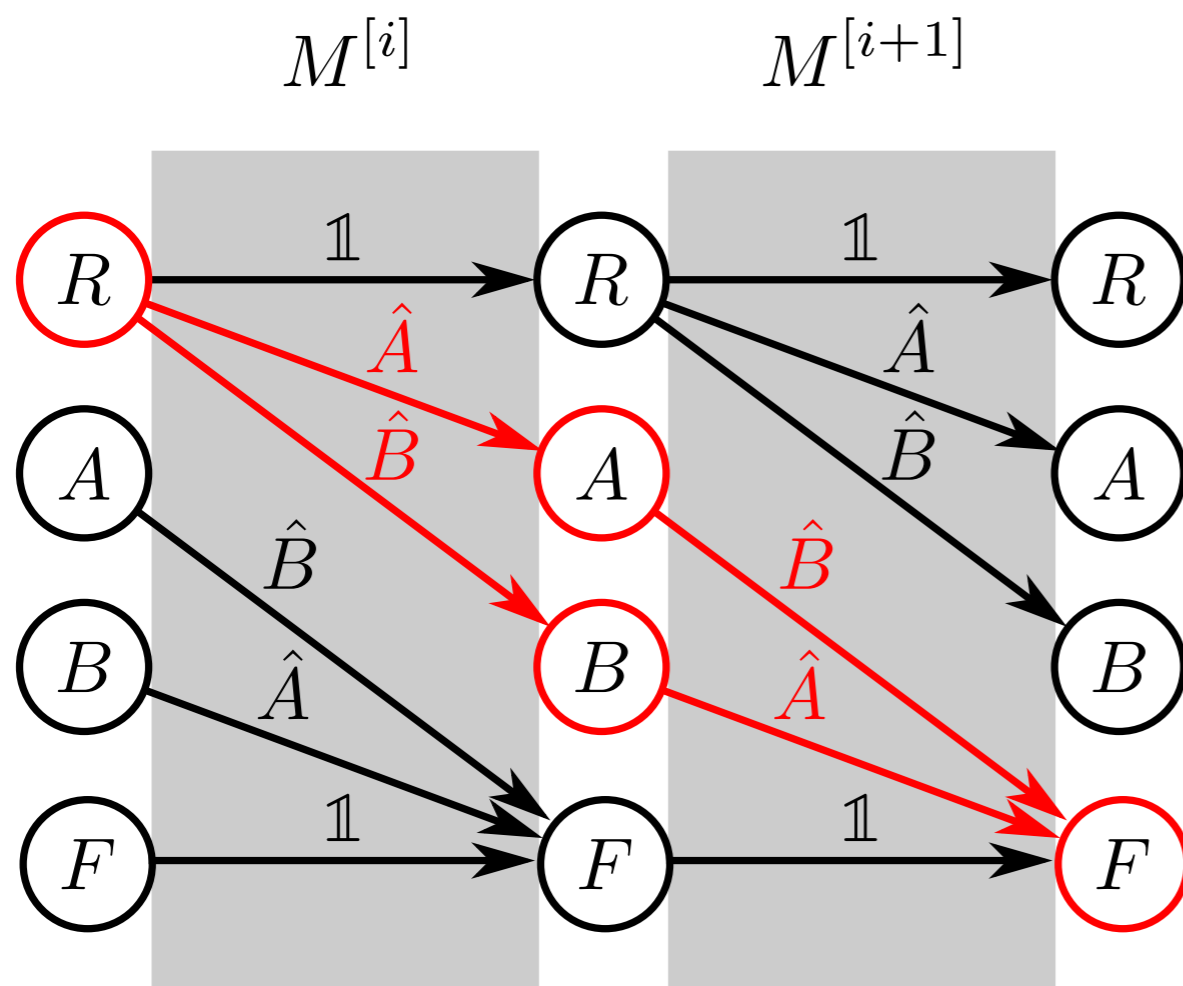
Density Matrix Renormalization Group (DMRG)

MPO representation of $\hat{O} = \sum_i \left(\hat{A}_i \hat{B}_{i+1} + \hat{B}_i \hat{A}_{i+1} \right)$

$$\begin{aligned} &= \hat{A} \otimes \hat{B} \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} \\ &+ \mathbb{1} \otimes \hat{A} \otimes \hat{B} \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} + \dots \\ &+ \hat{B} \otimes \hat{A} \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} \\ &+ \mathbb{1} \otimes \hat{B} \otimes \hat{A} \otimes \mathbb{1} \otimes \dots \otimes \mathbb{1} + \dots \end{aligned}$$

Density Matrix Renormalization Group (DMRG)

MPO representation of $\hat{O} = \sum_i \left(\hat{A}_i \hat{B}_{i+1} + \hat{B}_i \hat{A}_{i+1} \right)$



$$M = \begin{pmatrix} R & A & B & F \\ \mathbb{1} & \hat{A} & \hat{B} & 0 \\ 0 & 0 & 0 & \hat{B} \\ 0 & 0 & 0 & \hat{A} \\ 0 & 0 & 0 & \mathbb{1} \end{pmatrix} \begin{matrix} R \\ A \\ B \\ F \end{matrix}$$

Density Matrix Renormalization Group (DMRG)

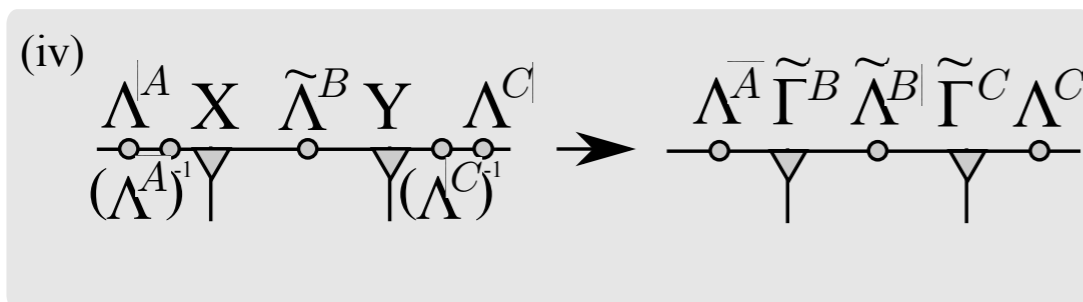
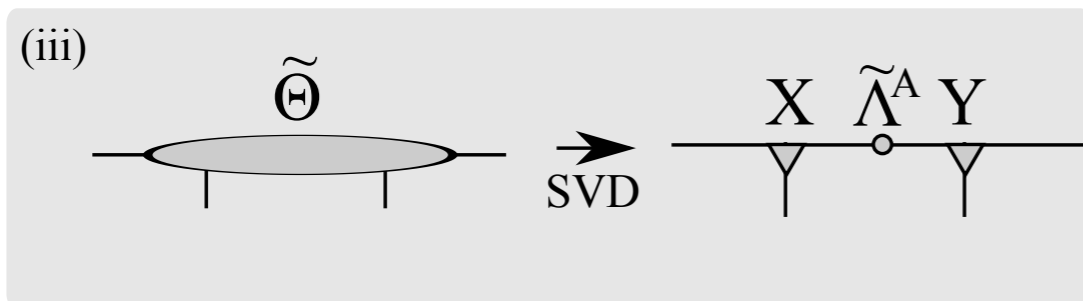
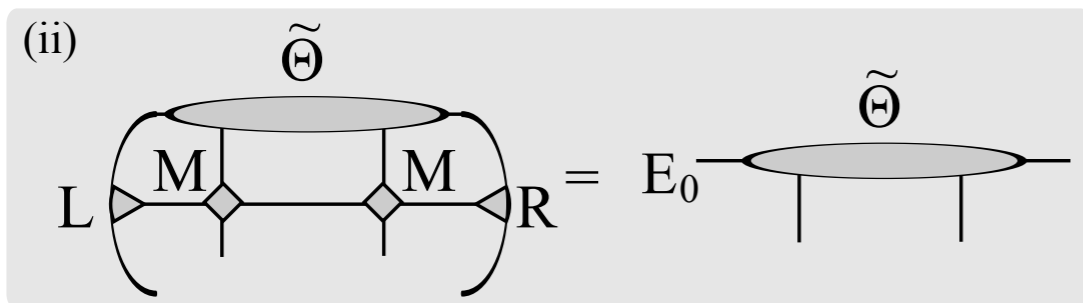
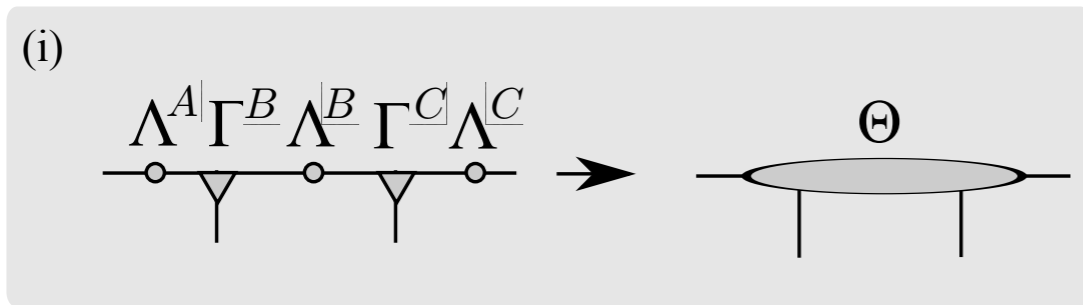
Find the **ground state** iteratively

$$H_{\alpha i \beta; \alpha' i' \beta'} = \begin{array}{c} \begin{array}{ccccccc} A^{[1]} & A^{[2]} & A^{[3]} & & A^{[5]} & A^{[6]} & A^{[7]} \\ \alpha & & & i & \beta & & \\ \alpha' & & & i' & \beta' & & \\ A^{[1]*} & A^{[2]*} & A^{[3]*} & & A^{[5]*} & A^{[6]*} & A^{[7]*} \end{array} \\ \langle \psi_0 | \\ H \\ | \psi_0 \rangle \end{array}$$

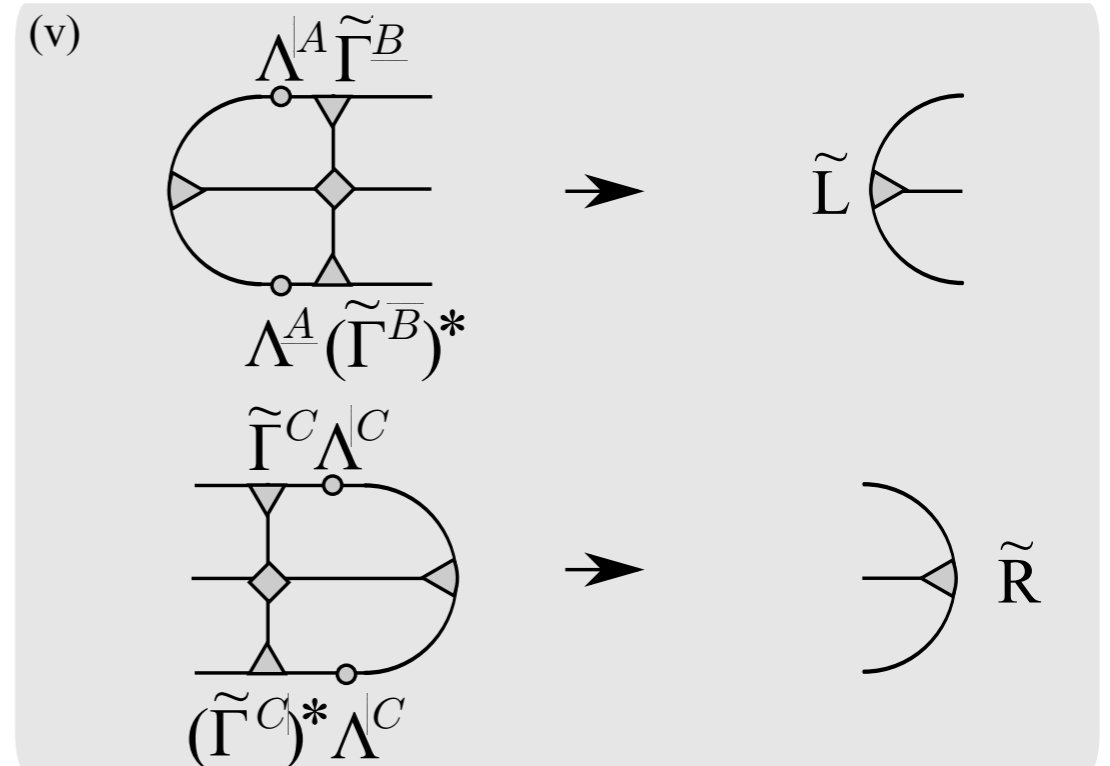
by locally minimizing energy of $H_{\alpha i \beta; \alpha' i' \beta'}$ (e.g., Lanczos)

Much faster convergence than TEBD + allows for long range interactions!

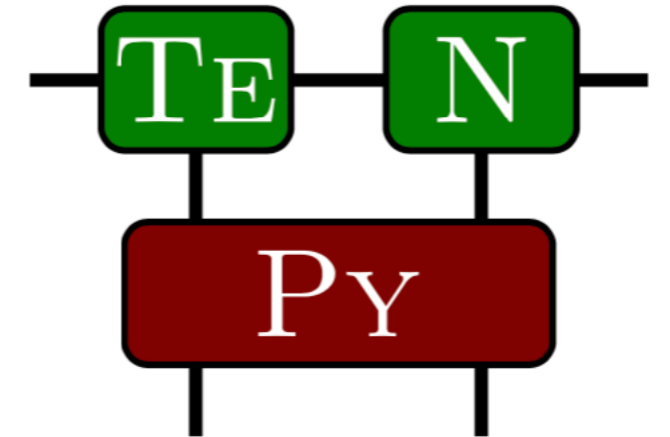
Density Matrix Renormalization Group (DMRG)



truncation



Tensor Network Python (TeNPy)



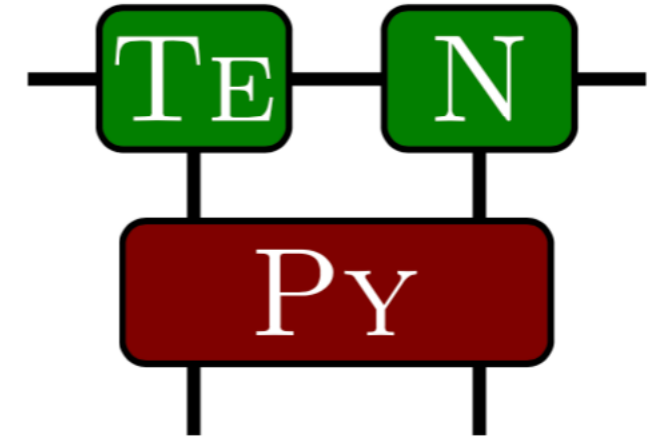
What is TeNPy

- ▶ Python 3 library for simulations with tensor network
<https://github.com/tenpy/tenpy>
- ▶ Object oriented, modular structure, and easy to install
- ▶ HTML documentation
<https://tenpy.readthedocs.io/en/latest/>
- ▶ (in)finite DMRG,TEBD;TDVP



Johannes Hauschild

Tensor Network Python (TeNPy)



Example: DMRG

Example

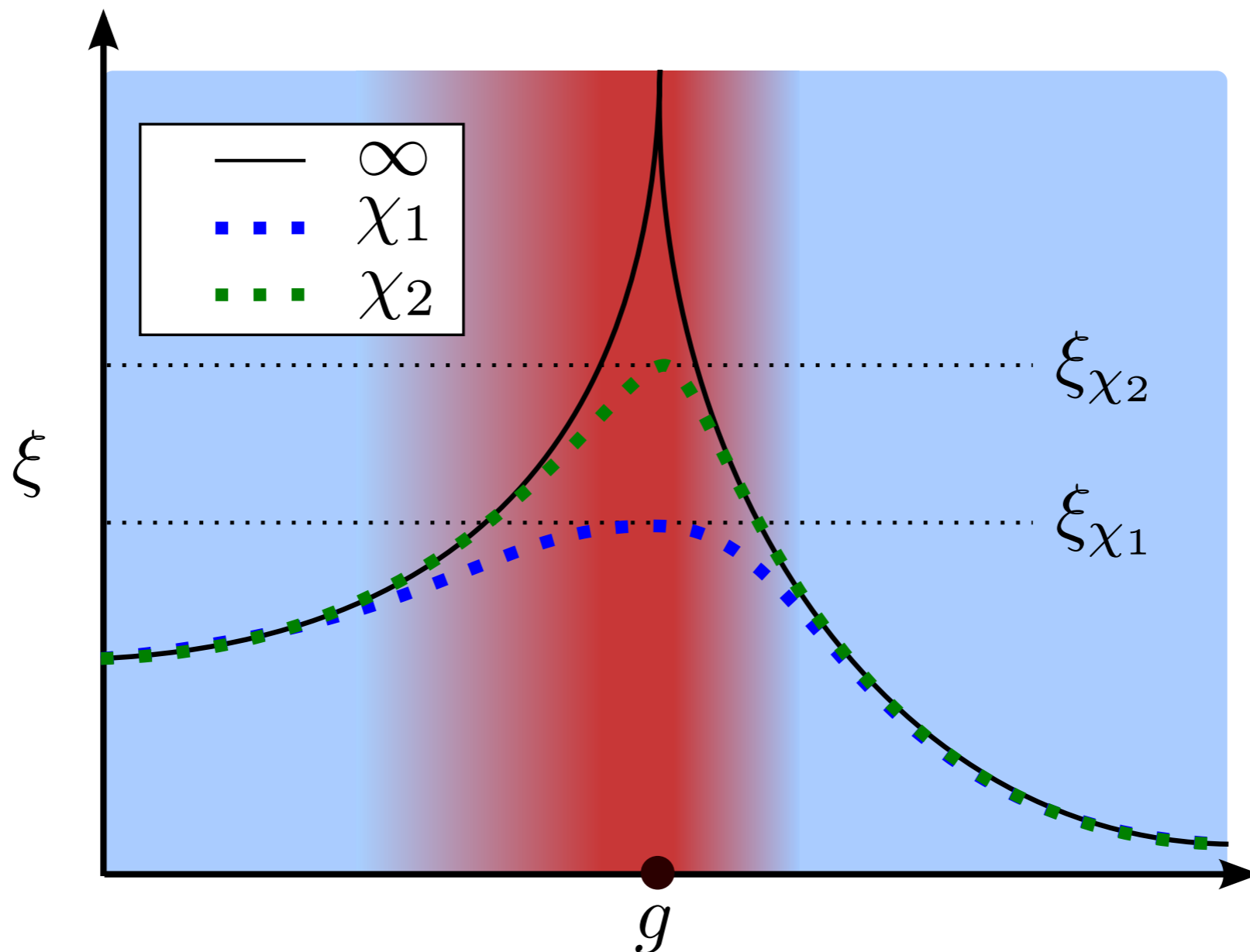
```
from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFChain
from tenpy.algorithms import dmrg

M = TFChain({'L': 16, 'J': 1., 'g': 1.5})
psi = MPS.from_product_state(M.lat.mps_sites(),
                             ['up']*16, 'finite')
dmrg_params = {'trunc_params': {'chi_max': 30,
                                'svd_min': 1.e-10}}
dmrg.run(psi, M, dmrg_params) # find ground state
print("E =", sum(M.bond_energies(psi)))
print("final bond dimensions: ", psi.chi)
```

Hauschild and FP, [arxiv:1805.00055](https://arxiv.org/abs/1805.00055)

Finite Entanglement Scaling

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



Tutorial: (C) TeNPy DMRG

<http://go.tum.de/475840>

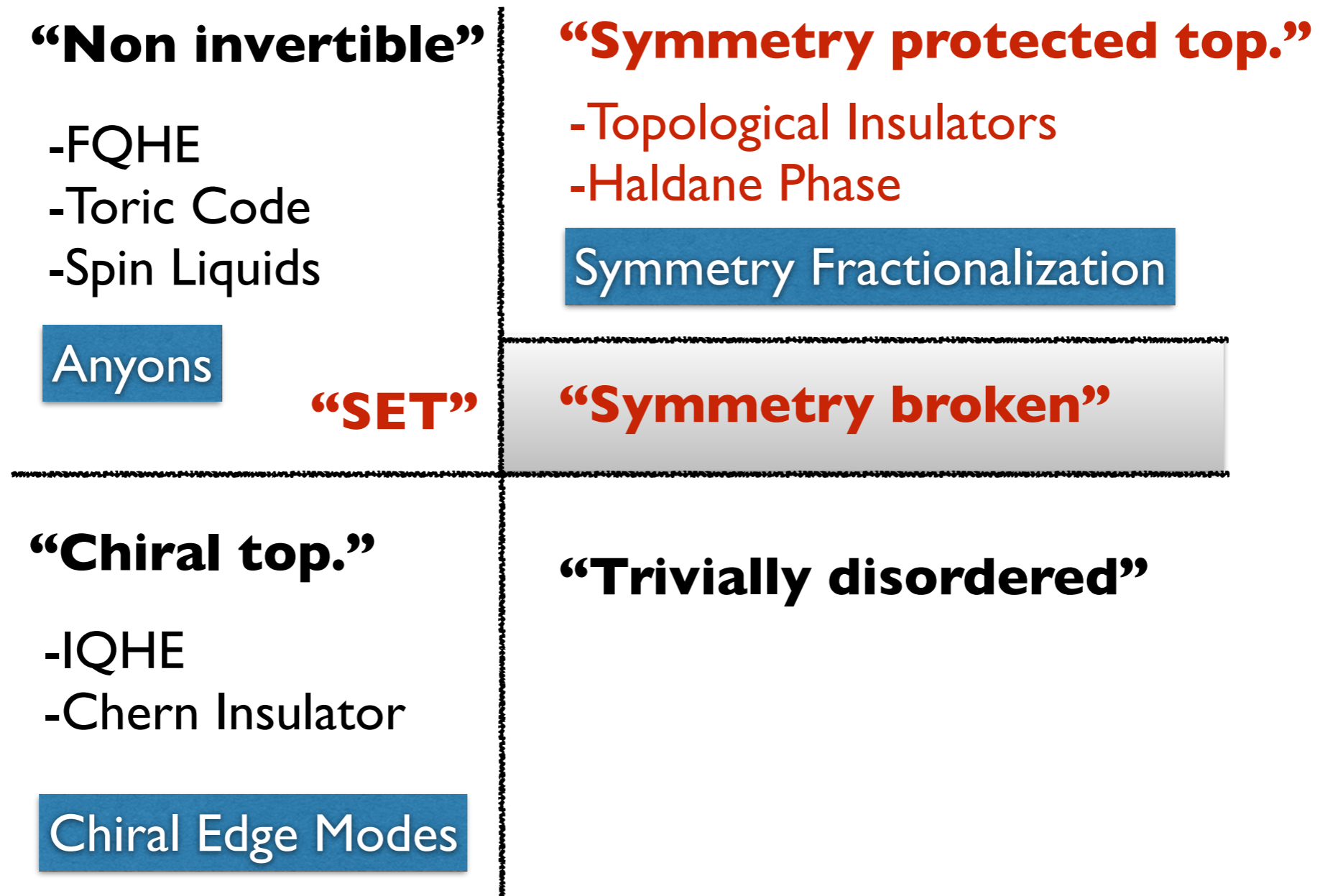
- I) Get familiar with the TeNPy interface:
<https://tenpy.github.io>
- II) Find the phase transition by plotting the magnetization as function of g
- III) Extract the central charge using “entanglement scaling”: $S = \frac{c}{6} \log \xi + \text{const}$

Tensor Networks and the Many-Body Problem

- I) Entanglement and Matrix-Product States
- II) Time Evolving Block Decimation
- III) Density-Matrix Renormalization Group
- IV) Extracting topological invariants
- V) (isometric Tensor-Network States)

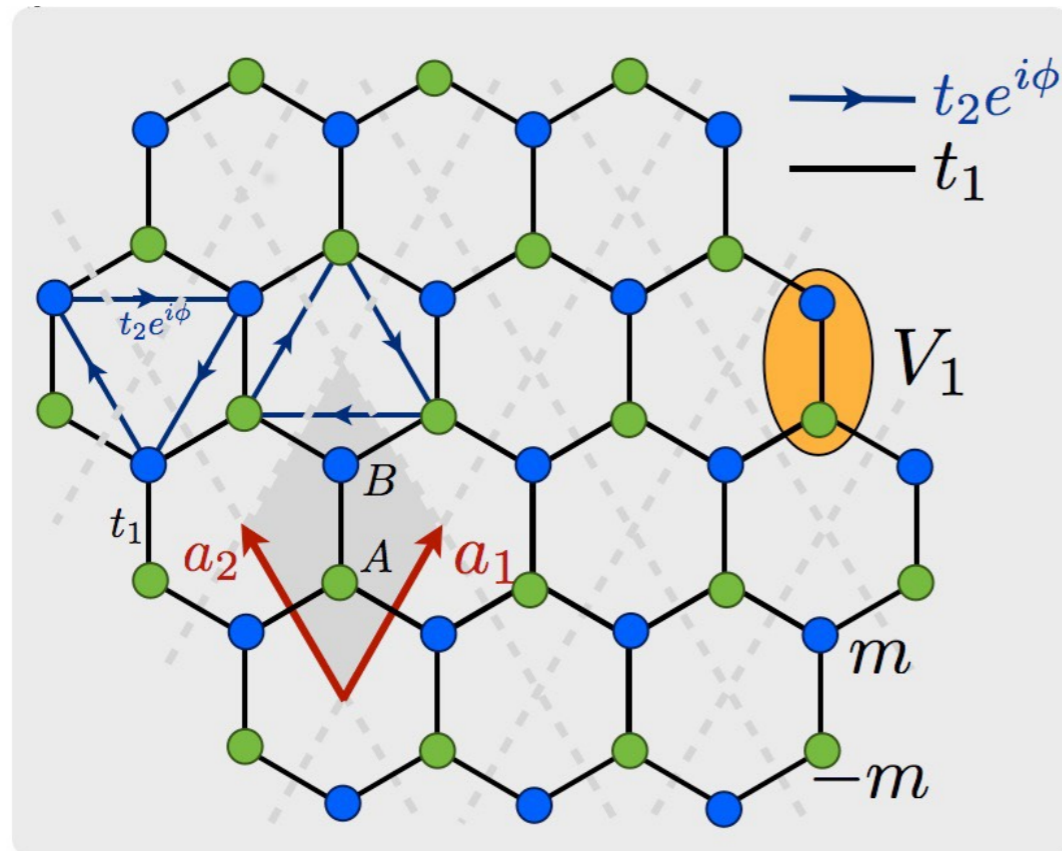


Topological Phases of Matter

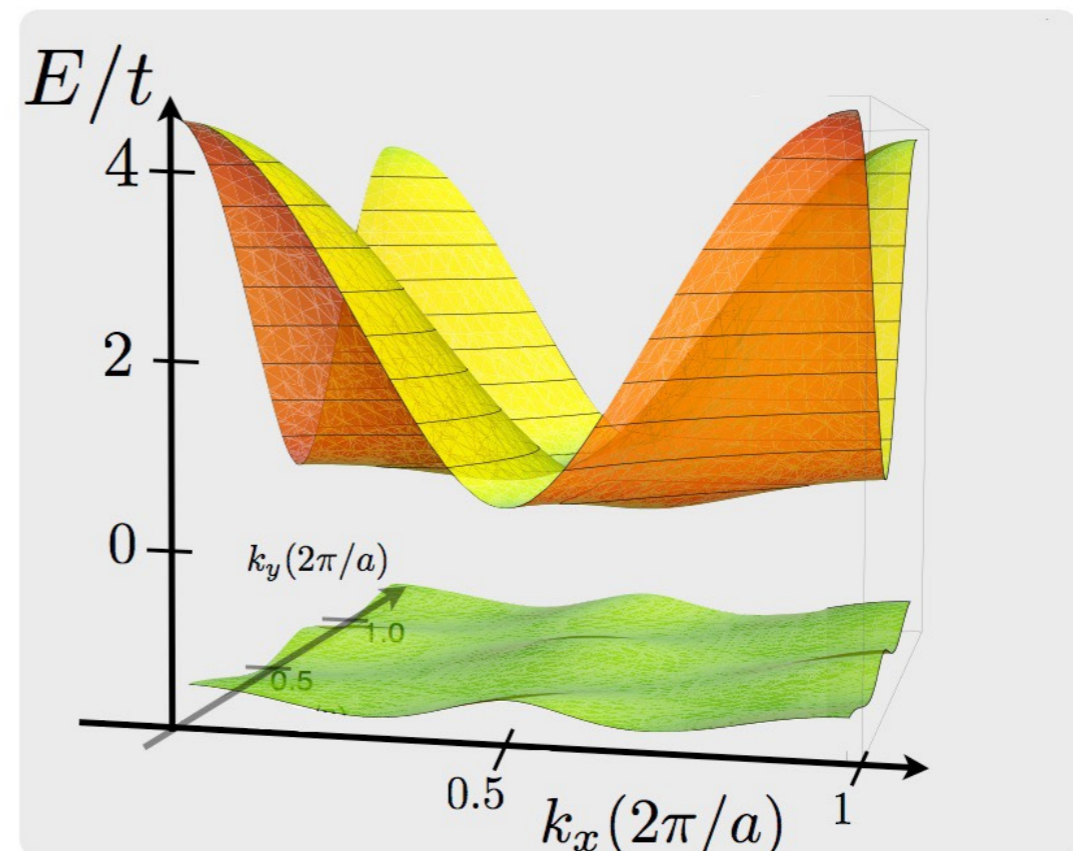


All phases can be identified using DMRG!

(Fractional) Chern Insulators



[Haldane '88]



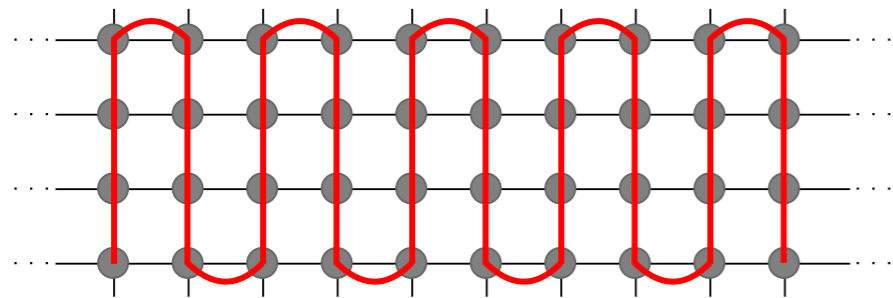
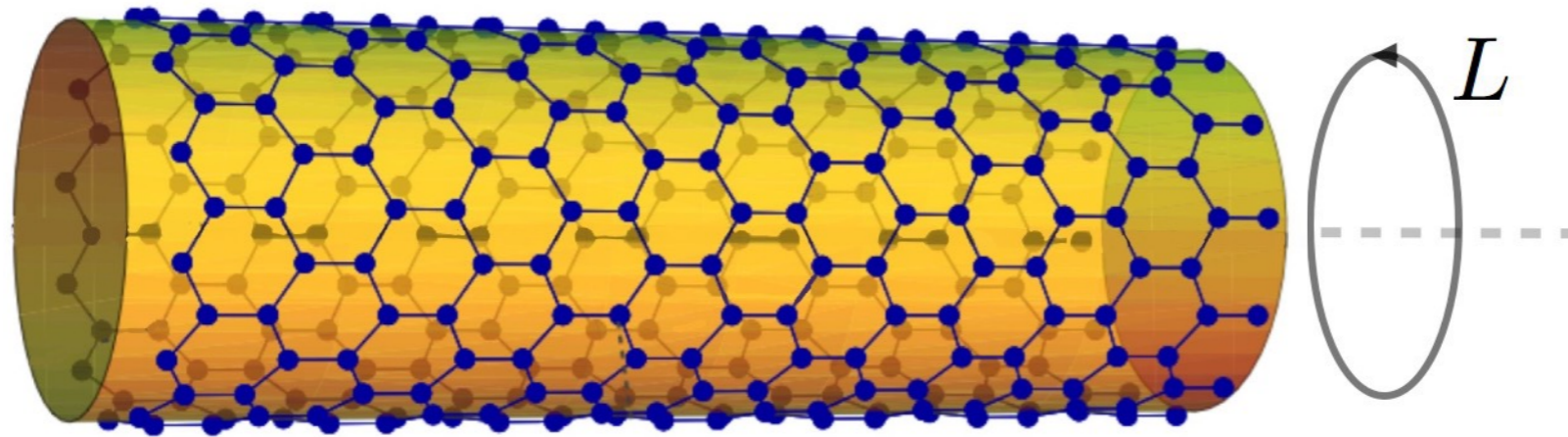
D. Sheng, Z.-C. Gu, K. Sun, and L. Shen '11
 N. Regnault and B.A. Bernevig '11
 S. Kourtis, T. Neupert, C. Chamon, and C. Mudry, '12
 S. Kourtis, J.W.F. Venderbos, and M. Daghofer '13

Chern Insulator ($\nu = 1$): Lattice version of the Integer Quantum Hall Effect

Fractional Chern Insulator (e.g., $\nu = 1/3$): Interactions are important!

DMRG for 2D Systems

DMRG on cylinders with circumference up to $L = 12$



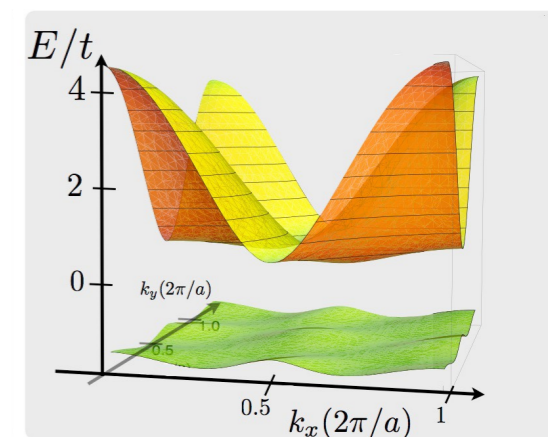
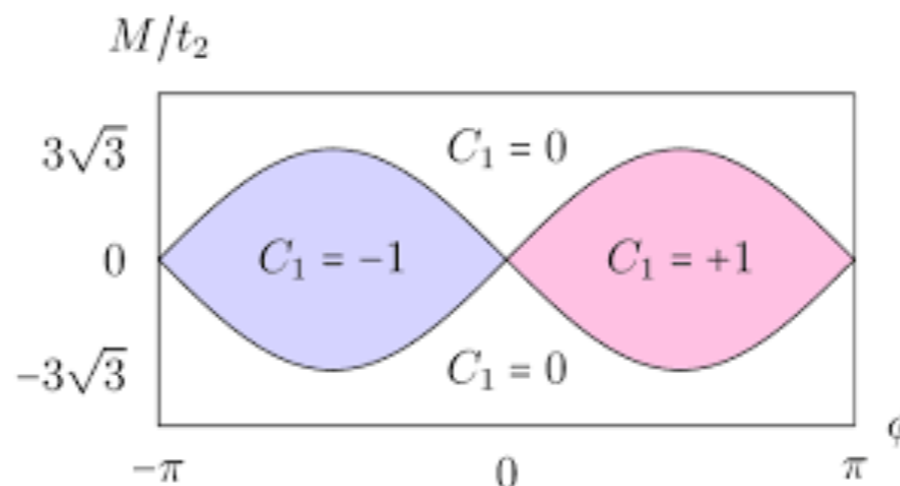
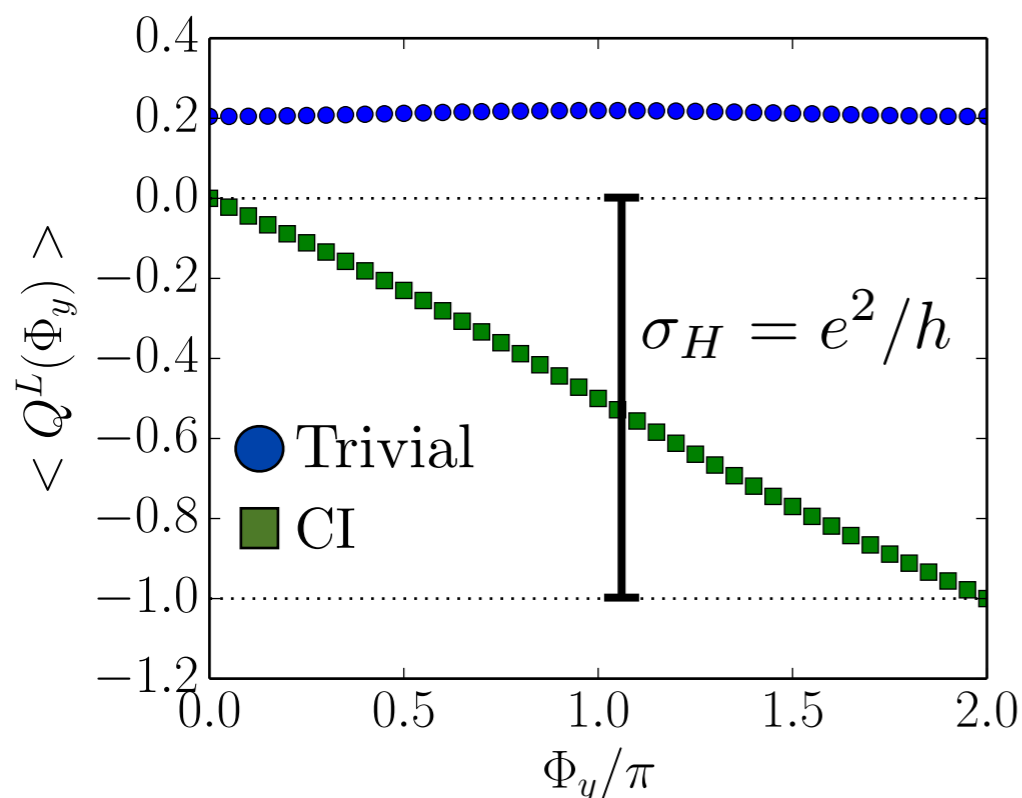
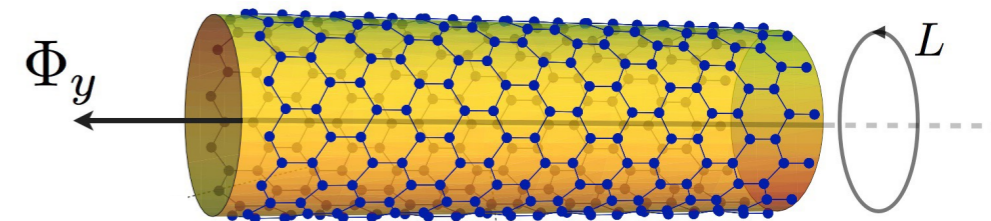
2D physics at cost of long range interaction in 1D representation!

- ▶ MPO representation of the Hamiltonian (bond dimension scales **polynomially** with L)
- ▶ Area law: MPS dimensions of the ground state grows **exponentially** with L !

Chern Insulators

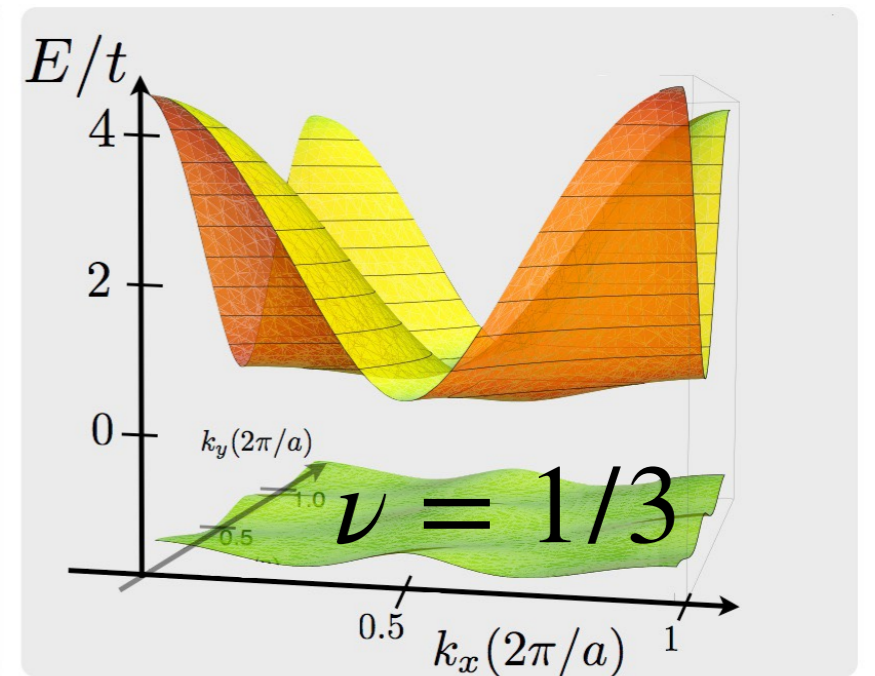
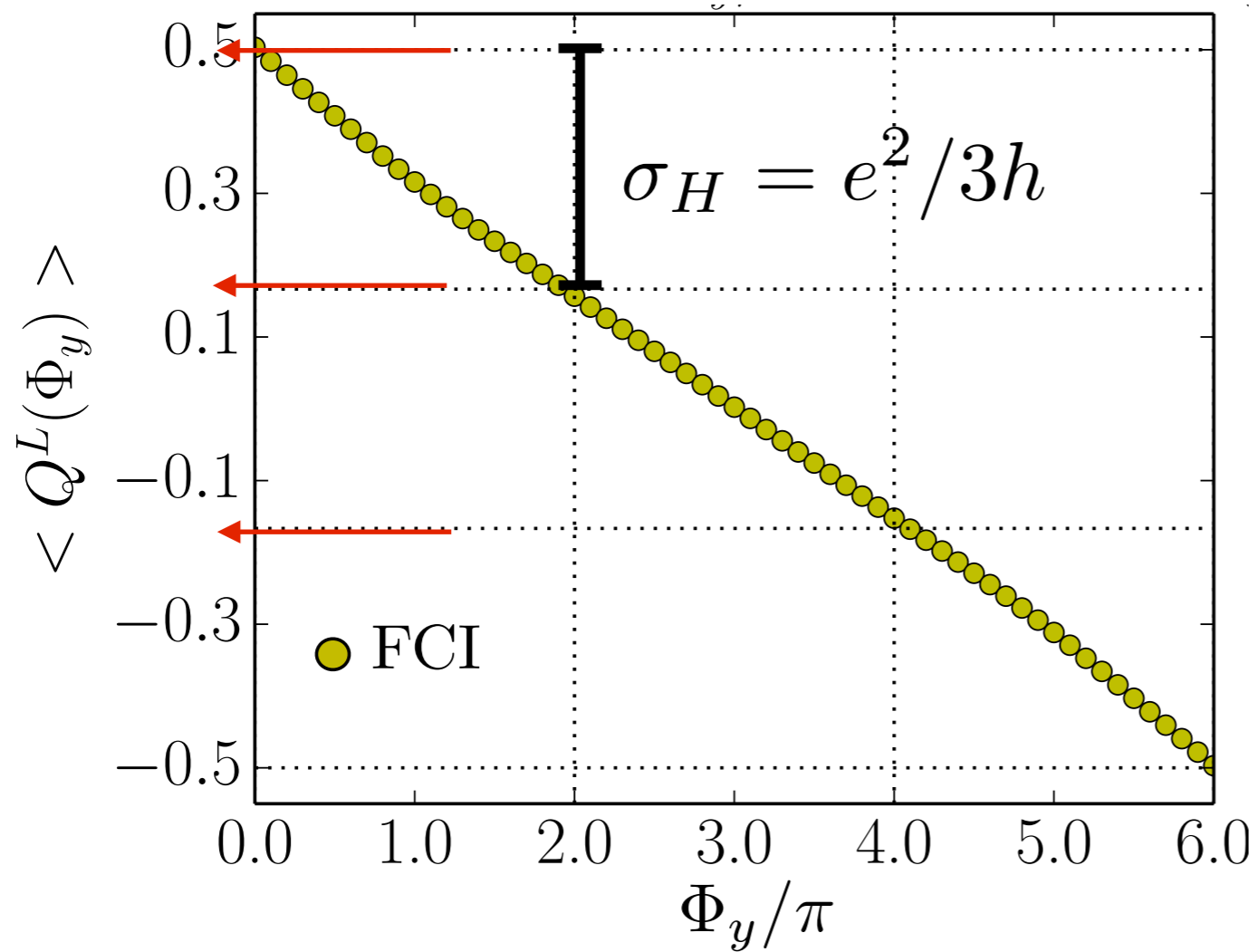
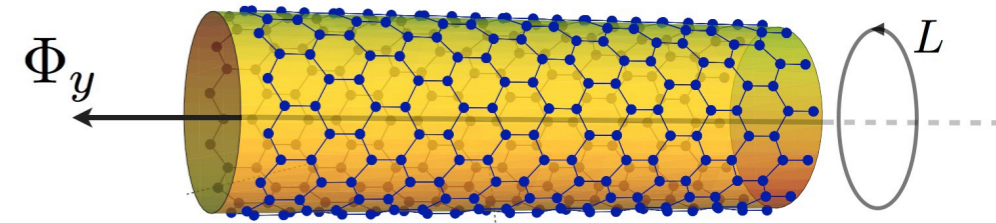
Laughlin charge pump

- ▶ Generate flux ϕ_y using complex hopping at the boundary
- ▶ Start from $\phi_y = 0$ and adiabatically insert a flux 2π
- ▶ Measure the charge pumped from left to right



Fractional Chern Insulators

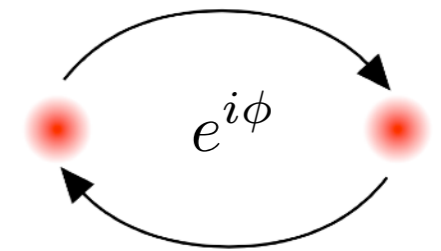
Laughlin charge pump



Fractional Chern Insulators: Top. Entanglement

Intrinsic topological order: Gapped quantum phases that are robust to any small (local) perturbation

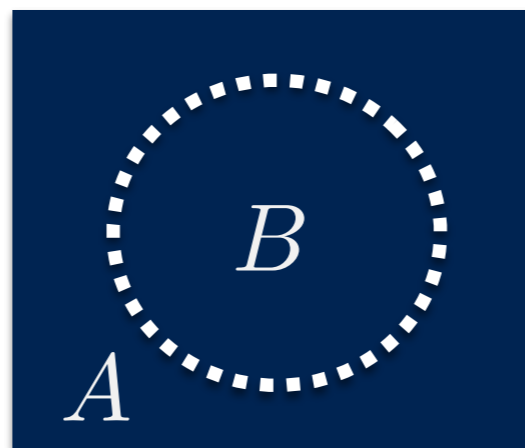
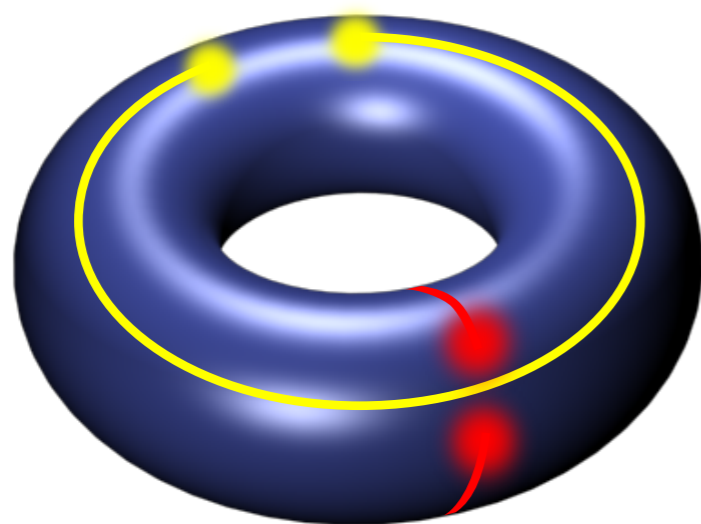
Characterized by quasiparticle excitations that obey **fractional statistics “anyons”** [Wen '90]



▶ Topological degeneracy on torus/cylinder (= number of anyons)

▶ Topological entanglement entropy $\gamma : S = \alpha L - \gamma$

[Kitaev and Preskill '06, Levin and Wen '06]



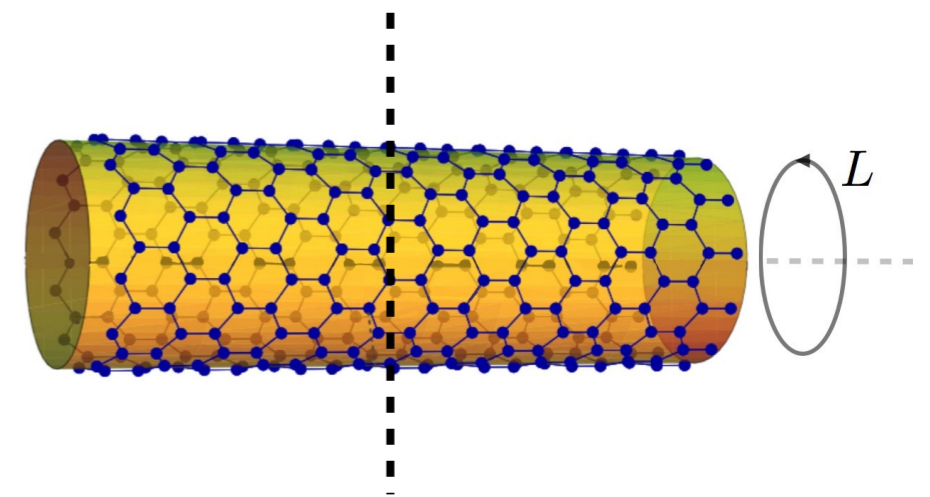
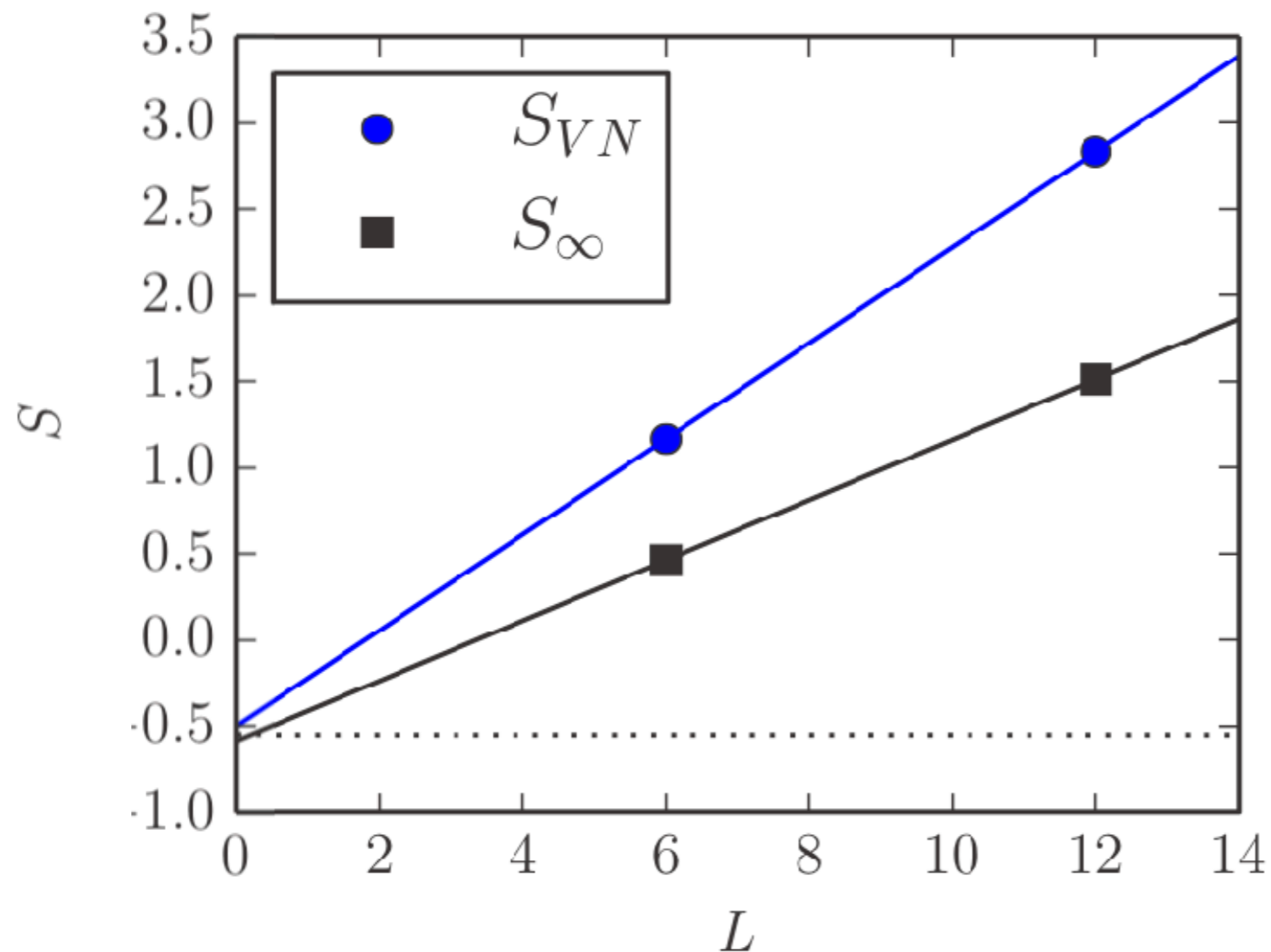
$$|\psi\rangle = \sum_{\alpha} \sqrt{p_{\alpha}} |\phi_{\alpha}^A\rangle |\phi_{\alpha}^B\rangle$$

$$S = - \sum_{\alpha} p_{\alpha} \log p_{\alpha}$$

$$\text{Abelian: } \gamma = \log(\sqrt{\#\text{anyons}})$$

Fractional Chern Insulators: Top. Entanglement

Topological entanglement in the FCI phase

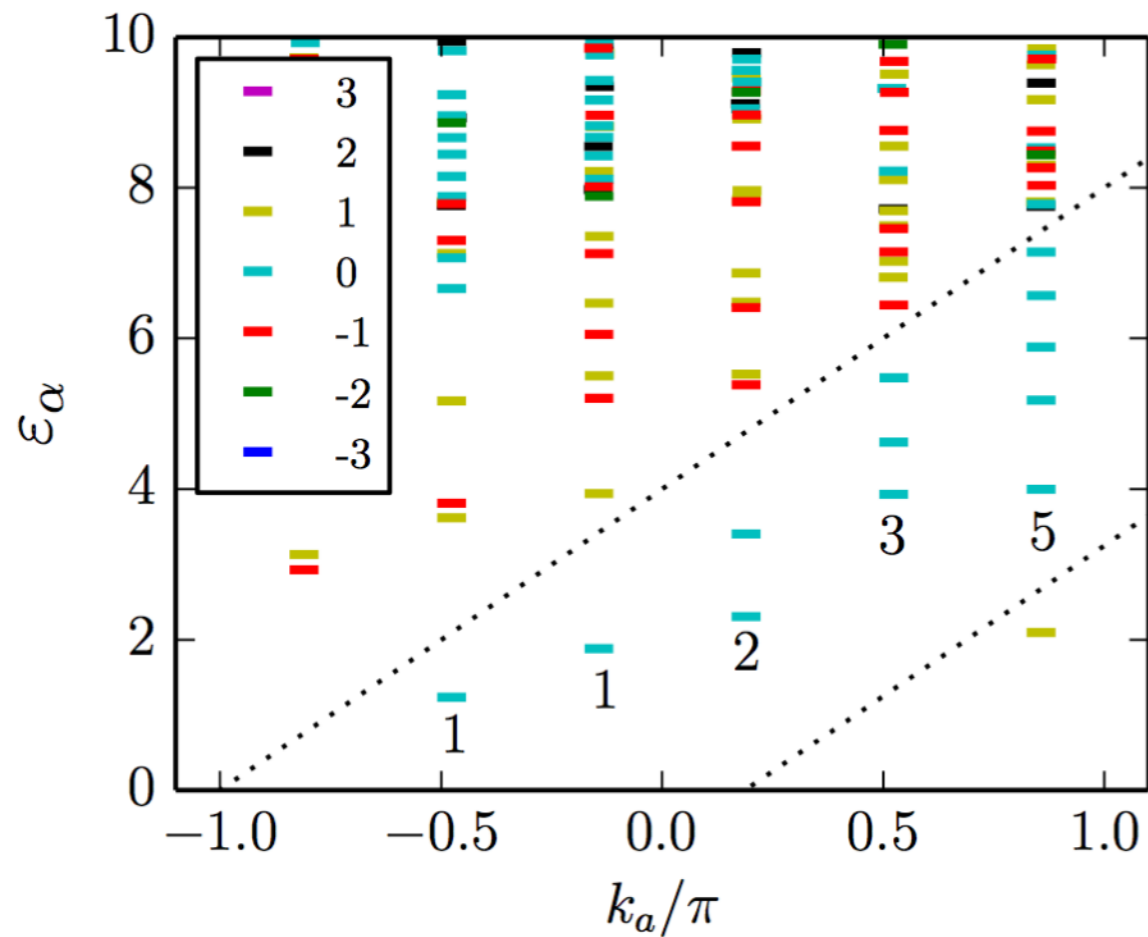


$$S = \alpha L - \gamma$$

$$\log \sqrt{3}$$

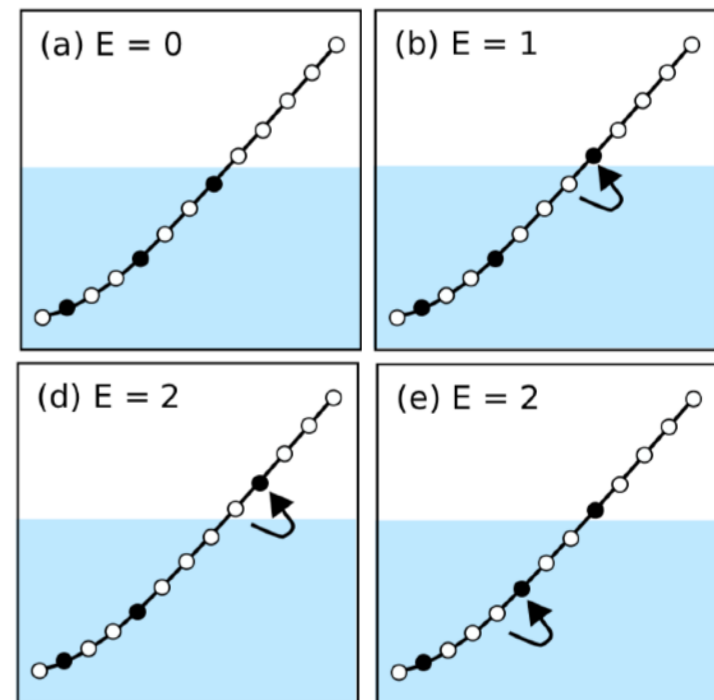
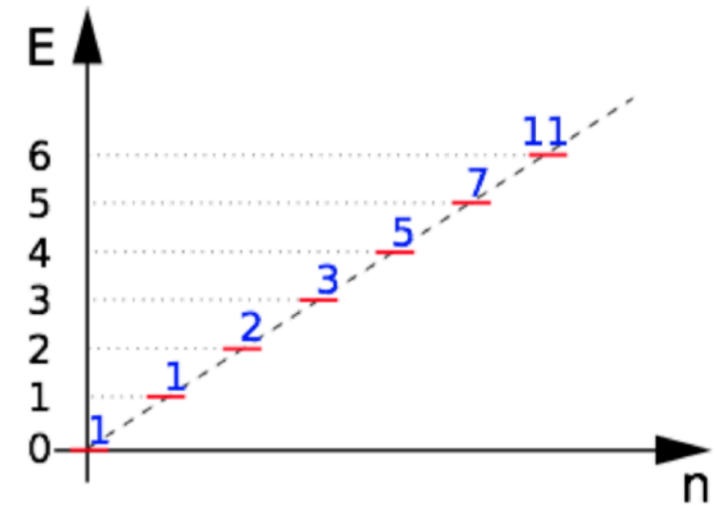
Fractional Chern Insulators: Chiral Edge States

Chiral edge states



[Li & Haldane '08]

$$\rho^{\text{red}} = \sum_{\alpha} \exp(-\epsilon_{\alpha}) |\phi_{\alpha}\rangle \langle \phi_{\alpha}|$$



Tutorial: (D) TeNPy Entanglement Spectrum

<http://go.tum.de/475840>

- I) Calculate the entanglement spectrum of the Haldane model. Can you get the right counting?
- II) Calculate the expectation value of the charge density operator and explore the regime of large interactions.

Tutorial: (E) TeNPy Laughlin Pump

<http://go.tum.de/475840>

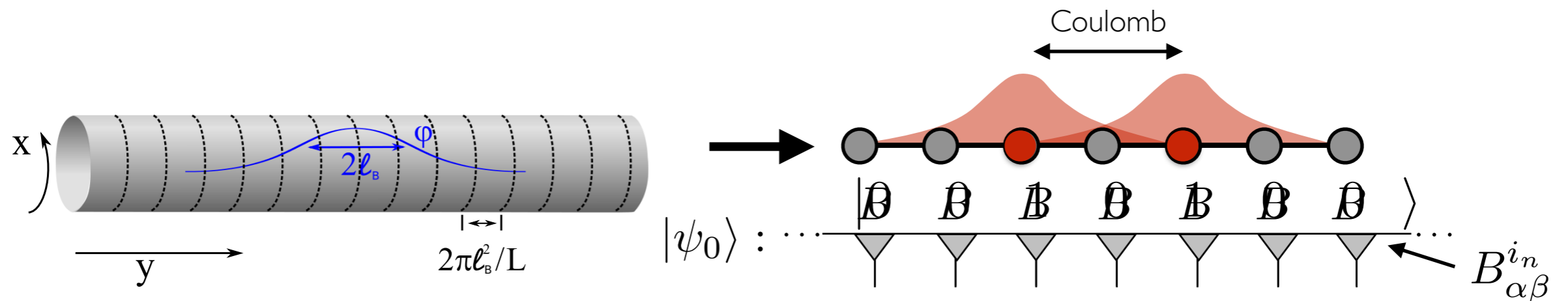
- I) Explore a few points in the phase diagram of the Haldane using the Laughlin pump.
- II) Open ended: Can you find parameters to stabilize an FCI?

Fractional Quantum Hall

Density Matrix Renormalization Group
to simulate FQHE on infinite cylinders

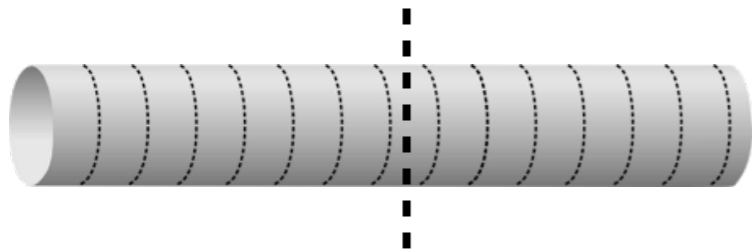
Orbitals in first Landau level are localized along
the cylinder: **Quasi 1D model**

[Tao & Taoless 88, Haldane & Rezayi '94; Bergholtz et al. '05, Seidel et al. '05]

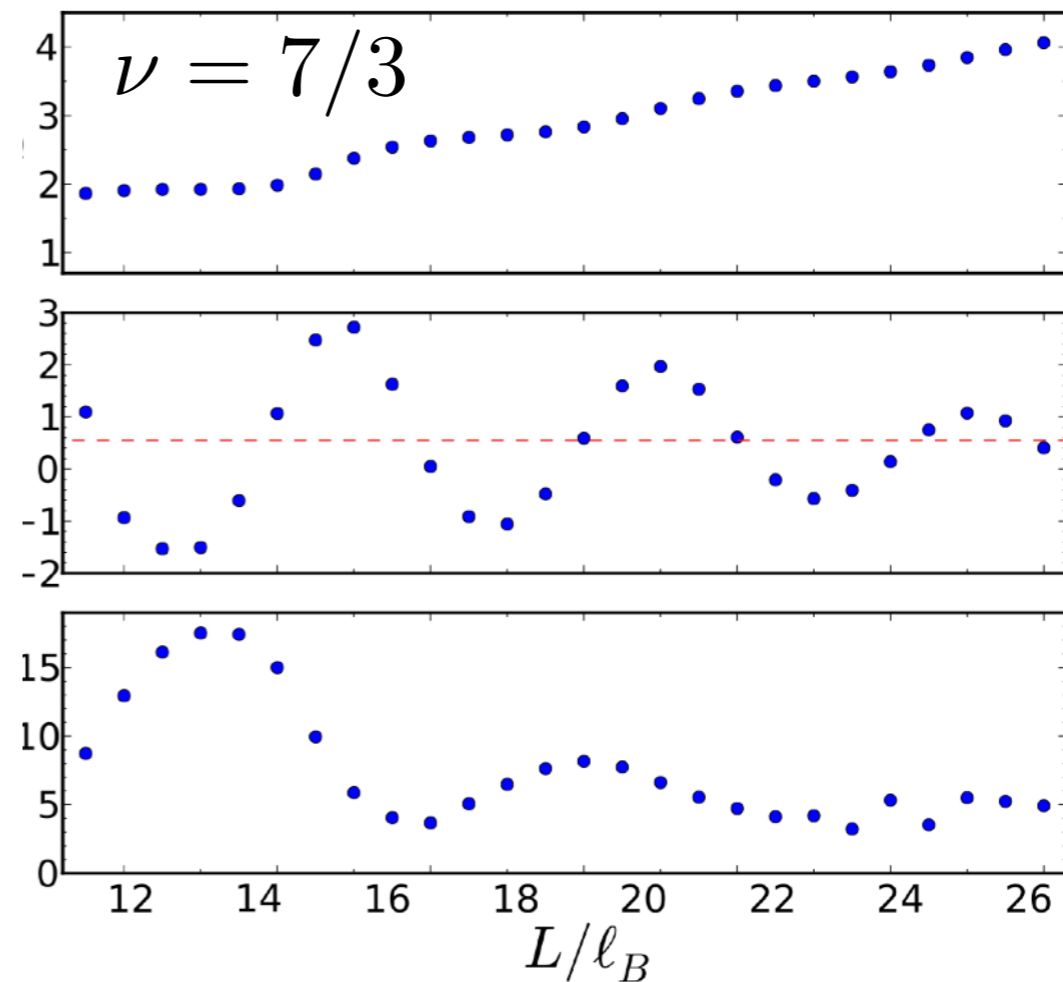
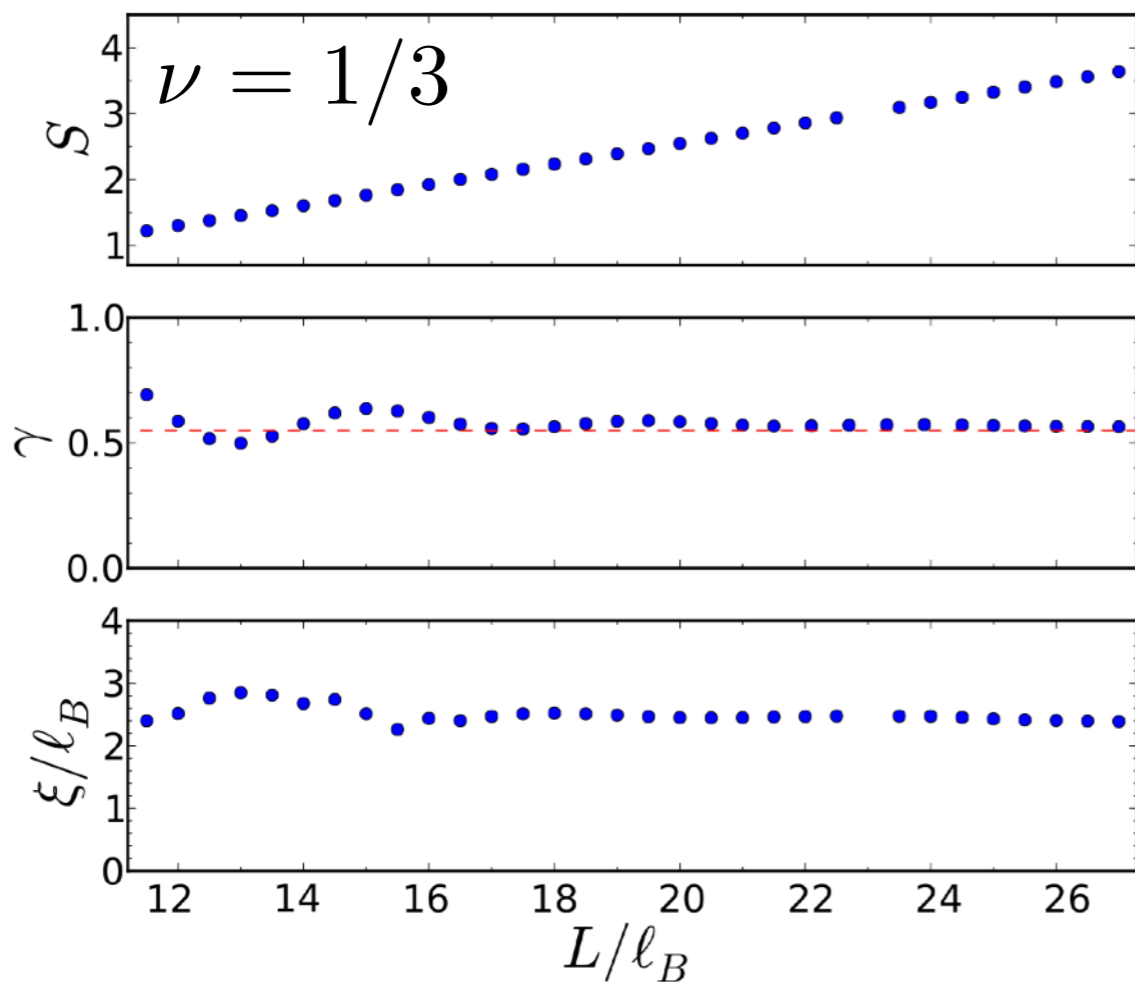


Fractional Quantum Hall

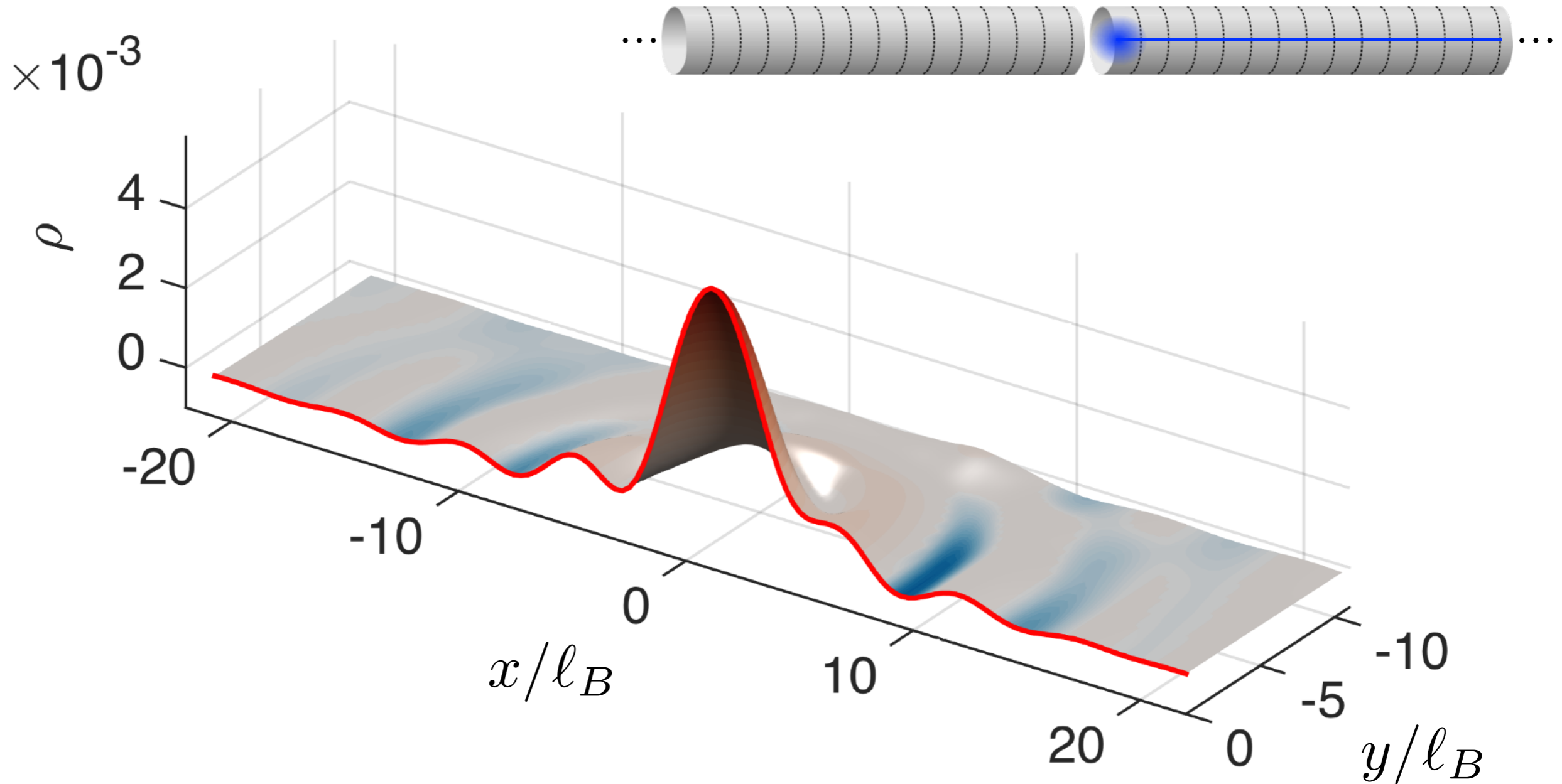
Topological entanglement entropy of the FQHE with Coulomb interactions (“minimally entangled states”)



$$S = \alpha L - \gamma$$



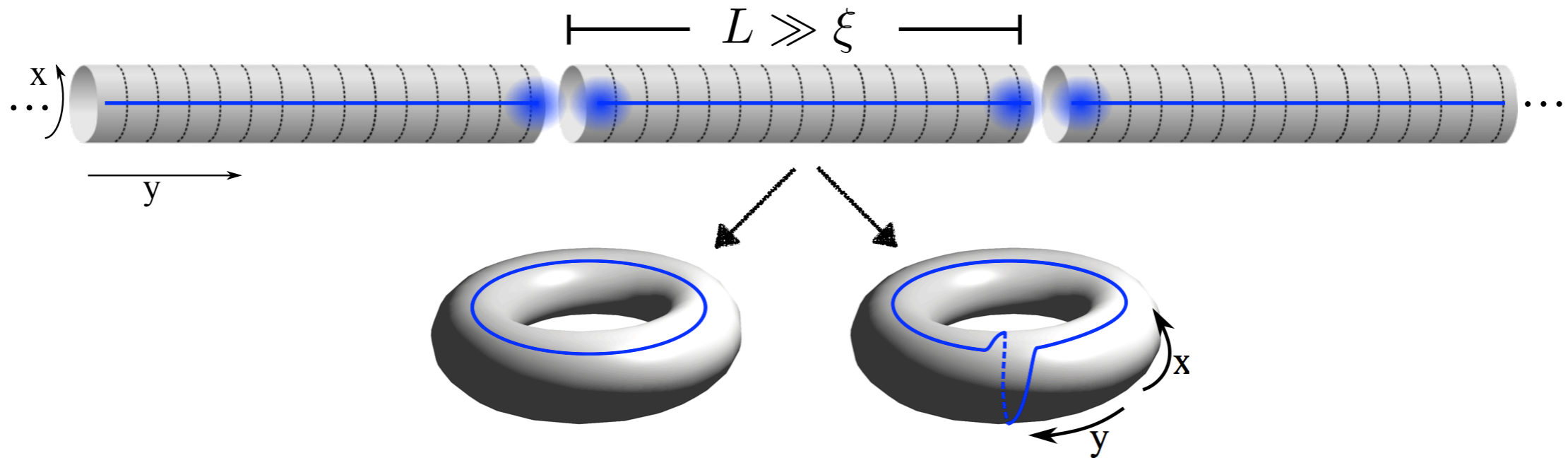
Fractional Quantum Hall



Density profile for Fibonacci anyons with charge $e/5$

Fractional Quantum Hall

Extracting topological content by adding a “twist”



Momentum polarization: **topological spin,**
central charge, Hall viscosity

$$U_{T;ab} = \delta_{ab} \exp \left[2\pi i \left(h_a - \frac{c}{24} - \frac{\eta_H}{2\pi\hbar} L_x^2 \right) \right]$$

Tensor Networks and the Many-Body Problem

- I) Entanglement and Matrix-Product States
- II) Time Evolving Block Decimation
- III) Density-Matrix Renormalization Group
- IV) Extracting topological invariants
- V) (isometric Tensor-Network States)



Matrix-Product States

Matrix-product states (MPS): Reduction of the number of variables: $d^L \rightarrow Ld\chi^2$ [M. Fannes et al. 92]

$$\psi_{j_1, j_2, j_3, j_4, j_5} = \begin{array}{c} M^{[1]} \quad M^{[2]} \quad M^{[3]} \quad M^{[4]} \quad M^{[5]} \\ \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \\ | \quad | \quad | \quad | \quad | \end{array} \quad \begin{array}{l} M^j_{\alpha, \beta} = \alpha \text{---} \bullet \text{---} \beta \\ | \\ j \\ \alpha, \beta = 1 \dots \chi \\ j = 1 \dots d \end{array}$$

Canonical form: Use the gauge degree of freedom ($A^j = XM^jX^{-1}$) to find a convenient representation

$$\begin{array}{c} A^{[1]} \quad A^{[2]} \quad \Lambda^{[3]} \quad B^{[4]} \quad B^{[5]} \\ \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \\ | \quad | \quad | \quad | \quad | \end{array} \quad \begin{array}{c} \Lambda \Gamma \\ \overbrace{A} \\ \left[\begin{array}{c} \bullet \text{---} \bullet \\ | \\ \bullet \text{---} \bullet \end{array} \right] = \mathbb{1} \\ A^* \end{array} \quad \begin{array}{c} \Gamma \Lambda \\ \overbrace{B} \\ \left[\begin{array}{c} \bullet \text{---} \bullet \\ | \\ \bullet \text{---} \bullet \end{array} \right] = \mathbb{1} \\ B^* \end{array} \quad (\text{Isometries})$$

Center matrix Λ represents wave function

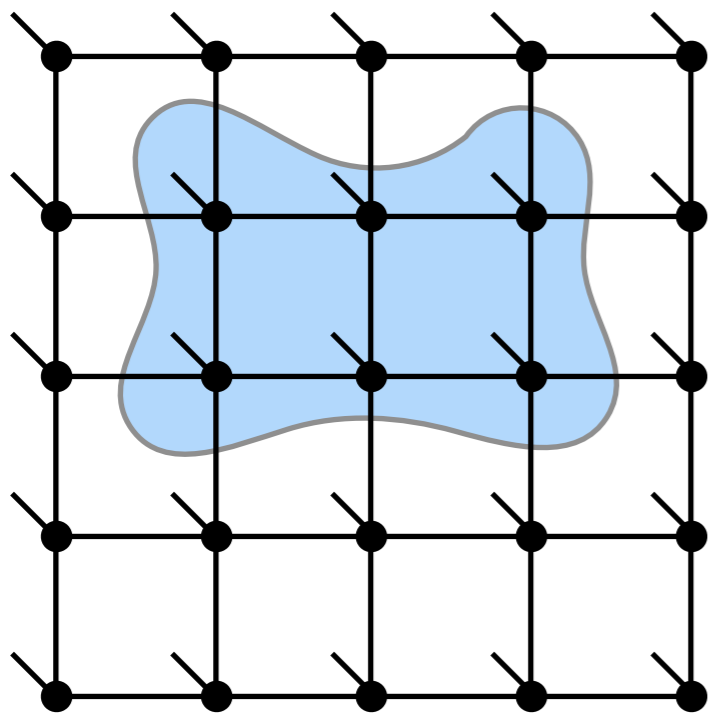
$$|\psi\rangle = \sum_{\alpha, \beta, j} \Lambda^j_{\alpha, \beta} |\alpha\rangle |j\rangle |\beta\rangle \quad (\text{orthogonal states } |j\rangle, |\alpha\rangle, |\beta\rangle)$$

Tensor Network States in 2D

MPS capture 1D area law \rightarrow Exponential scaling in 2D

$$\psi_{j_1, j_2, j_3, j_4, j_5} \approx \begin{array}{c} M^{[1]} \quad M^{[2]} \quad M^{[3]} \quad M^{[4]} \quad M^{[5]} \\ \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \text{---} \bullet \\ | \quad | \quad | \quad | \quad | \end{array}$$

How to generalize the MPS approach to 2D?



$$T_{\alpha, \beta, \gamma, \delta}^j = \begin{array}{c} \diagup \\ \bullet \\ \diagdown \\ | \\ \text{---} \end{array}$$

- ▶ **Tensor Network States (TNS)**

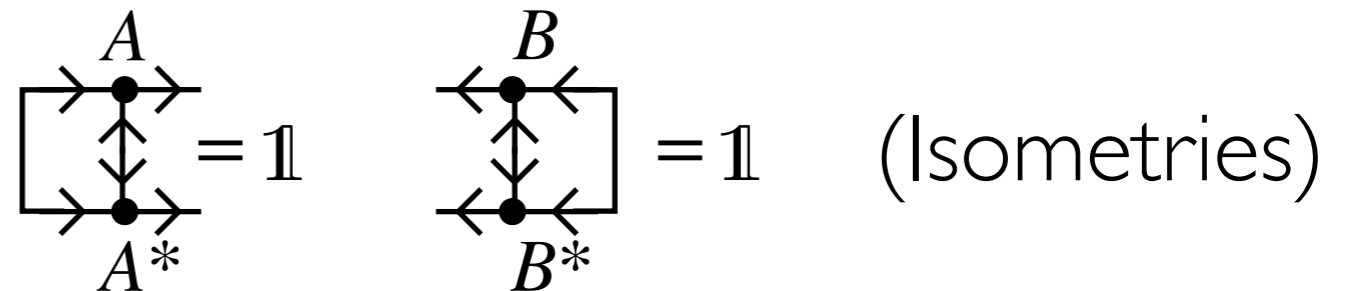
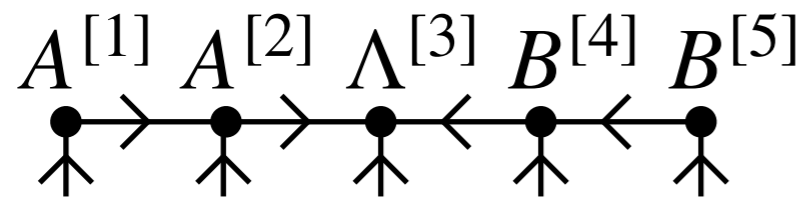
[Maeshima et al. '01, Verstraete and Cirac '04]

- ▶ **Capture 2D area law*** 😊

- ▶ Difficult to handle numerically:
Exact contraction of the 2D network
is still **exponentially hard** 😞

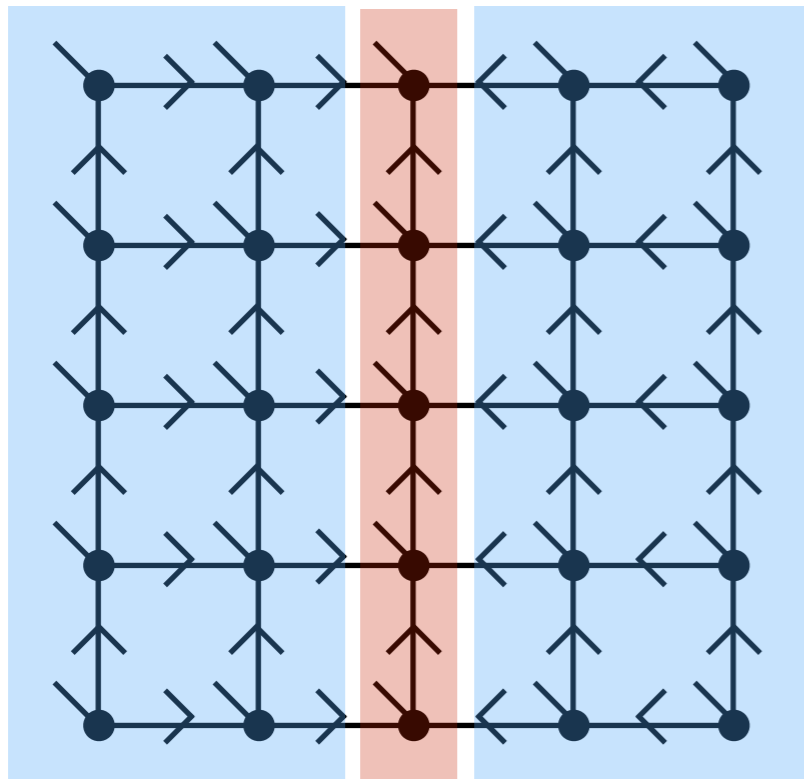
Isometric Tensor Network States in 2D

Recall: **Canonical form of 1D MPS**



Isometric TNS

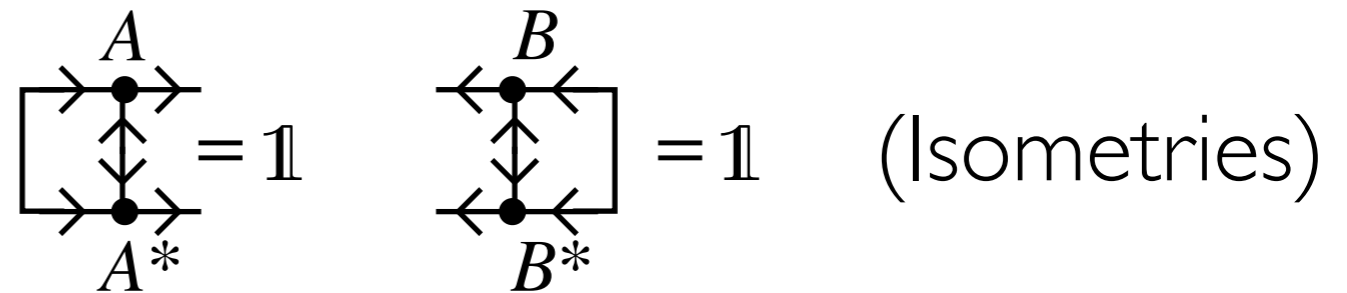
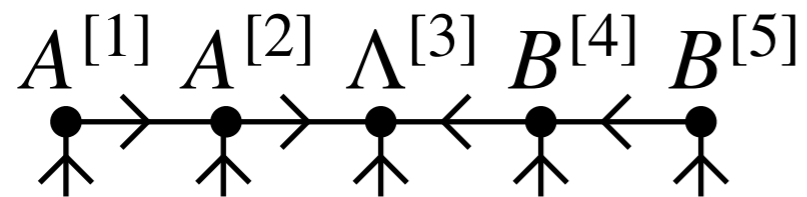
$A^{[1]} A^{[2]} \Lambda^{[3]} B^{[4]} B^{[5]}$



- ▶ Isometric tensors are **efficiently contractable**
- ▶ Orthogonality center column is a **1D MPS**: Standard DMRG techniques
- ▶ Subset of TNS: Unclear what its variational power is!

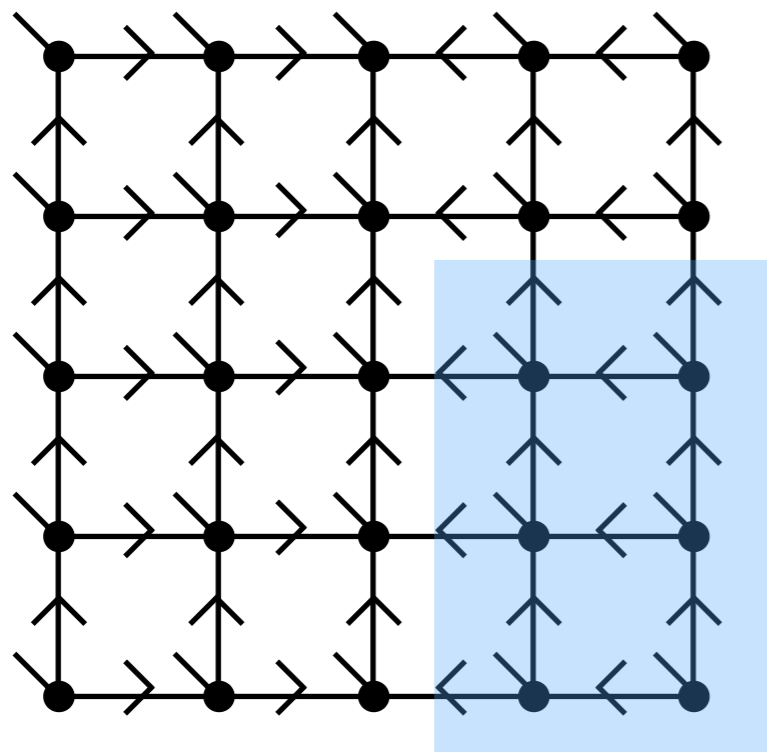
Isometric Tensor Network States in 2D

Recall: **Canonical form of 1D MPS**



Isometric TNS

$A^{[1]} A^{[2]} \Lambda^{[3]} B^{[4]} B^{[5]}$



- ▶ **Subregions** with only outgoing arrows have isometric boundary maps
- ▶ **Causal structure**: time flows opposite to the direction of the arrows

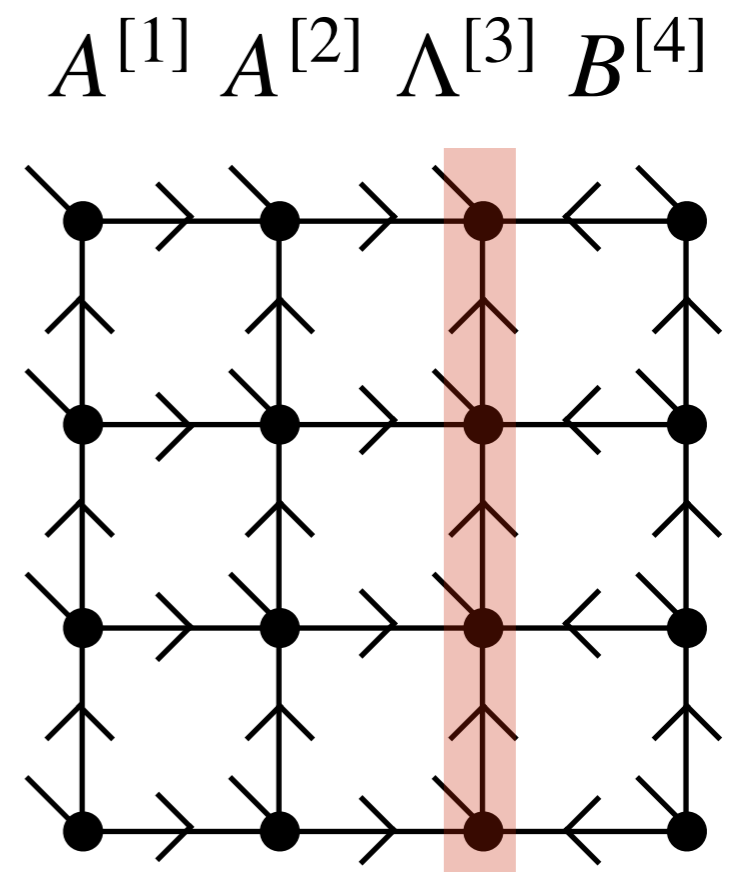
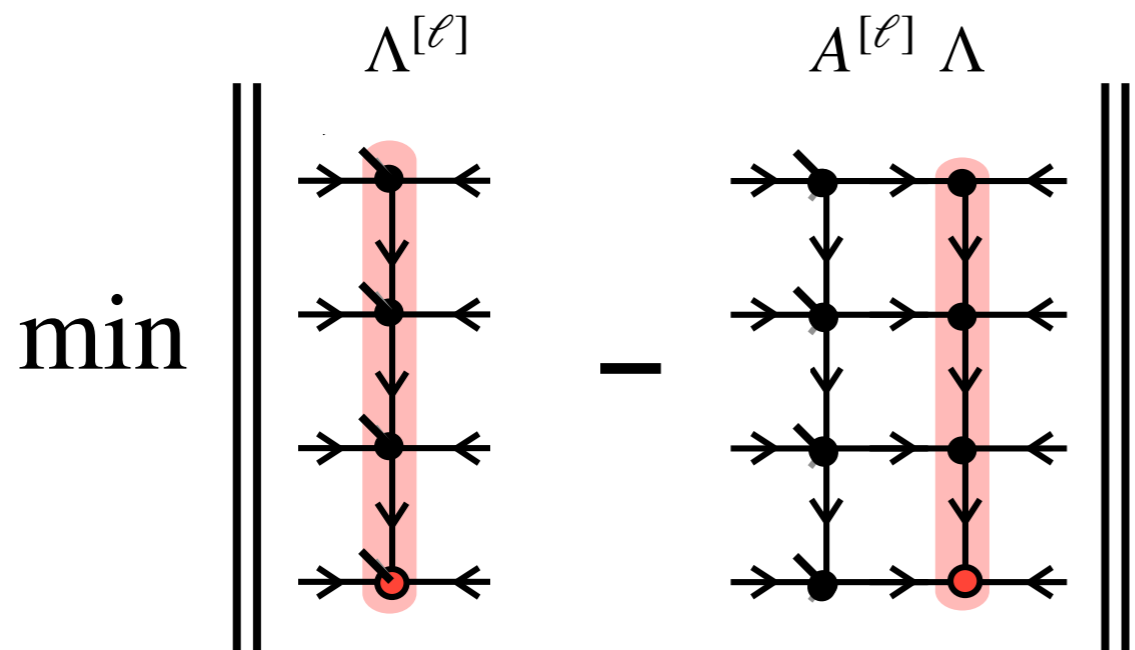
Isometric Tensor Network States in 2D

How to shift the orthogonality center?

Recall: **ID MPS** $\Lambda^\ell B^{[\ell+1]} = A^{[\ell]} \Lambda^{[\ell+1]}$ solved by QR or SVD

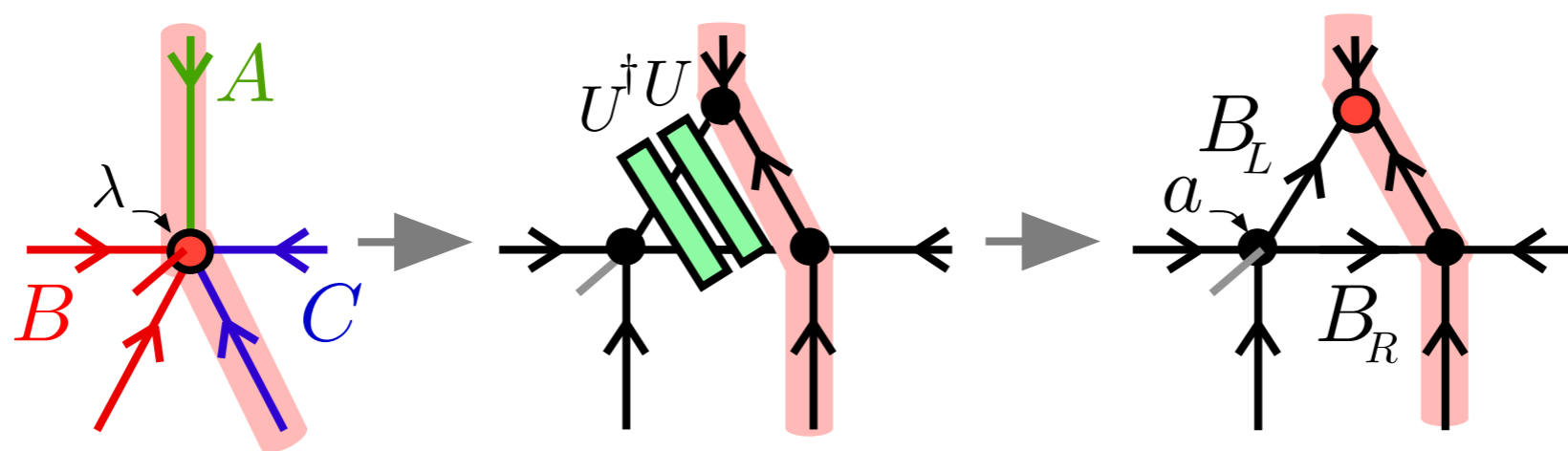
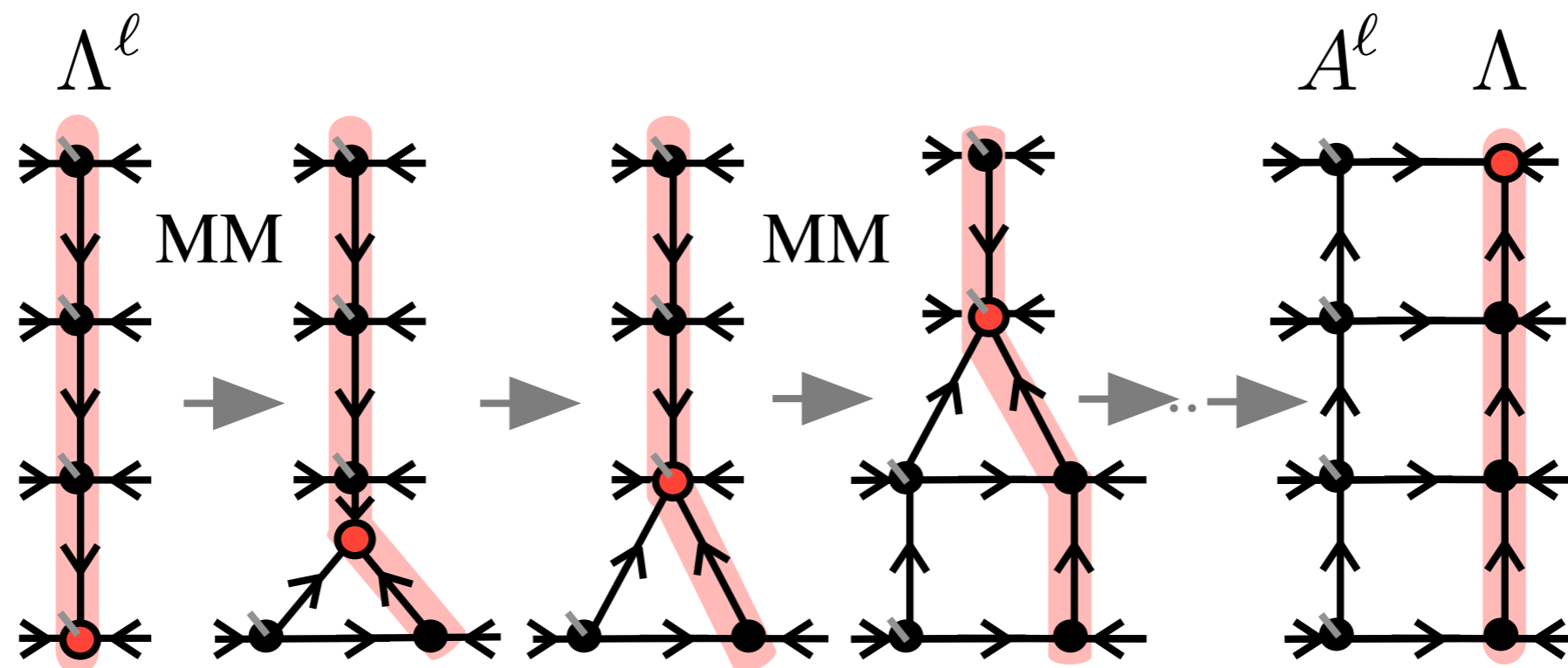
Not possible for 2D TNS as it would destroy the locality of Λ

Solve the variational problem:



Isometric Tensor Network States in 2D

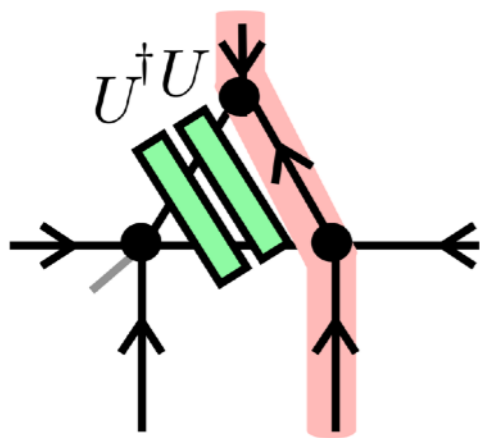
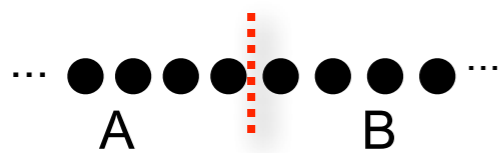
Sequential splitting based on disentangling: **“Moses Move” (MM)**



Finding the disentangler

Variationally disentangle the state: $S_2 = -\ln \text{Tr} \rho_{\text{red}}^2$.

minimize Renyi entropies

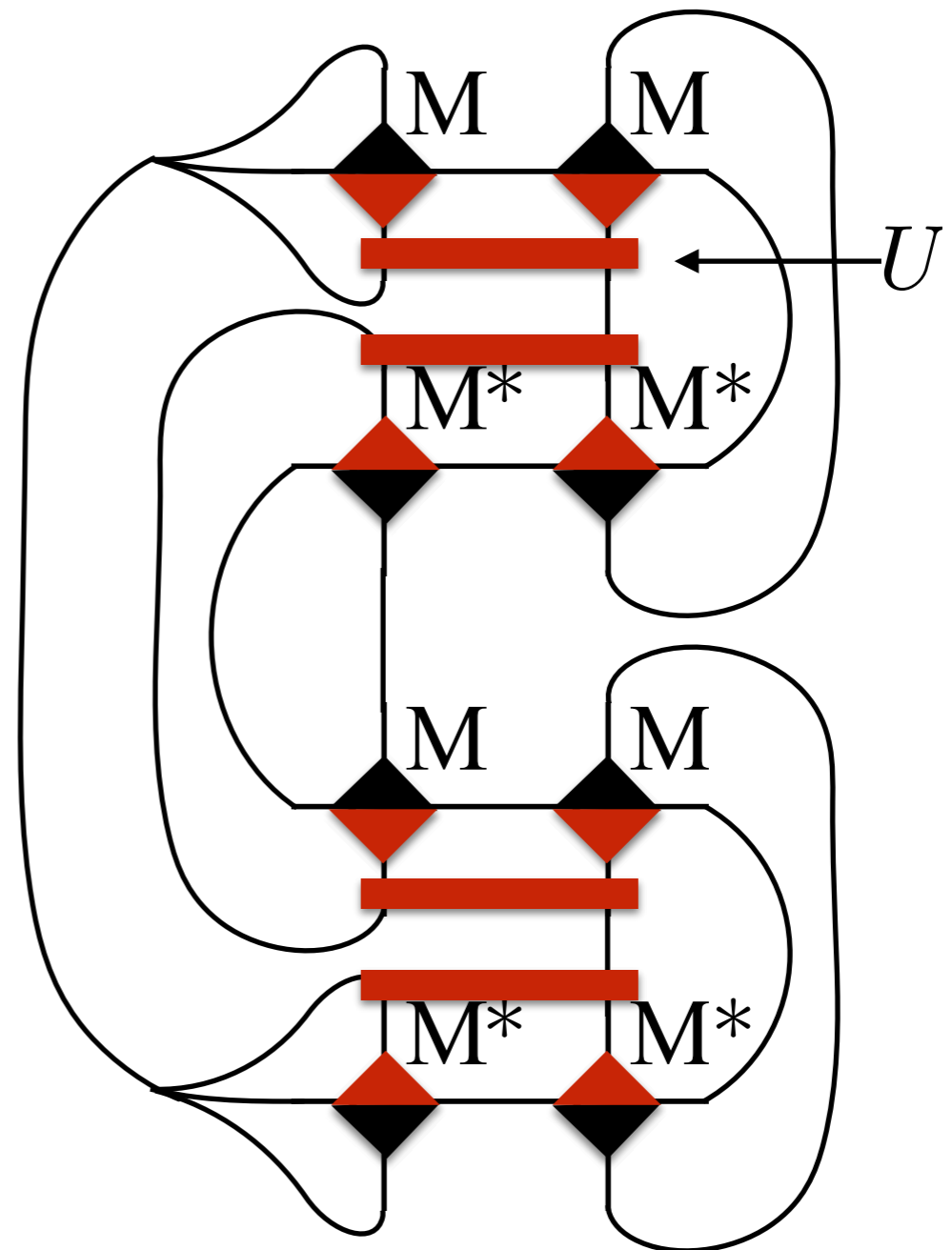


$|\tilde{\psi}\rangle :$

$\tilde{\rho}_{\text{red.}} :$

$\text{Tr} \tilde{\rho}_{\text{red.}}^2 :$

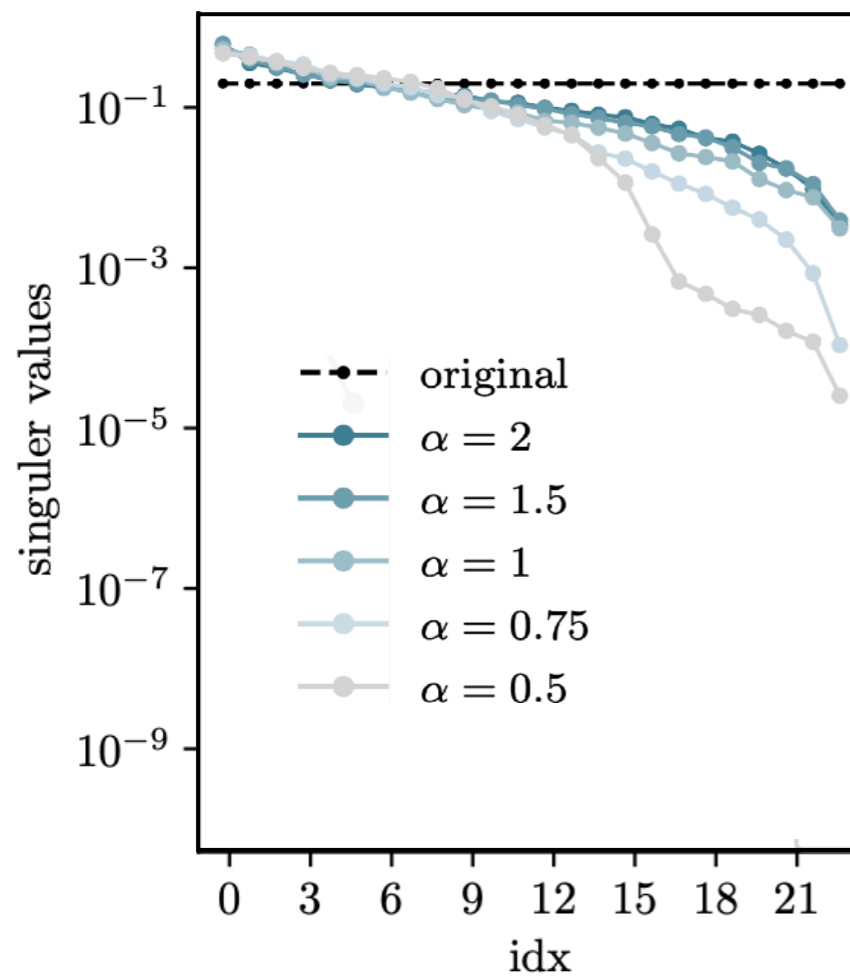
$\tilde{\rho}_{\text{red.}} :$



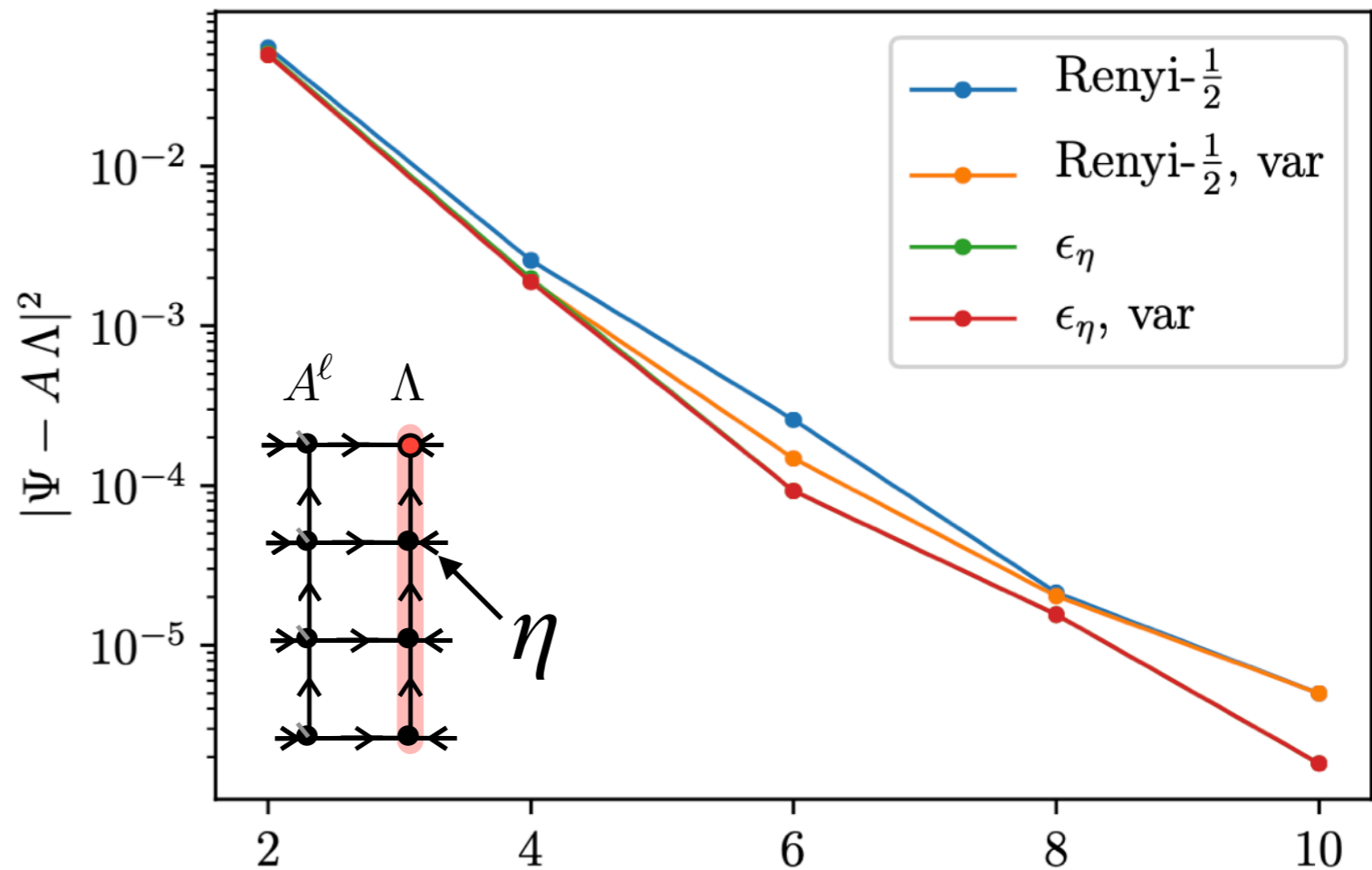
- ▶ Other Rényi entropies can also be minimized

Finding the disentangler

Role of the disentangler:

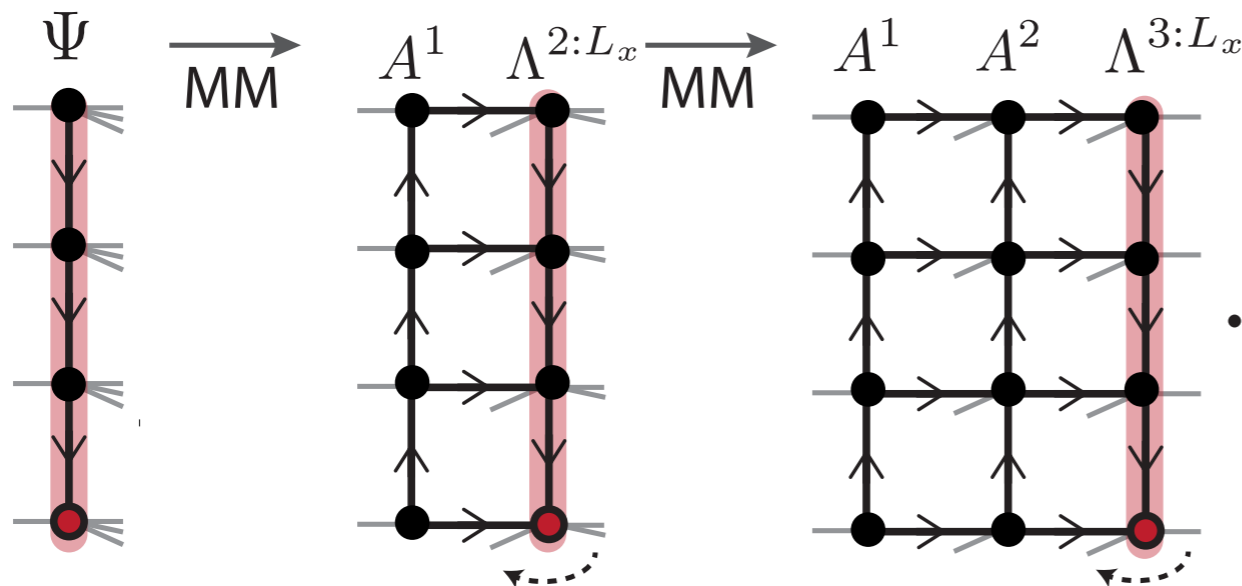


Variational vs. Moses Move:



Convert quasi 1D MPS to isometric TNS

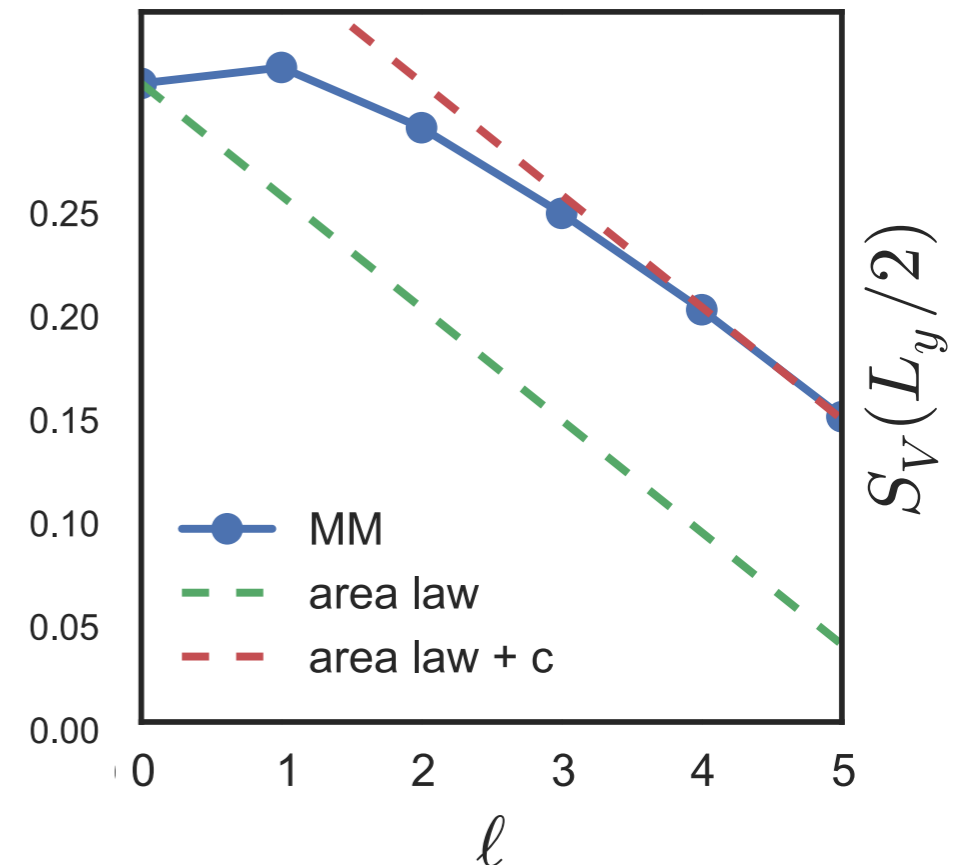
“Peel off” layers from MPS representation of 2D state



- ▶ **Sequentially disentangle the state**
- ▶ **Efficient compression**

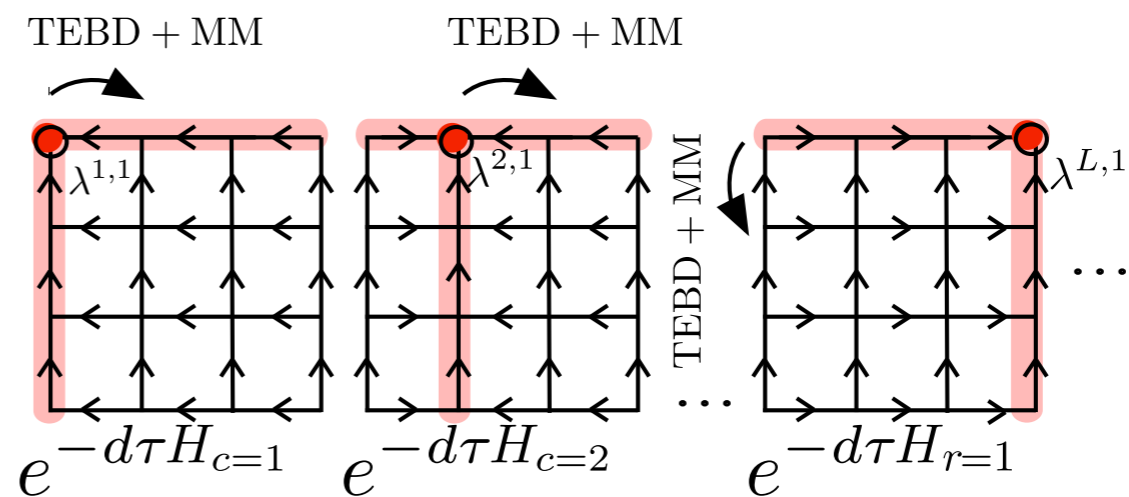
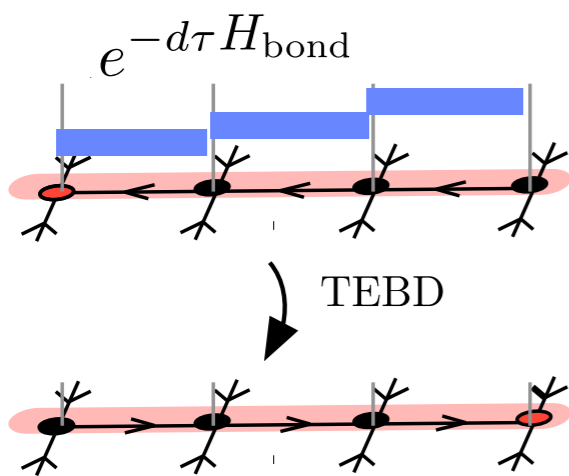
2D transverse field Ising Model ($g = 3.5$)

$$H = - \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - g \sum_i \sigma_i^x$$



(I) Time evolution of 2D Hamiltonians (TEBD²)

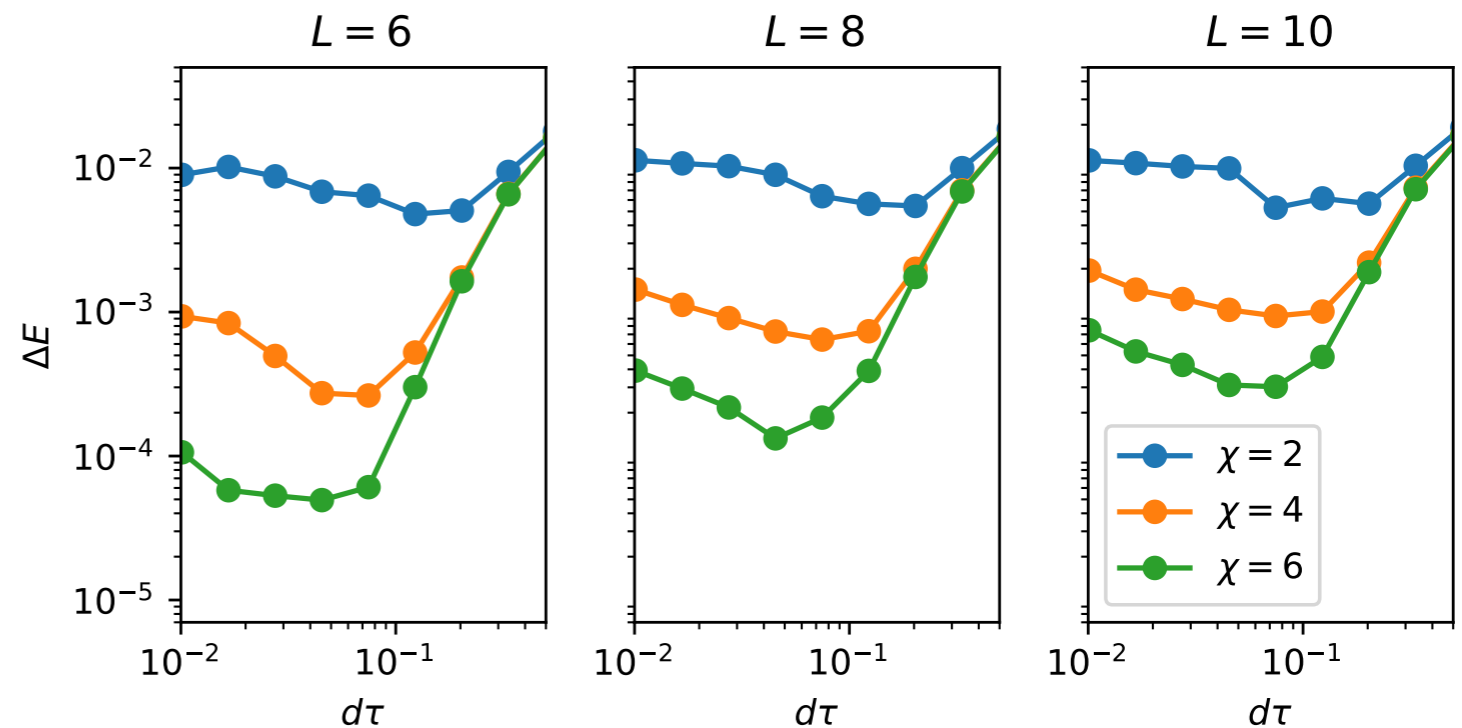
Sequentially apply **1D Time-Evolving Block Decimation (TEBD)** algorithm on the center columns/rows: 2nd order [Vidal '03]



2D transverse field Ising Model ($g = 3.5$)

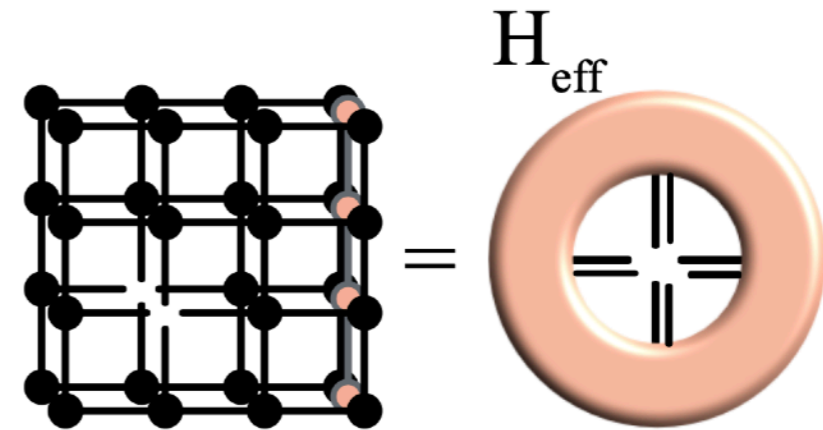
$$H = - \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - g \sum_i \sigma_i^x$$

Imaginary time evolution: $|\psi_0\rangle$



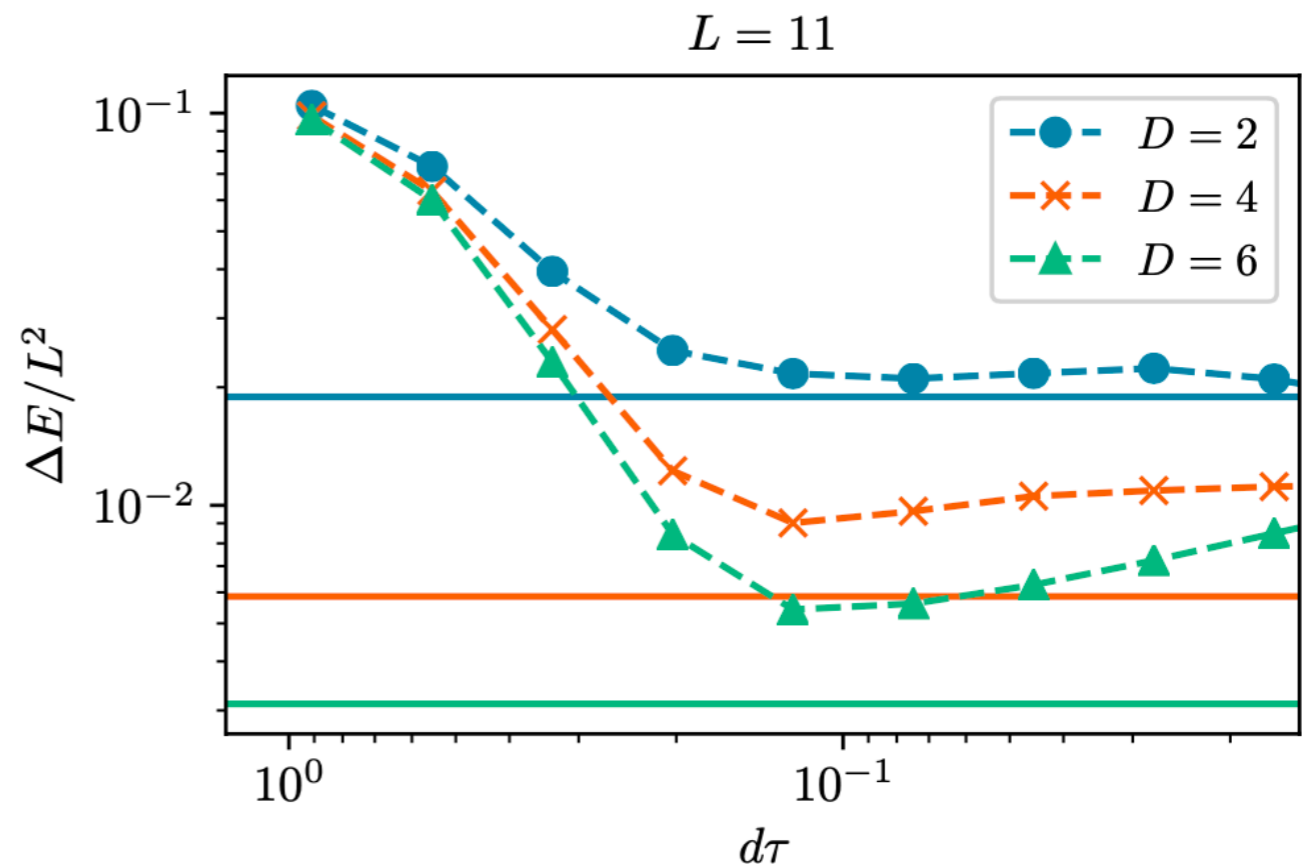
(II) Variational optimization (DMRG²)

Iteratively minimize the energy by sequentially optimizing the isometries



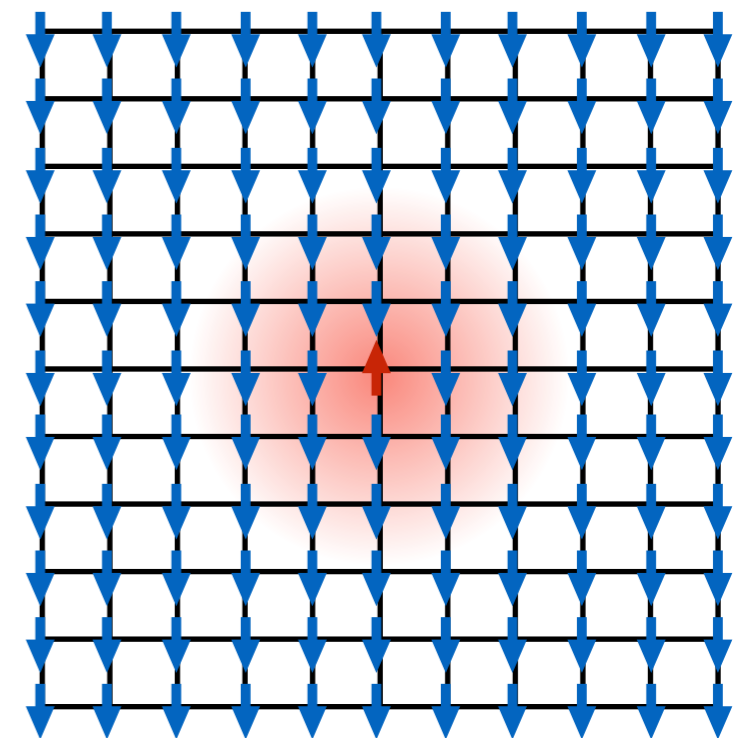
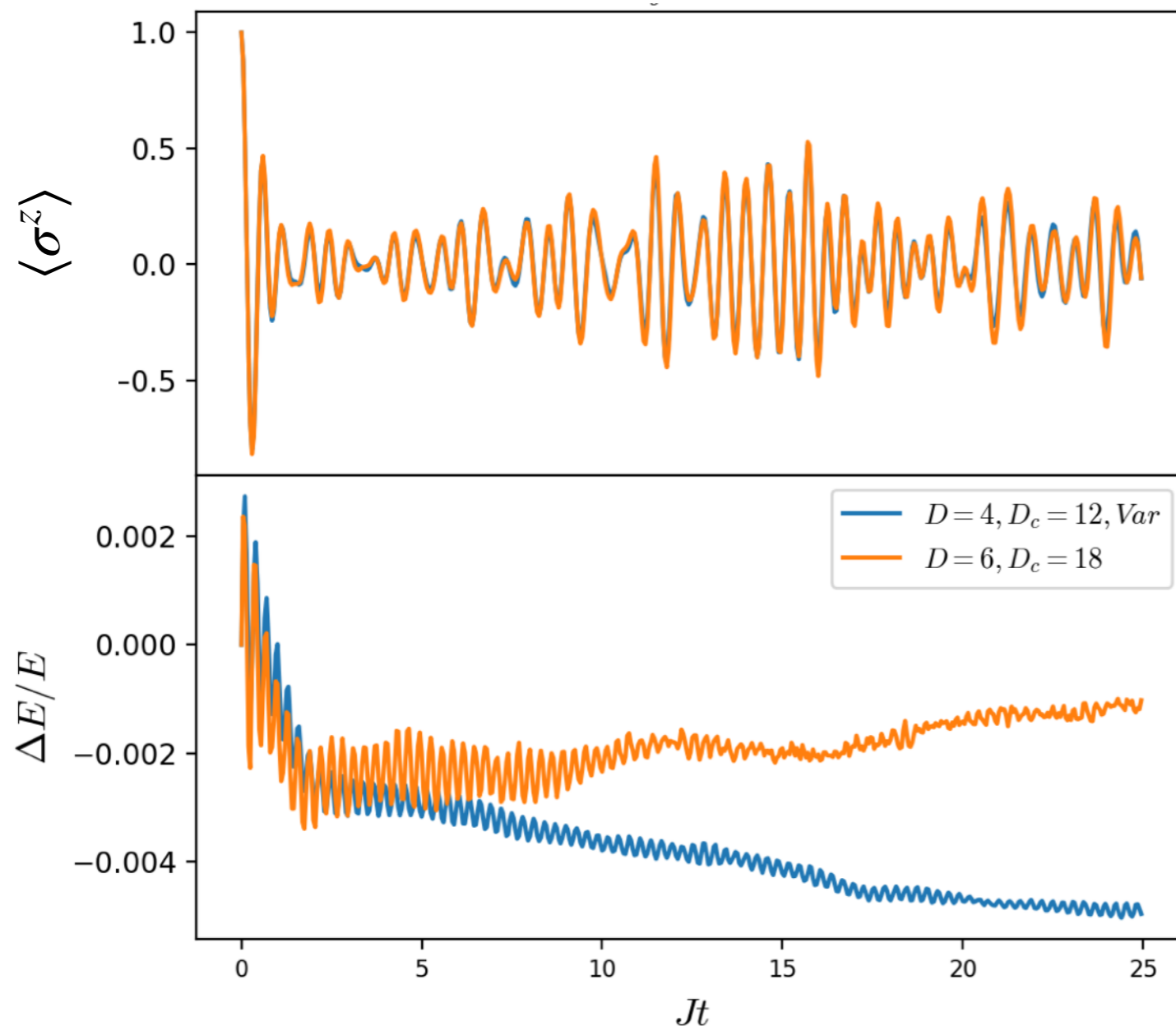
2D transverse field Ising Model ($g = 3.0$)

$$H = - \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - g \sum_i \sigma_i^x$$



(III) Dynamical spin structure factors from isoTNS

Real time evolution of $|\psi_0(t)\rangle = e^{-iHt} \sigma^y |\psi_0\rangle$ for the transverse field Ising model (paramagnetic phase)



- **Good convergence at small bond dimension χ**

(III) Dynamical spin structure factors from isoTNS

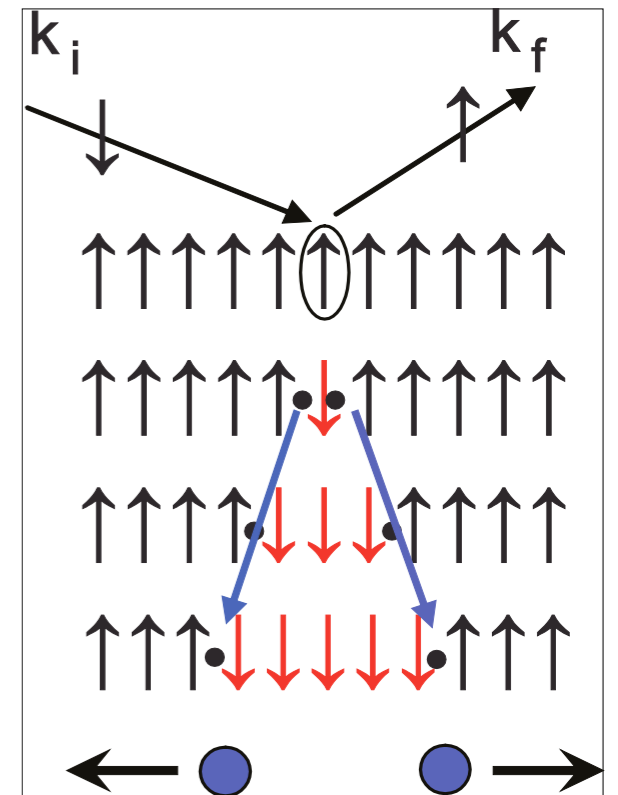
Numerical calculation of the **dynamical structure factor**

$$S(k, \omega) = \sum_x \int_{-\infty}^{\infty} dt e^{-i(kx + \omega t)} C(x, t)$$

with $C(x, t) = \langle \psi_0 | \sigma_x^y(t) \sigma_0^y(0) | \psi_0 \rangle$

(1) Find the ground state $|\psi_0\rangle$: DMRG²

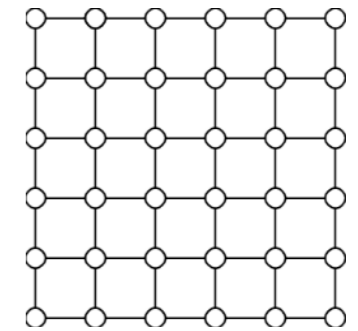
(2) Time evolve $\sigma_0^y |\psi_0\rangle$ to obtain $C(x, t)$



Slow growth of entanglement: Long times!

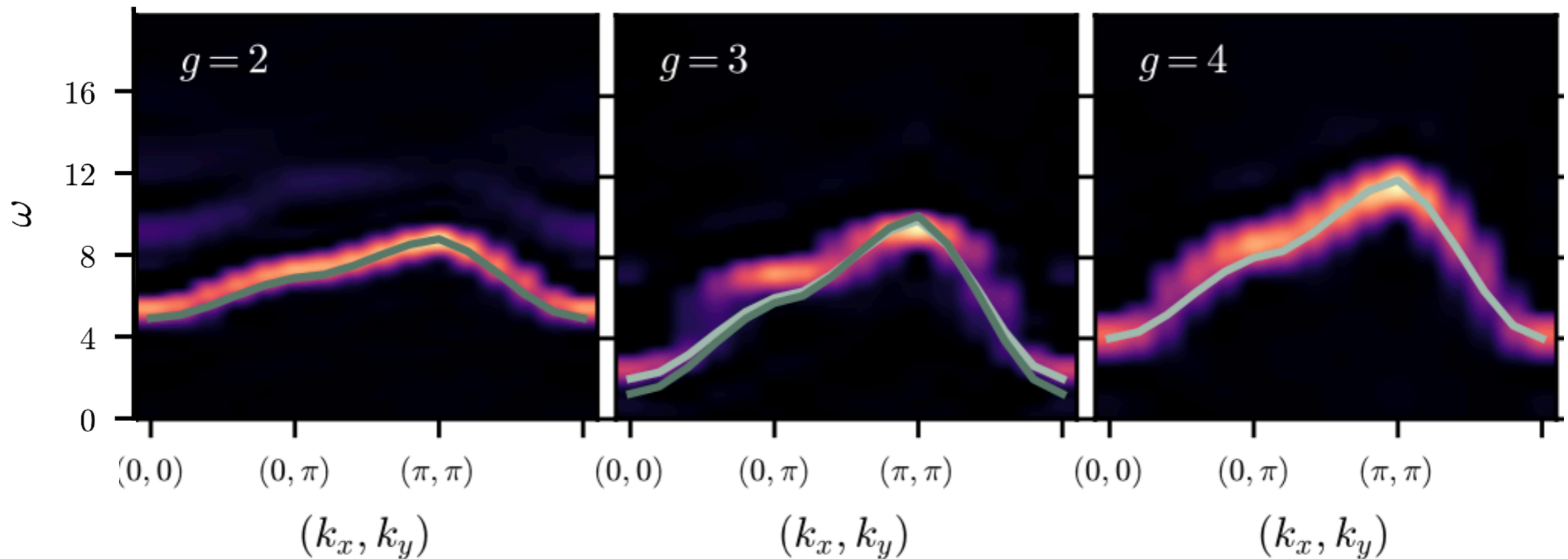
(III) Dynamical spin structure factors from isoTNS

Dynamical structure factor: Transverse field Ising



$$H = - \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z - g \sum_i \sigma_i^x$$

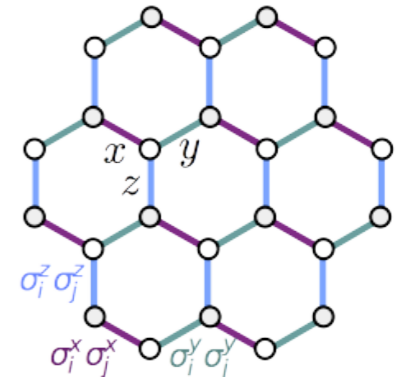
$S^{yy}(k, \omega)$



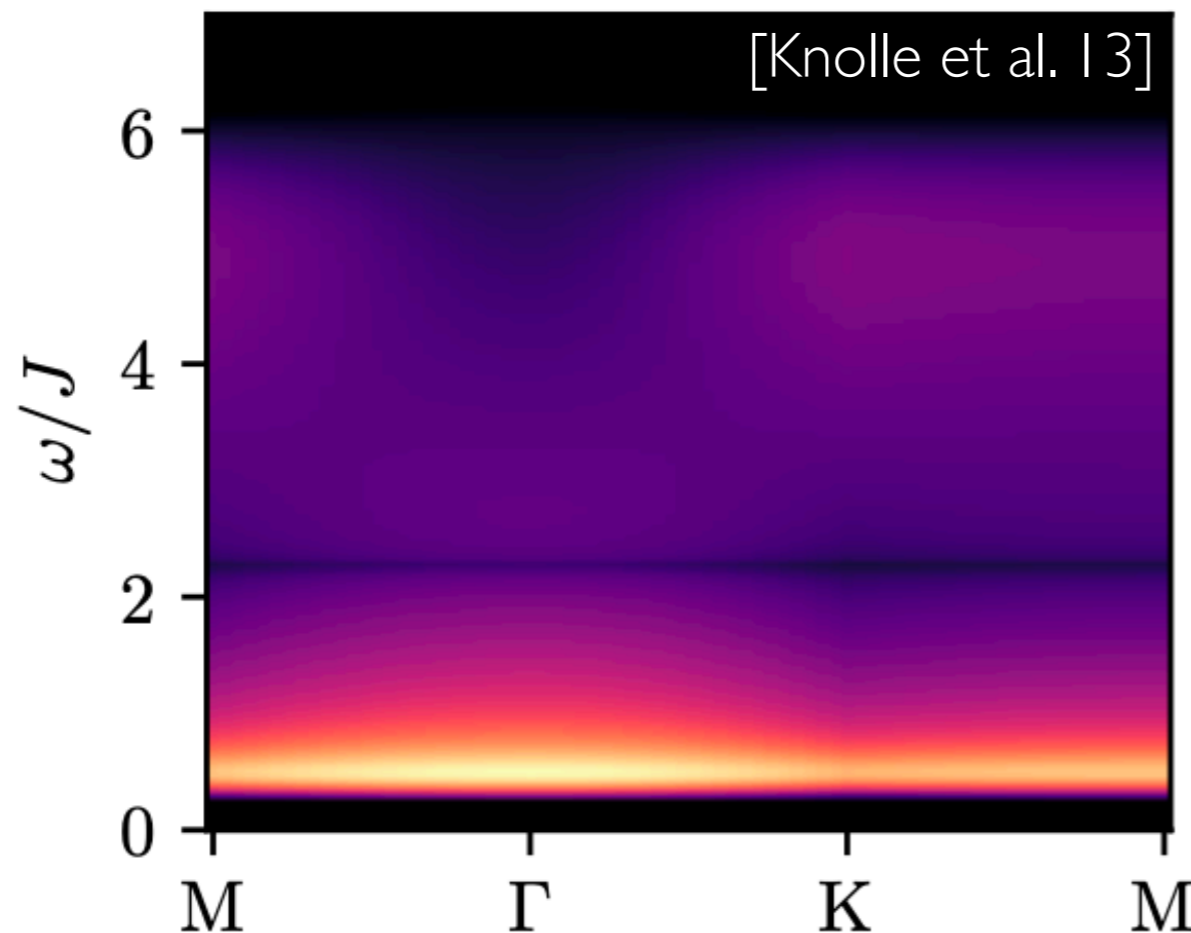
(III) Dynamical spin structure factors from isoTNS

Dynamical structure factor: Kitaev model

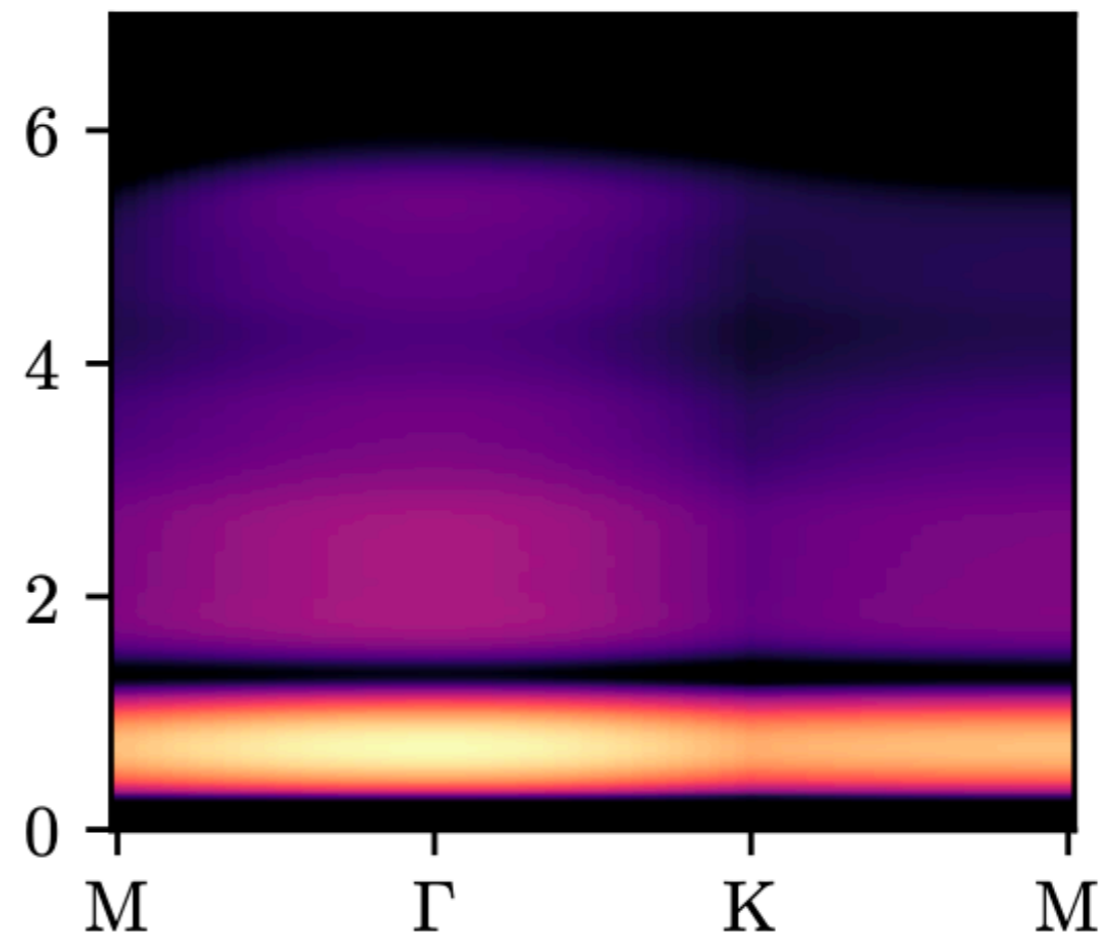
$$H = J \sum_{\langle i,j \rangle} \sigma_i^\alpha \sigma_j^\alpha$$



exact $S(\mathbf{k}, \omega)$



isoTNS $S(\mathbf{k}, \omega)$

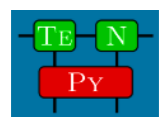


[Lin, Zaletel and FP; work in progress]

Tensor networks and the many-body problem

- I) Entanglement and Matrix-Product States
- II) Time Evolving Block Decimation
- III) Density-Matrix Renormalization Group
- IV) Extracting topological invariants
- V) (isometric Tensor-Network States)

Python toolbox for MPS/TPS simulations:



<https://github.com/tenpy/tenpy>

Lecture notes on MPS:

Hauschild and FP, [arxiv:1805.00055](https://arxiv.org/abs/1805.00055)

Thank You!