Title: Matrix product states and 1d quantum systems

Speakers: Frank Pollmann

Collection: Online School on Ultra Quantum Matter

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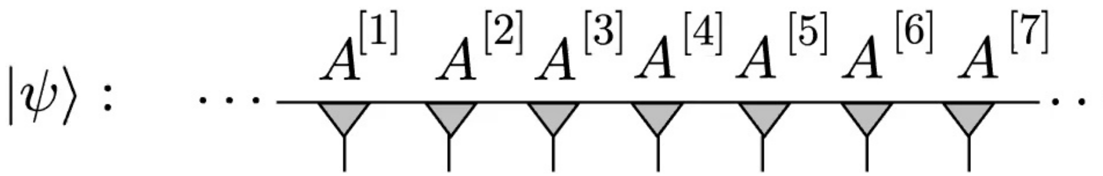
Matrix Product States and 1D Quantum Systems

Frank Pollmann (TUM)



Online School on Ultra Quantum Matter

Complexity of a quantum many-body problem

Many-body Hilbert space

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

N spin-1/2 particles: dim=2^L

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

- Full diagonalization up to ~20 sites
- Sparse methods up to ~40 sites

Matrix-Product States

Many-body Hilbert space

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

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

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

Matrix-Product States

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

Why is it a good representation?

Matrix product states and 1d quantum systems

I) Entanglement and Matrix-Product States

II) Time Evolving Block Decimation

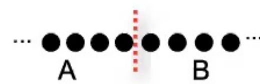
III) Density-Matrix Renormalization Group

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**)



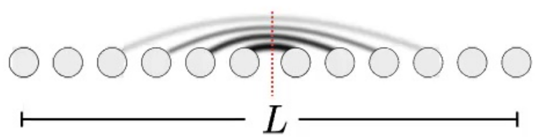
$$|\psi\rangle = \sum_{i,j} C_{i,j} |i\rangle_A \otimes |j\rangle_B = \sum_{\alpha} \Lambda_\alpha |\alpha\rangle_A \otimes |\alpha\rangle_B, \ \langle \alpha | \alpha' \rangle = \delta_{\alpha\alpha'}$$

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



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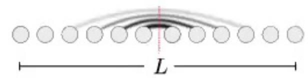

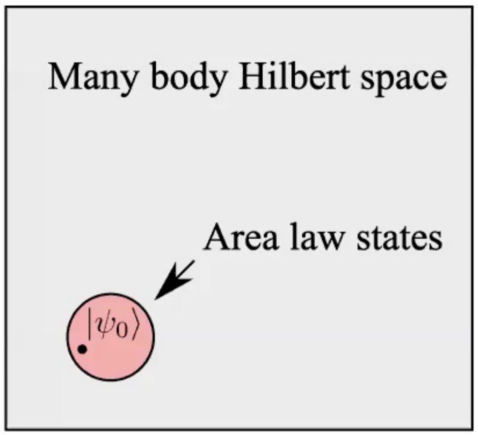

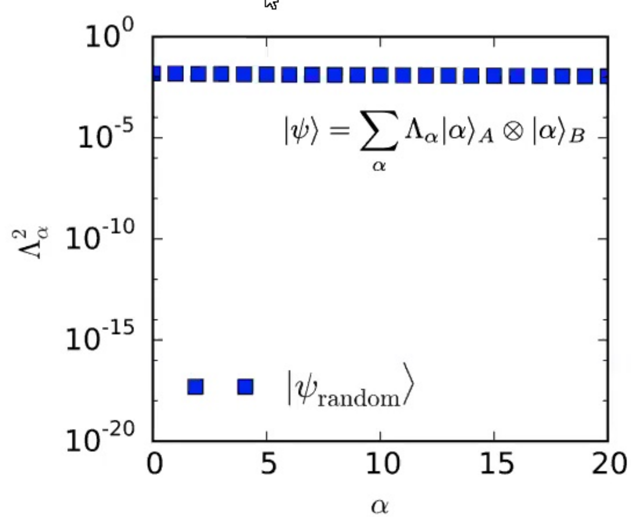

All ground states live in a tiny corner of the Hilbert space!

Entanglement

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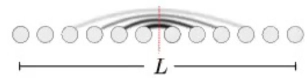

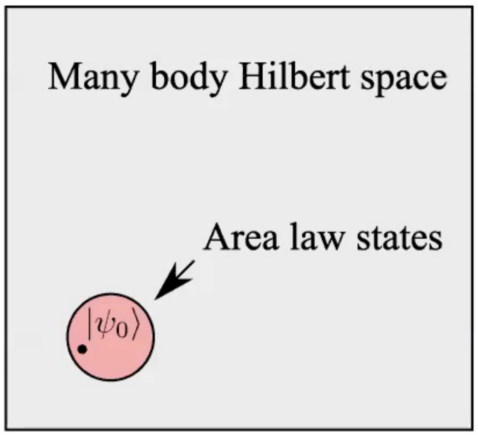

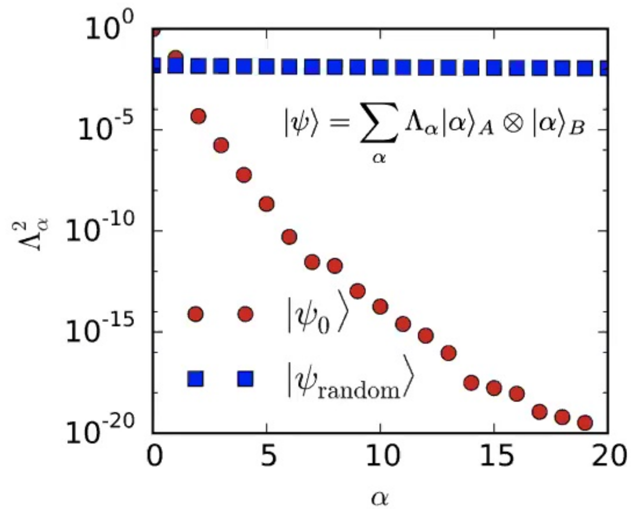

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SVD Compression

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)

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

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

Compression of quantum states

Compression of quantum states

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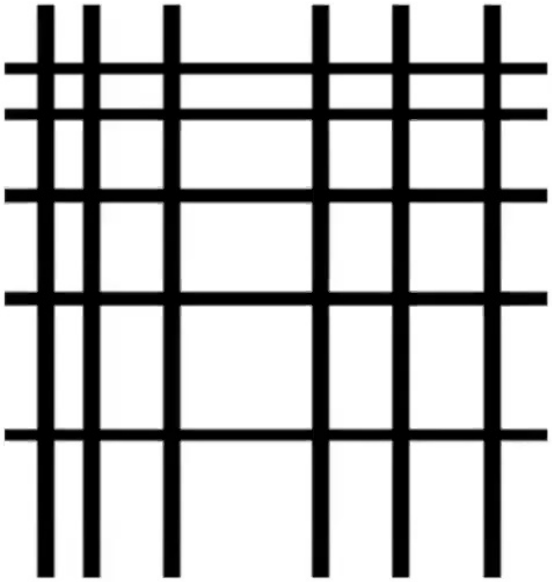
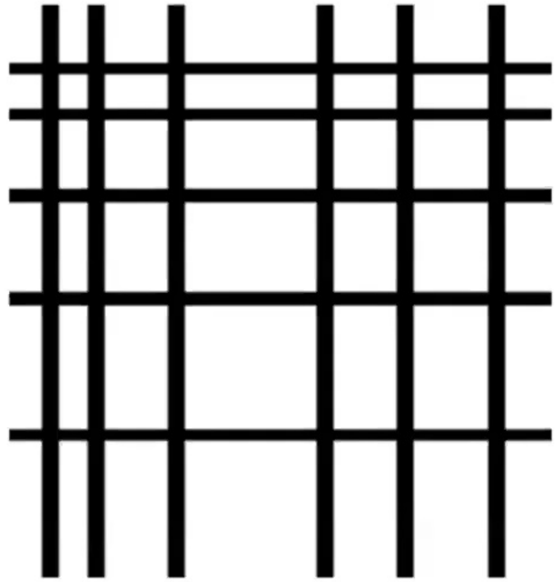
Important features visible already for < 16 states!

Compression of quantum states

Compression of quantum states



$\chi = 500$



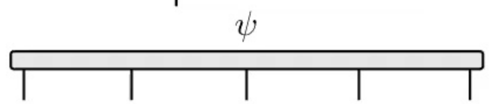
$\chi = 1$

[Mondrian]

Matrix-Product States

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

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



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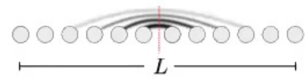

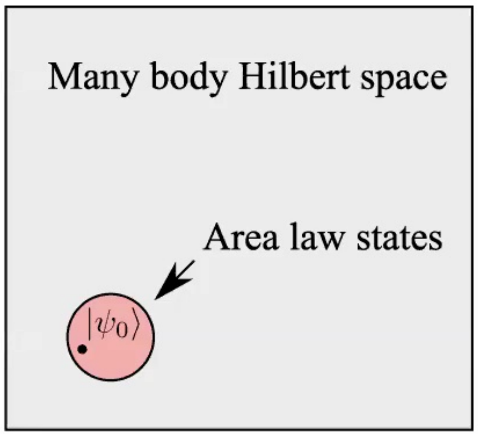

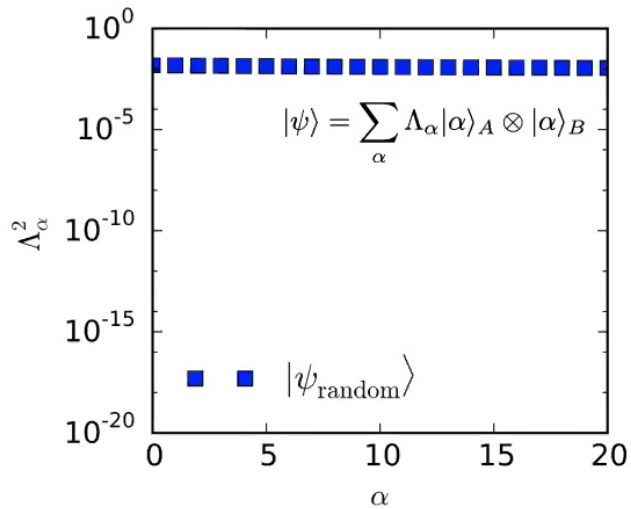

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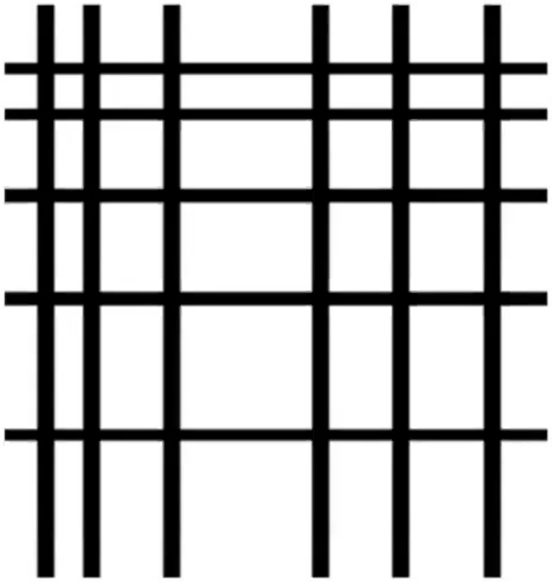

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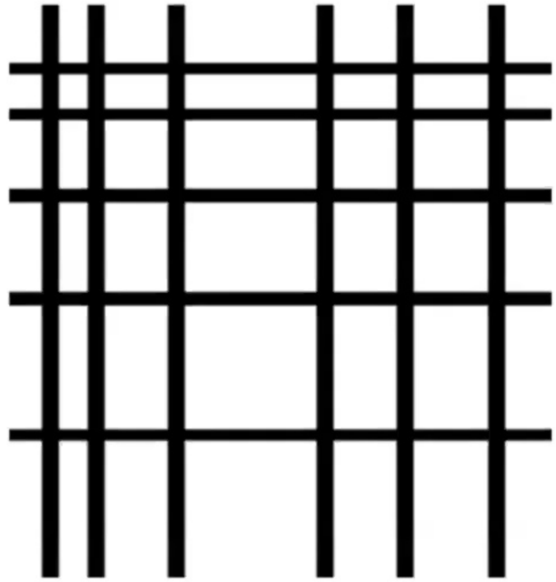

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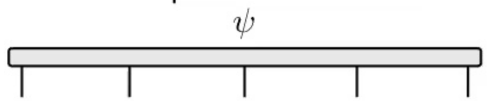
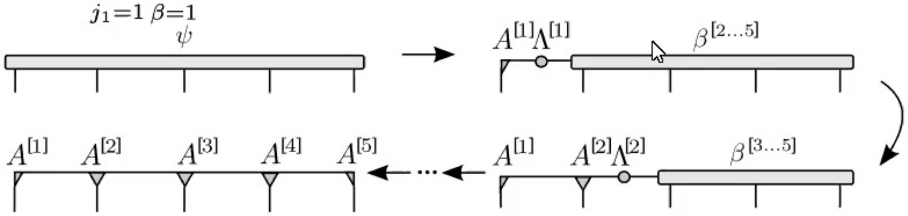
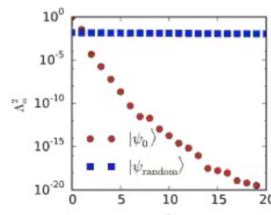


Successive Schmidt decompositions

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





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

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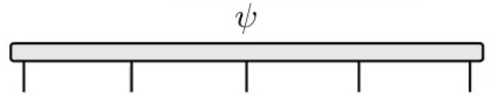

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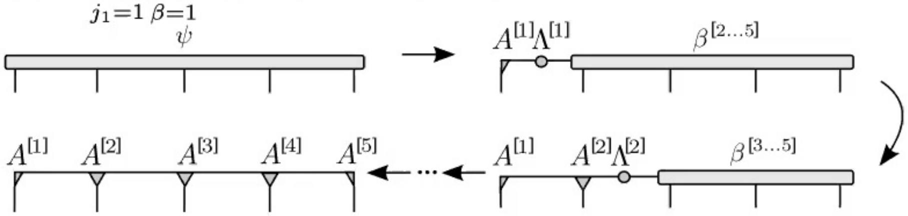

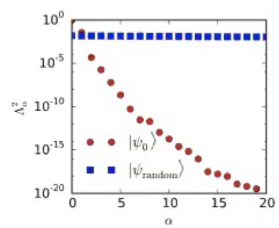

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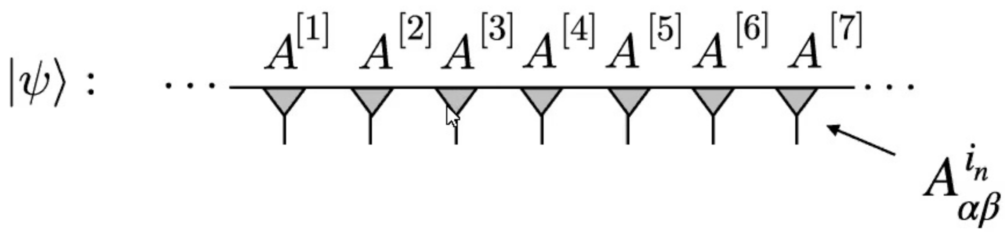
MPS are tailored to describe 1D systems with an area law!

MPS and the canonical form

From now on: Leave out site indices!



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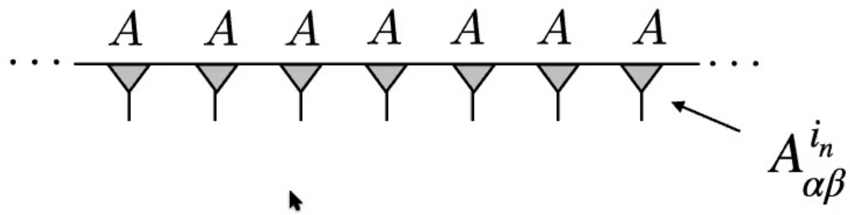
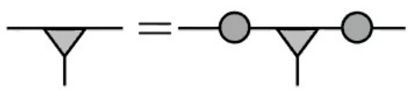
$|\psi\rangle :$



MPS is not unique

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



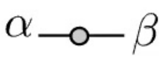
➡ $\tilde{A}^{i_n}$ describes the same state!

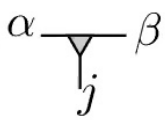
MPS and the canonical form

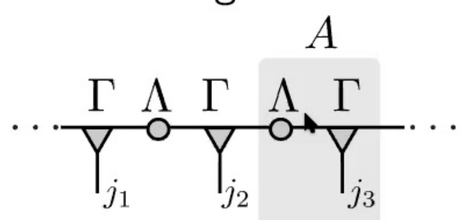
Choose a convenient representation in **Canonical Form**:
Bond index corresponds to Schmidt decomposition! [Vidal '03]

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

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

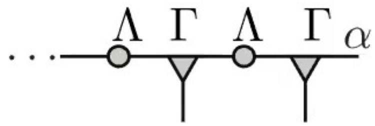
$\Lambda_{\alpha\beta} =$  : Diagonal matrix with Schmidt values

$\Gamma^{j}_{\alpha\beta} =$  : Tensor relating to Schmidt basis

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

MPS and the canonical form

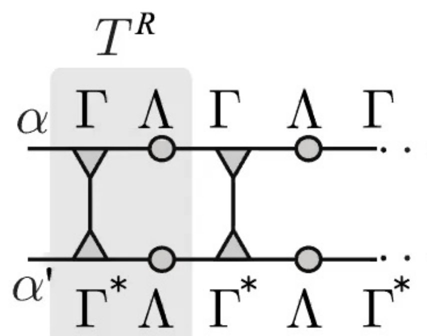
Schmidt states in terms of the MPS:

$|\alpha\rangle_L =$ 

$|\alpha\rangle_R =$ 

Orthogonality:

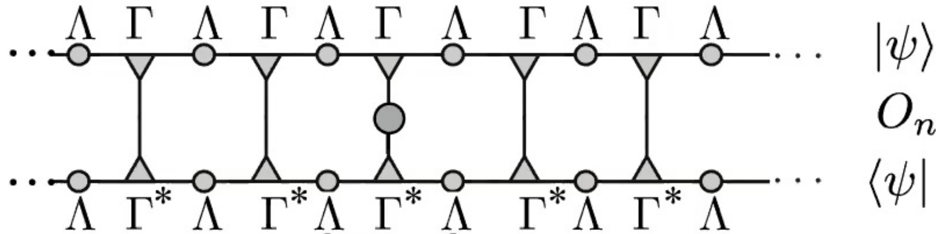
$$\langle \alpha' | \alpha \rangle_R = \delta_{\alpha'\alpha} \equiv$$



MPS and the canonical form

Efficient evaluation of **expectation values**:

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



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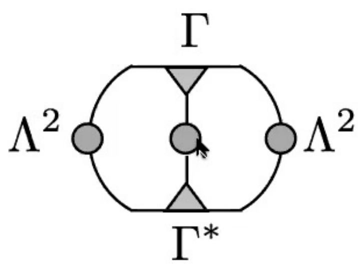
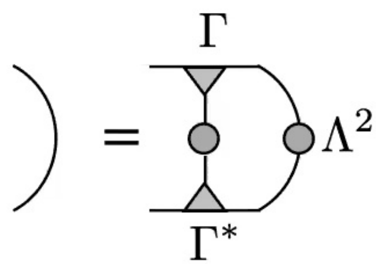


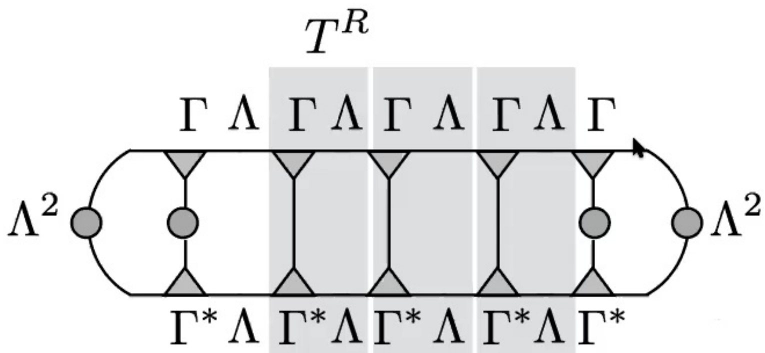
using



MPS and the canonical form

Efficient evaluation of **correlation functions**:

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



Matrix Product States and 1D Quantum Systems

I) Entanglement and Matrix-Product States

II) Time Evolving Block Decimation

III) Density-Matrix Renormalization Group

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.

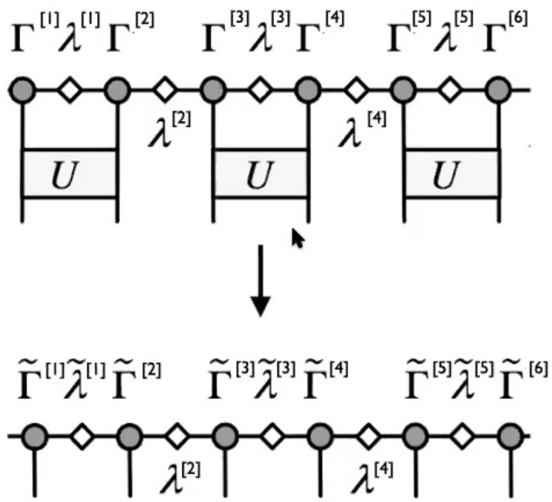
Two chains of two-site gates

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

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

Time evolving block decimation

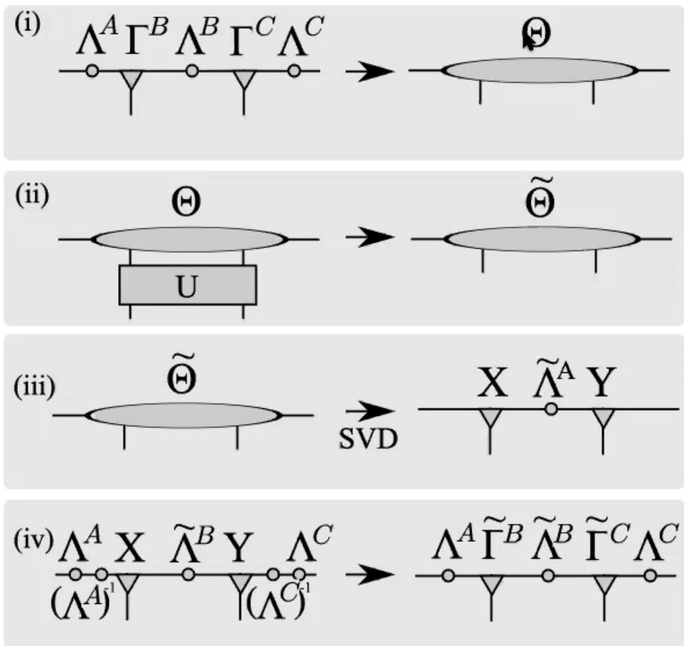
Time Evolving Block Decimation algorithm (TEBD)



How do we get the original form back?

Time evolving block decimation

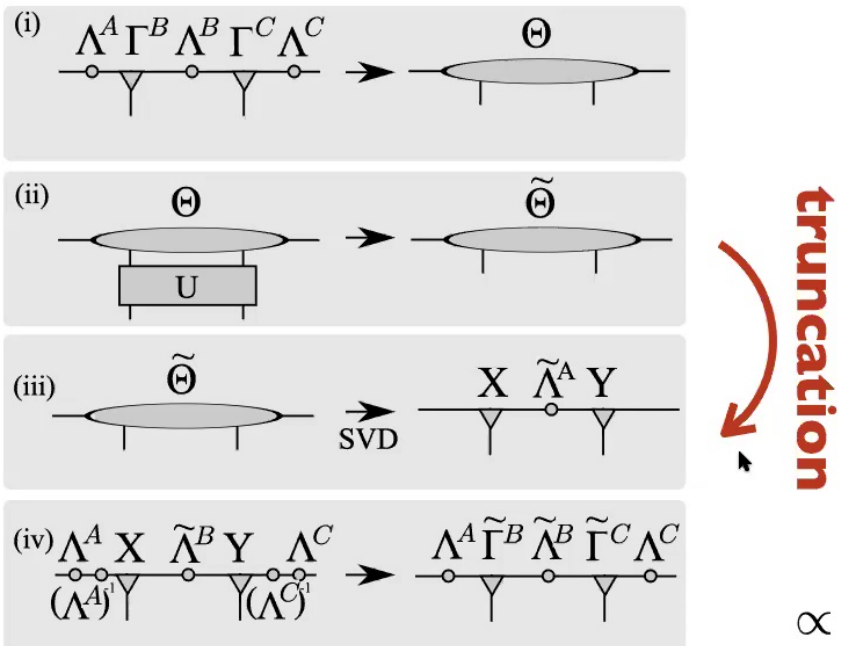
Time Evolving Block Decimation (TEBD) algorithm [Vidal '03]



$\propto d^3 \chi^3$

Time evolving block decimation

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



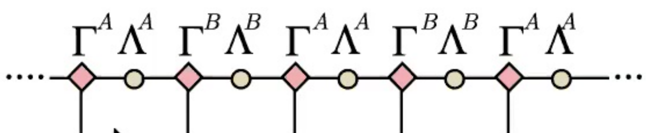
$\propto d^3 \chi^3$

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

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

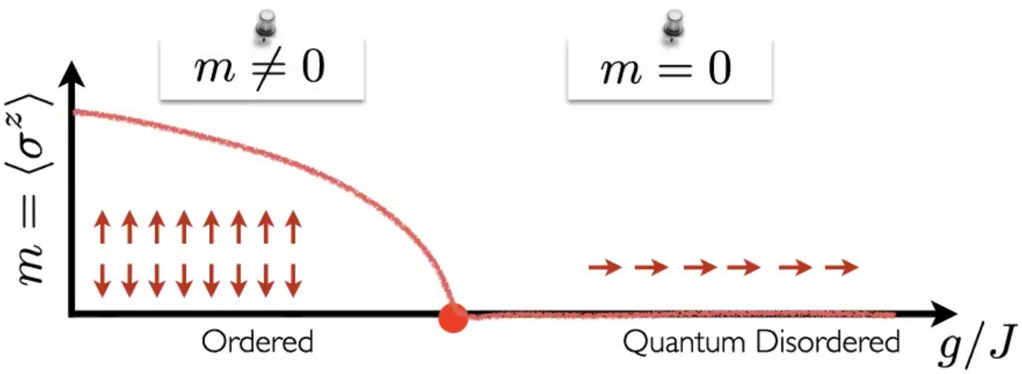


Quantum Ising Model

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

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

↑↑↑↓↓↓↑↑



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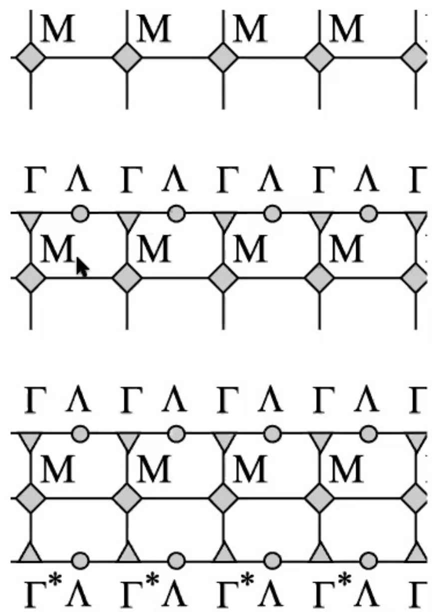
Density matrix renormalization group (DMRG)

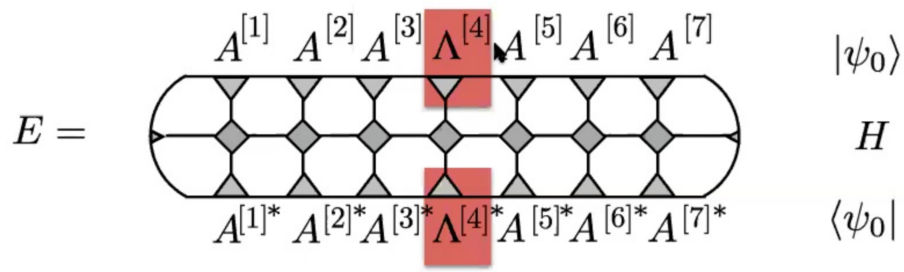
Matrix-Product operators: Generalization of MPS to the space of linear operators

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



Density matrix renormalization group (DMRG)

Find the **ground state** iteratively



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

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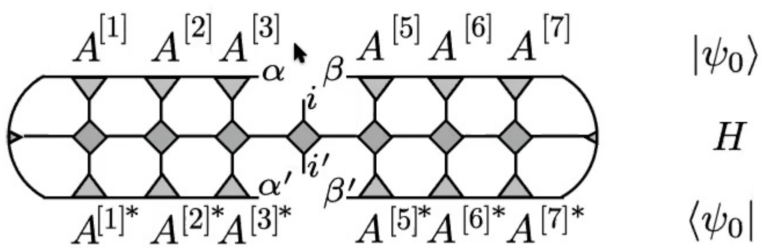
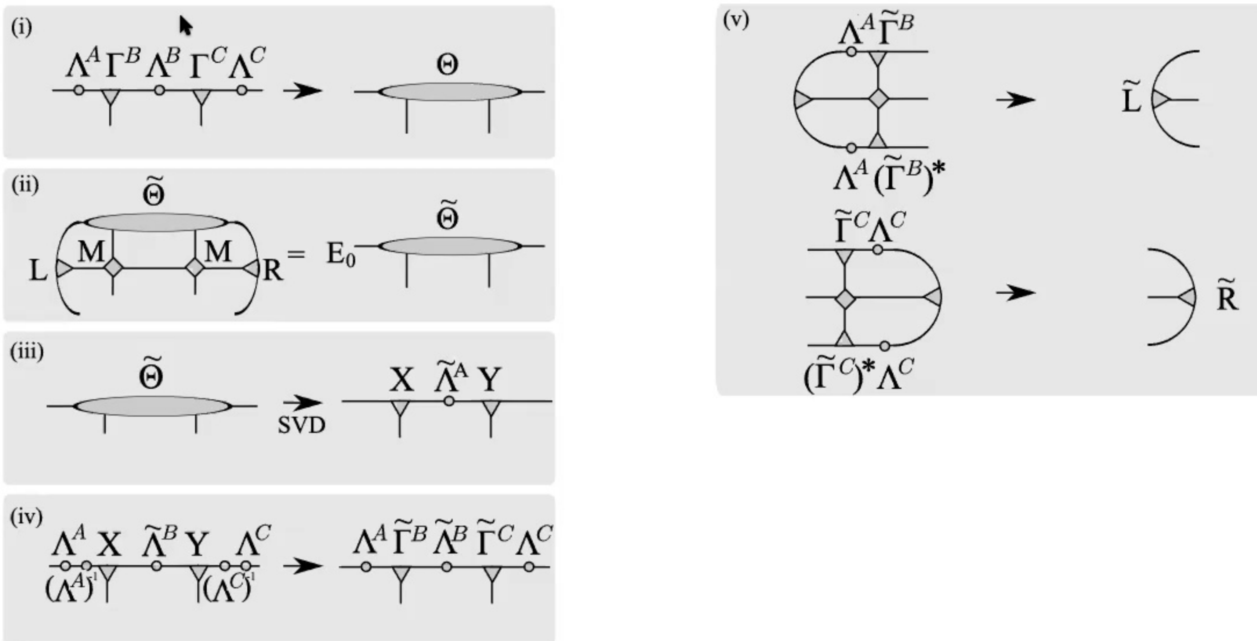


by locally minimizing energy of $H_{\alpha i \beta;\alpha' i' \beta'}$ (e.g., Lanczos)

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

Density matrix renormalization group (DMRG)



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.github.io
- (in)finite DMRG, TEBD, TDVP, …

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Tensor Network Python (TeNPy)

Example: DMRG

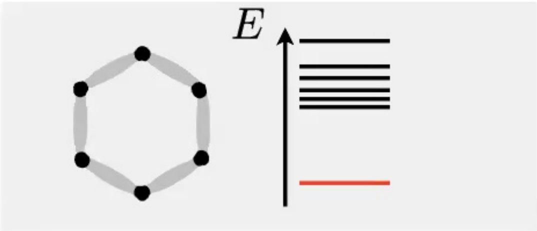
Example

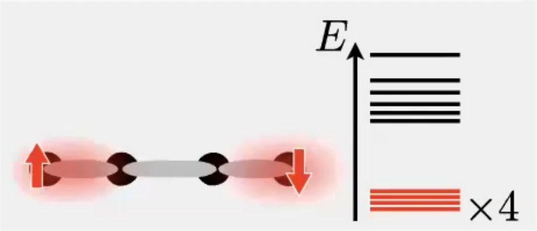
```
from tenpy.networks.mps import MPS
from tenpy.models.tf_ising import TFIChain
from tenpy.algorithms import dmrg

M = TFIChain({'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)
```

Symmetry protected topological phases

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: Protected by symmetry [Affleck et al '87]





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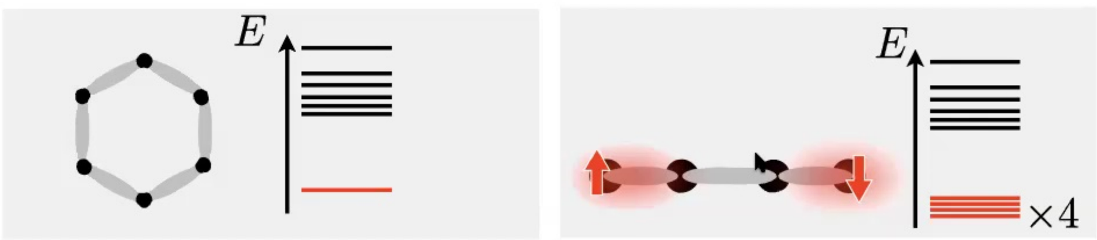
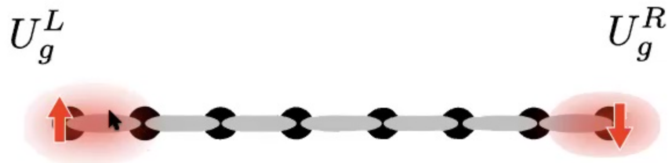


Edge spins have been observed in the NMR profile close to the chain ends of Mg-doped Y_2BaNiO_5 [S.H. Glarum, et al., Tedoldi et al. '99]

Symmetry protected topological phases

Local Hamiltonian and gapped 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** $H^2[G, U(1)]$ [Schur 1911]

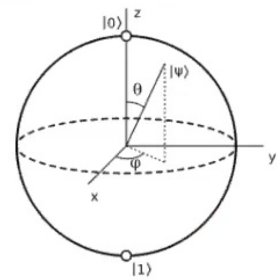
FP, A.M. Turner, E. Berg, and M. Oshikawa, Phys. Rev. B **81**, 064439 (2010).

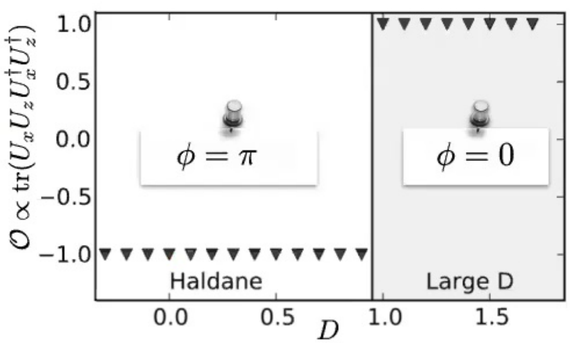
Symmetry protected topological phases

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

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

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





$U_x U_z = e^{i\phi} U_z U_x,\ \phi = 0, \pi$

(spin-1 vs. spin

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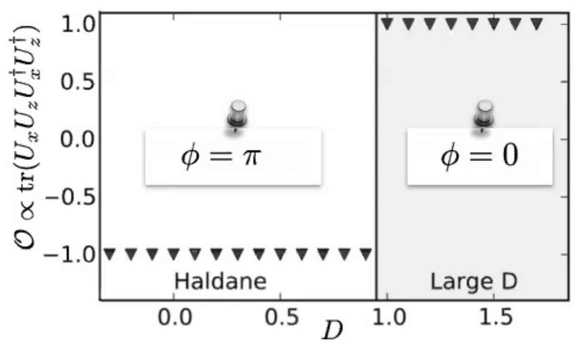

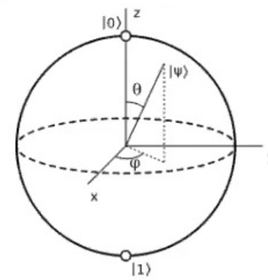

$U_x U_z = e^{i\phi} U_z U_x, \; \phi = 0, \pi$

(spin-1 vs. spin

- Non-local order parameters
- Degeneracies in the entanglement spectrum

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Matrix Product States and 1D Quantum Systems

I) Entanglement and Matrix-Product States

II) Time Evolving Block Decimation

III) Density-Matrix Renormalization Group

Tutorials:

SVD Compression https://colab.research.google.com/drive/1_4V66KqRXHMR-CQl18eqkQBu9EZqw2KM
TEBD Algorithm https://colab.research.google.com/drive/1G_8r4lfiCYKHLmhrFKH4NT4Q2ZWdTNRT
DMRG Algorithm (TeNPy): Ising model https://colab.research.google.com/drive/1V9VAop9_37p2FuqVANH1GGCThtZDD_GM
DMRG Algorithm (TeNPy): S-1 SPT model https://colab.research.google.com/drive/1A1V7_y75BtnLmUUoDPOw26y41eCGbl3b

(Documentation of TeNPy: https://tenpy.readthedocs.io/en/latest/)

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.github.io
- (in)finite DMRG, TEBD, TDVP, …

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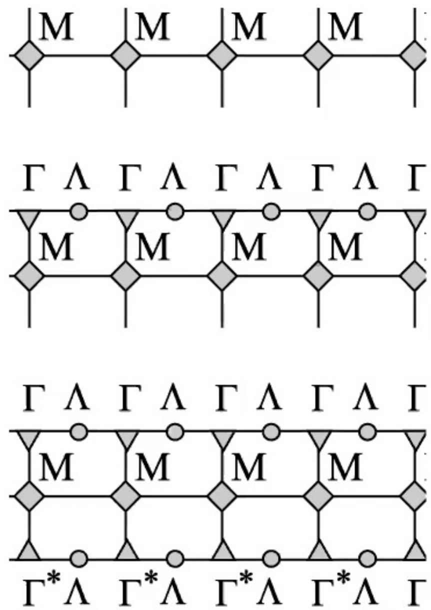
Density matrix renormalization group (DMRG)

Matrix-Product operators: Generalization of MPS to the space of linear operators

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



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