Matrix Product States for Beginners

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Today's menu

- Singular Value Decomposition.
- Tensors: Contractions and Projections
- Reduced density matrix.
- Entanglement (von Neumann) entropy.
- Matrix Product States: example with N=3.
- Important example: AKLT model.
- Why MPS?

Some basic references

- Ulrich Schollwöck, *Annals of Physics* **326** 96–192 (2011)

The density-matrix renormalization group in the age of matrix product states

Ulrich Schollwöck *

- Román Orús *Annals of Physics* **349** 117–158 (2014)

A practical introduction to tensor networks: Matrix product states and projected entangled pair states

Román Orús *

Institute of Physics, Johannes Gutenberg University, 55099 Mainz, Germany

- E. Miles Stoudenmire Lecture Notes/Slides IF-USP (2018)

Mini-course on
Tensor Networks and Applications
IFUSP, São Paulo, April 16-20, 2018.

http://www.fmt.if.usp.br/~gtlandi/courses/mini-course-tensor-networks

SVD

Consider a numerical SVD example:

$$M = \begin{bmatrix} 0.435839 & 0.223707 & 0.10 \\ 0.435839 & 0.223707 & -0.10 \\ 0.223707 & 0.435839 & 0.10 \\ 0.223707 & 0.435839 & -0.10 \end{bmatrix}$$

Can decompose as

$$\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix} \begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0.200 \end{bmatrix} \begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Keep fewer and fewer singular values:

$$\underset{U}{\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix}} \underset{\Lambda}{\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0.200 \end{bmatrix}} \underset{V}{\begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}$$

$$= M = \begin{bmatrix} 0.435839 & 0.223707 & 0.10 \\ 0.435839 & 0.223707 & -0.10 \\ 0.223707 & 0.435839 & 0.10 \\ 0.223707 & 0.435839 & -0.10 \end{bmatrix}$$

$$||M - M||^2 = 0$$

Keep fewer and fewer singular values:

$$\underset{U}{\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix}} \underset{\Lambda}{\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0.300 & 0 \\ 0 & 0 & 0 \end{bmatrix}} \underset{V}{\begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 \quad 0 & 0 & 1 \end{bmatrix}}$$

$$= M_2 = \begin{bmatrix} 0.435839 & 0.223707 & 0 \\ 0.435839 & 0.223707 & 0 \\ 0.223707 & 0.435839 & 0 \\ 0.223707 & 0.435839 & 0 \end{bmatrix}$$

$$||M_2 - M||^2 = 0.04 = (0.2)^2$$

Keep fewer and fewer singular values:

$$\underbrace{\begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} 0.933 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}}_{\Lambda} \underbrace{\begin{bmatrix} 0.707107 & 0.707107 & 0 \\ -0.707107 & 0.707107 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{V}$$

$$= M_3 = \begin{bmatrix} 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \end{bmatrix}$$

Truncating SVD =

Controlled approximation for M

$$||M_3 - M||^2 = 0.13 = (0.3)^2 + (0.2)^2$$

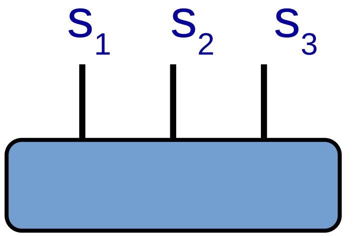
Tensors

Quantum state:

$$|\Psi\rangle = \sum_{s_1 s_2 s_3} \Psi_{s_1 s_2 s_3} |s_1\rangle |s_2\rangle |s_3\rangle$$

Graphic representation:

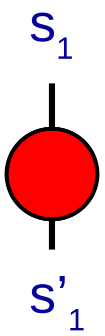
$$\Psi_{s_1 s_2 s_3}$$



Local operator:

$$\hat{A}(1) = \sum_{s_1 s_1'} A_{s_1 s_1'} |s_1\rangle\langle s_1'|$$

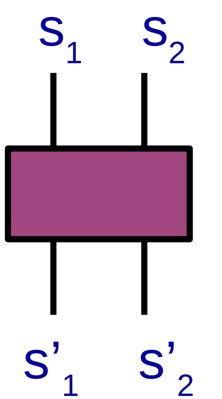
$$A_{s_1 s_1'}$$



Two-site operator:

$$\hat{U}(1,2) = \sum_{\substack{s_1 s_2 \\ s_1' s_2'}} U_{\substack{s_1 s_2 \\ s_1' s_2'}} |s_1\rangle |s_2\rangle \langle s_1'| \langle s_2'|$$

$$U_{\substack{s_1 s_2 \\ s_1' s_2'}}$$

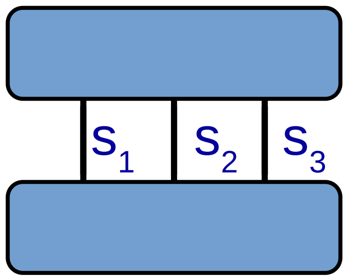


Contractions and projections

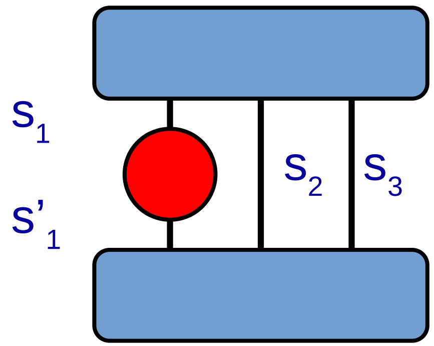
Full contractions (scalars):

$$\sum_{s_1 s_2 s_3} \Psi^*_{s_1 s_2 s_3} \Psi_{s_1 s_2 s_3}$$

$$\langle \Psi | \Psi \rangle$$



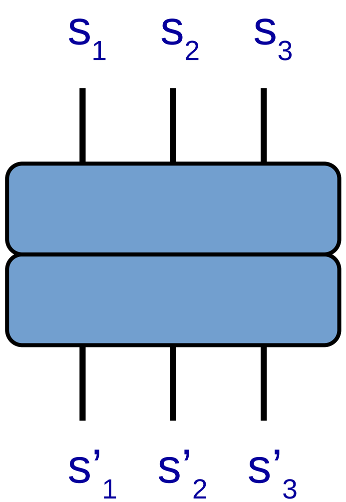
$$\langle \Psi | \hat{A}(1) | \Psi \rangle$$



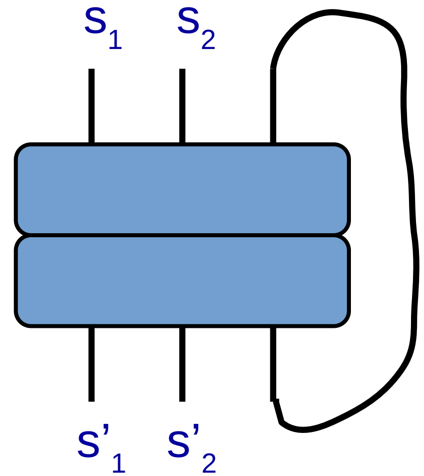
$$\sum_{\substack{s_1 s_1' \\ s_2 s_3}} \Psi^*_{s_1 s_2 s_3} A_{s_1 s_1'} \Psi_{s_1' s_2 s_3}$$

Projectors:

$$|\Psi\rangle\langle\Psi|$$



$$\mathrm{Tr}_{(3)} |\Psi\rangle\langle\Psi|$$

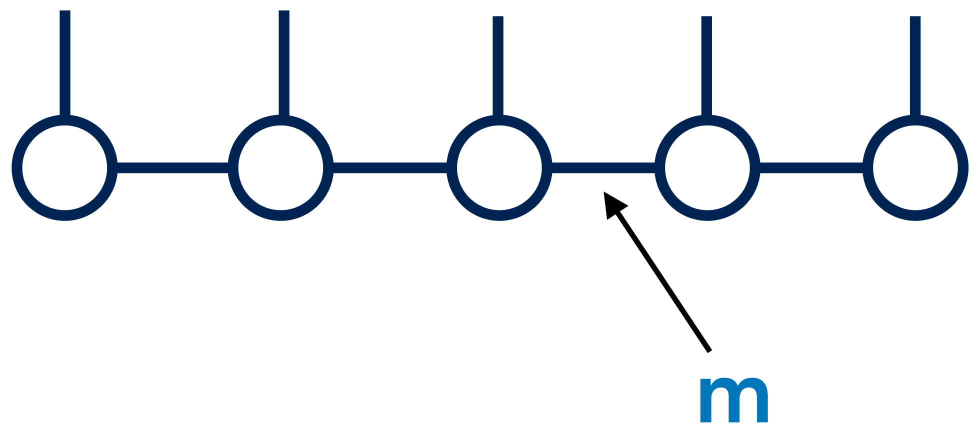


Reduced Density Matrix

Entanglement Entropy

MPS

Key facts about matrix product states



- linear size of matrices (dimension of bond indices) known as the *bond dimension* **m** (sometimes χ or D)

- for large enough **m**, can represent *any state* (**m** = $2^{N/2}$)

- entanglement of left-right cut bounded by log(**m**), so boundary law guaranteed

Examples of Matrix Product States

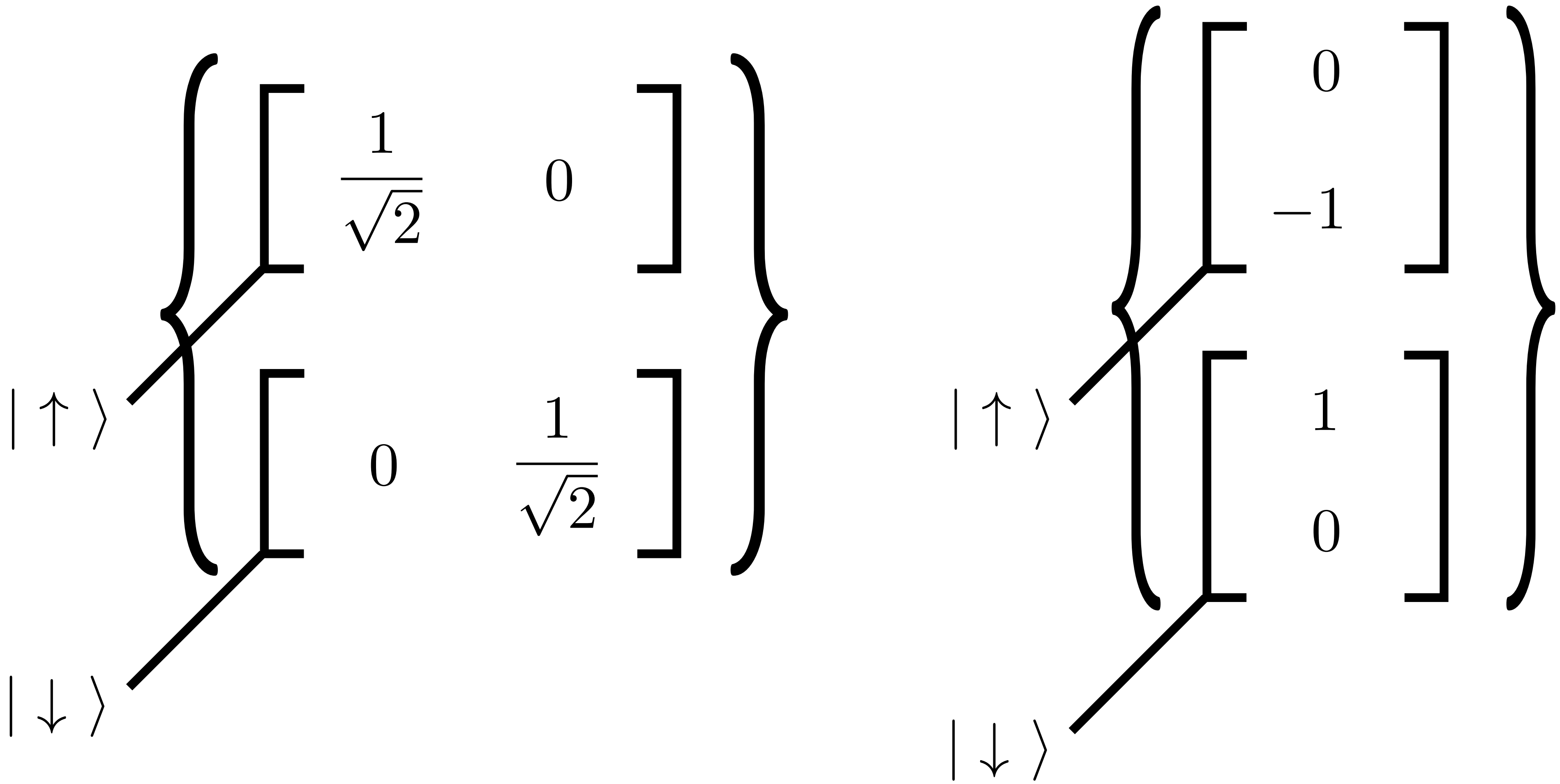
Example #1: singlet state

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

$$= \begin{bmatrix} \frac{1}{\sqrt{2}}|\uparrow\rangle & \frac{1}{\sqrt{2}}|\downarrow\rangle \end{bmatrix} \begin{bmatrix} |\downarrow\rangle \\ -|\uparrow\rangle \end{bmatrix}$$

How to see this is an MPS?

$$\begin{bmatrix} \frac{1}{\sqrt{2}}|\uparrow\rangle & \frac{1}{\sqrt{2}}|\downarrow\rangle \end{bmatrix} \begin{bmatrix} |\downarrow\rangle \\ -|\uparrow\rangle \end{bmatrix} =$$



Example #2: AKLT wavefunction

The AKLT wavefunction is the exact ground state of the following S=1 Hamiltonian

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

In the same phase as S=1 Heisenberg model, plus 'small' perturbation of $(\mathbf{S}\cdot\mathbf{S})^2$ biquadratic term

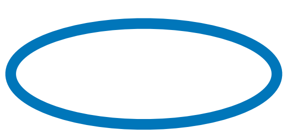
Can construct AKLT wavefunction as follows

Start with 2N spin 1/2's in singlet pairs

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

Can construct AKLT wavefunction as follows

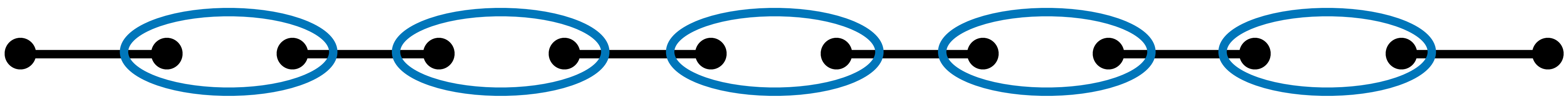
Act on pairs of S=1/2's with projection operator P

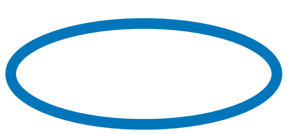


$$= \hat{P} = |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$

Can construct AKLT wavefunction as follows

Act on pairs of S=1/2's with projection operator P

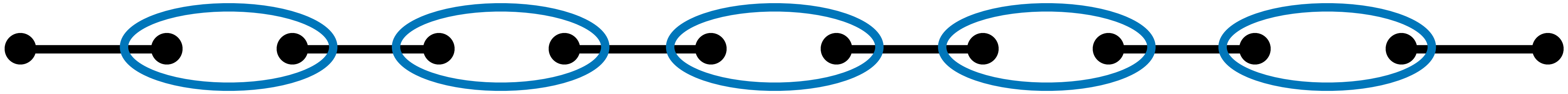




$$= \hat{P} = |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$

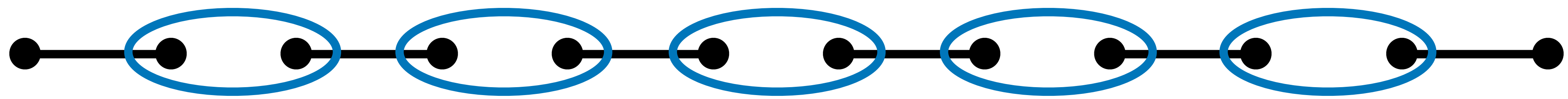
Can construct AKLT wavefunction as follows

After projection, blue ovals are S=1 spins



Can construct AKLT wavefunction as follows

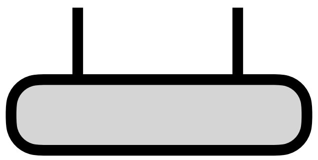
After projection, blue ovals are S=1 spins



Can predict interesting properties:

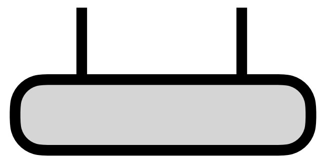
- doubly degenerate entanglement spectrum
- emergent S=1/2 edge spins

Tensor approach to AKLT

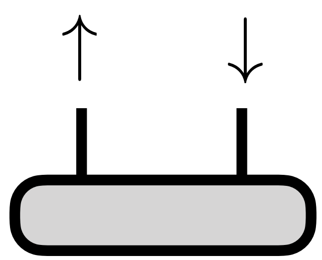


$$= \frac{1}{\sqrt{2}}|\uparrow\rangle|\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle|\uparrow\rangle$$

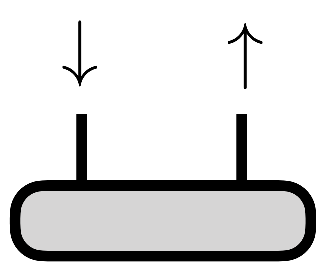
Tensor approach to AKLT



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

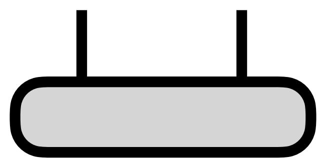


$$= \frac{1}{\sqrt{2}}$$

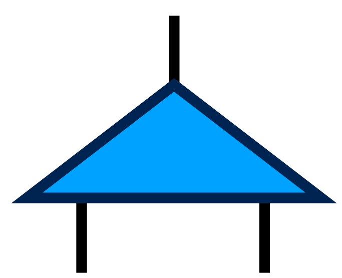


$$= -\frac{1}{\sqrt{2}}$$

Tensor approach to AKLT

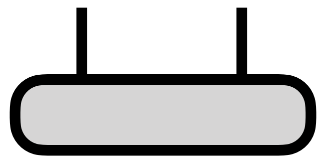


$$= \frac{1}{\sqrt{2}} |\uparrow\rangle |\downarrow\rangle - \frac{1}{\sqrt{2}} |\downarrow\rangle |\uparrow\rangle$$

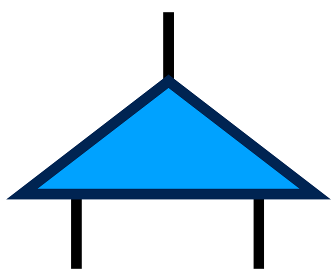


$$= |+\rangle\langle\uparrow\uparrow| + |0\rangle \frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$

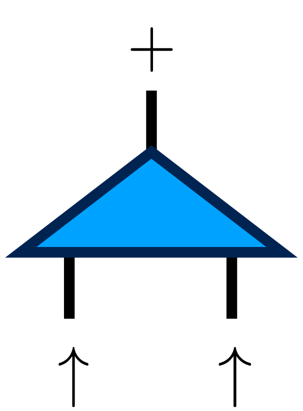
Tensor approach to AKLT



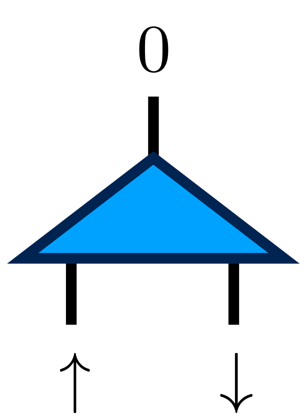
$$= \frac{1}{\sqrt{2}}|\uparrow\rangle|\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\rangle|\uparrow\rangle$$



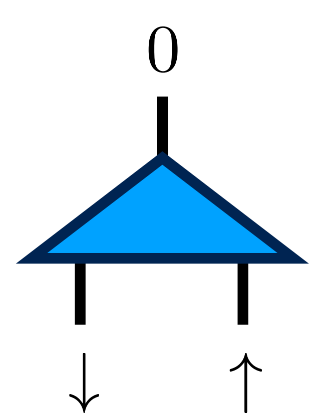
$$= |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$



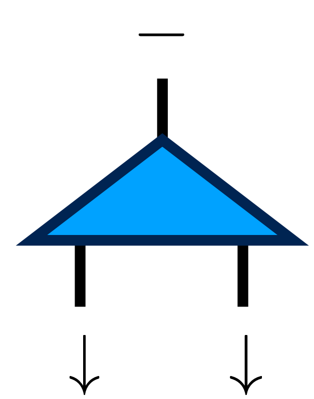
$= 1$



$= \frac{1}{\sqrt{2}}$

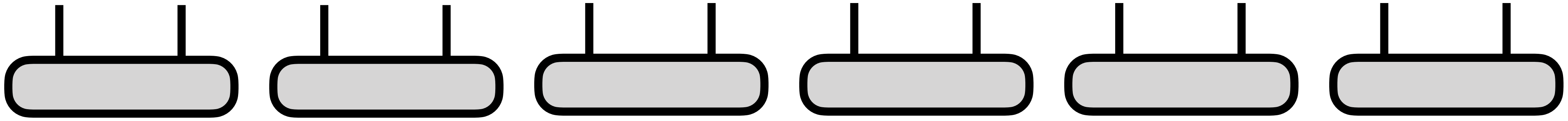


$= \frac{1}{\sqrt{2}}$

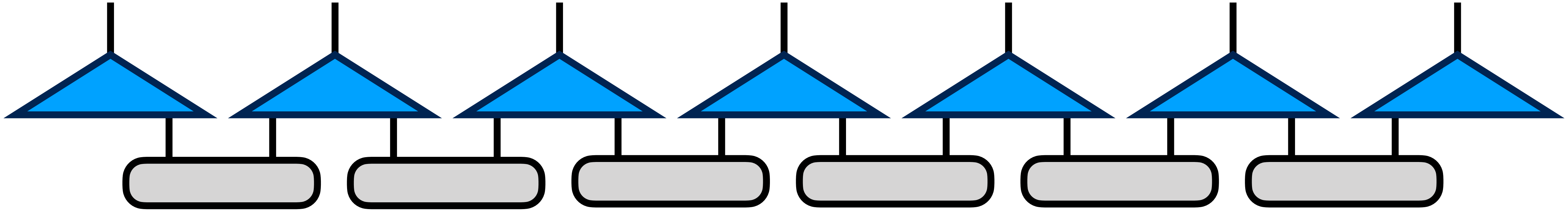


$= 1$

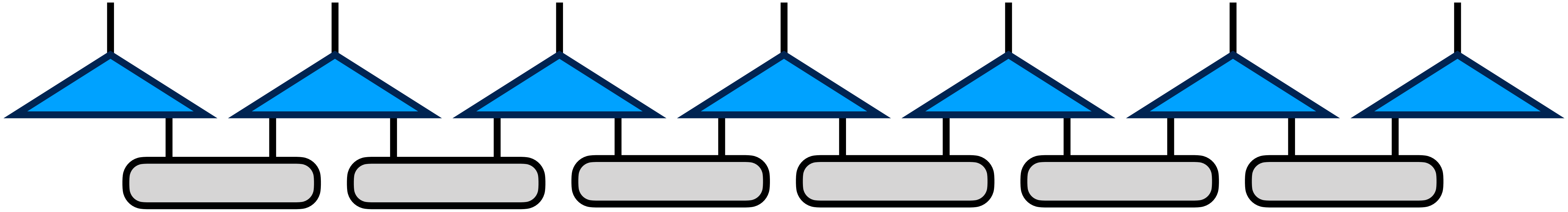
Tensor approach to AKLT



Tensor approach to AKLT

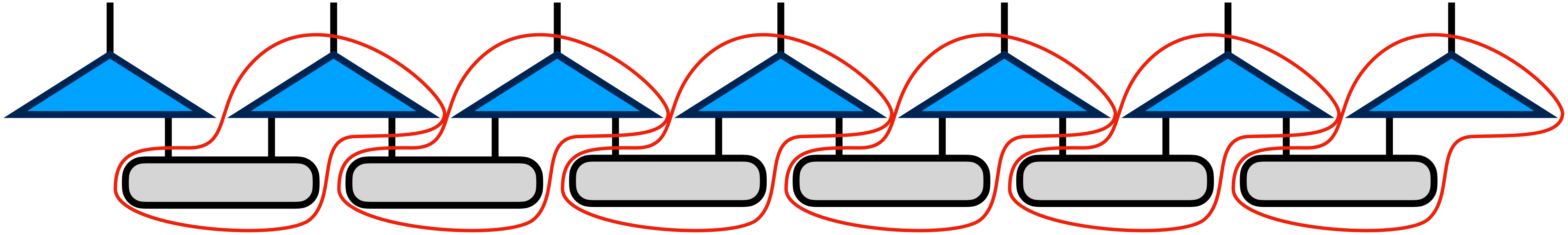


Put into MPS form



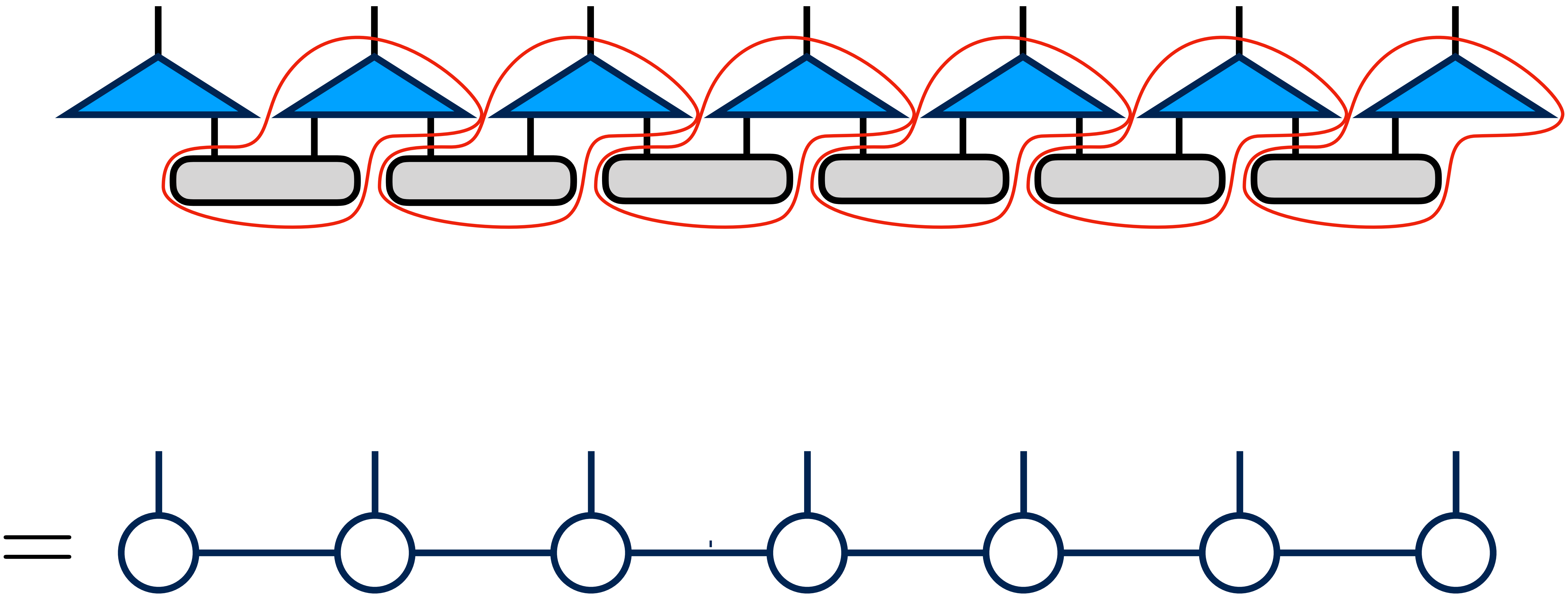
Put into MPS form

Contract pairs of tensors:



Put into MPS form

Contract pairs of tensors:



Nice form of AKLT matrix product state with periodic boundary conditions

Can actually show the following:

$$|\Psi_{\mathrm{AKLT}}\rangle = \mathrm{Tr}\left[M^{s_1} M^{s_2} M^{s_3} \cdots M^{s_N}\right] |s_1 s_2 s_3 \ldots s_N\rangle$$

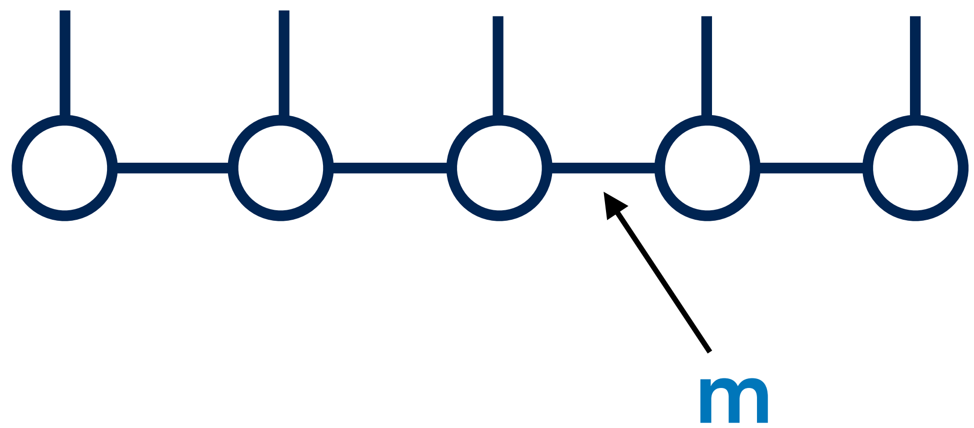
where

$$M^{+} = \sqrt{\frac{2}{3}}\ \sigma^{+}$$

$$M^{0} = -\sqrt{\frac{1}{3}}\ \sigma^{z}$$

$$M^{-} = -\sqrt{\frac{2}{3}}\ \sigma^{-}$$

Key facts about matrix product states



- linear size of matrices (dimension of bond indices) known as the *bond dimension* **m** (sometimes χ or D)

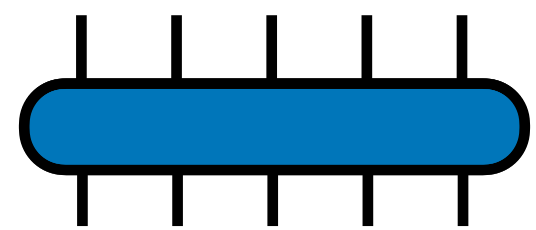
- for large enough **m**, can represent *any state* (**m** = $2^{N/2}$)

- entanglement of left-right cut bounded by log(**m**), so boundary law guaranteed

Many-Body Entanglement

What is the maximum amount of entanglement?

ρ_A is a $2^{N/2} \times 2^{N/2}$ matrix



$2^{N/2}$ eigenvalues, trace has to be 1

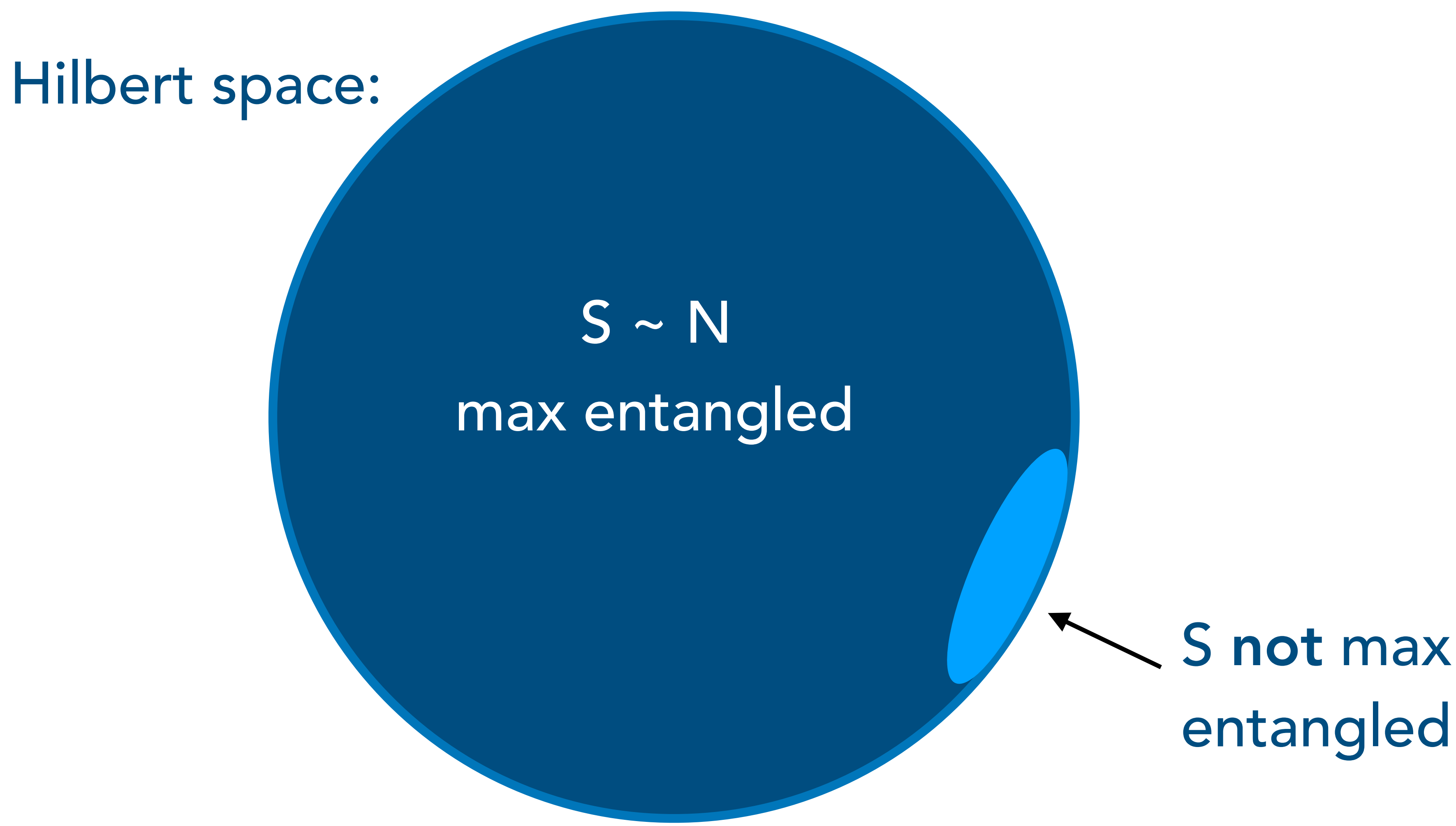
maximum entropy if all eigenvalues same, $p_n \equiv 2^{-N/2}$

$$S_{\mathrm{vN}} = -\sum_{n=1}^{2^{N/2}} p_n \ln(p_n) = -2^{N/2} \frac{1}{2^{N/2}} \ln(2^{-N/2})$$

$$= \frac{N}{2} \ln(2) \sim N$$ "volume law"

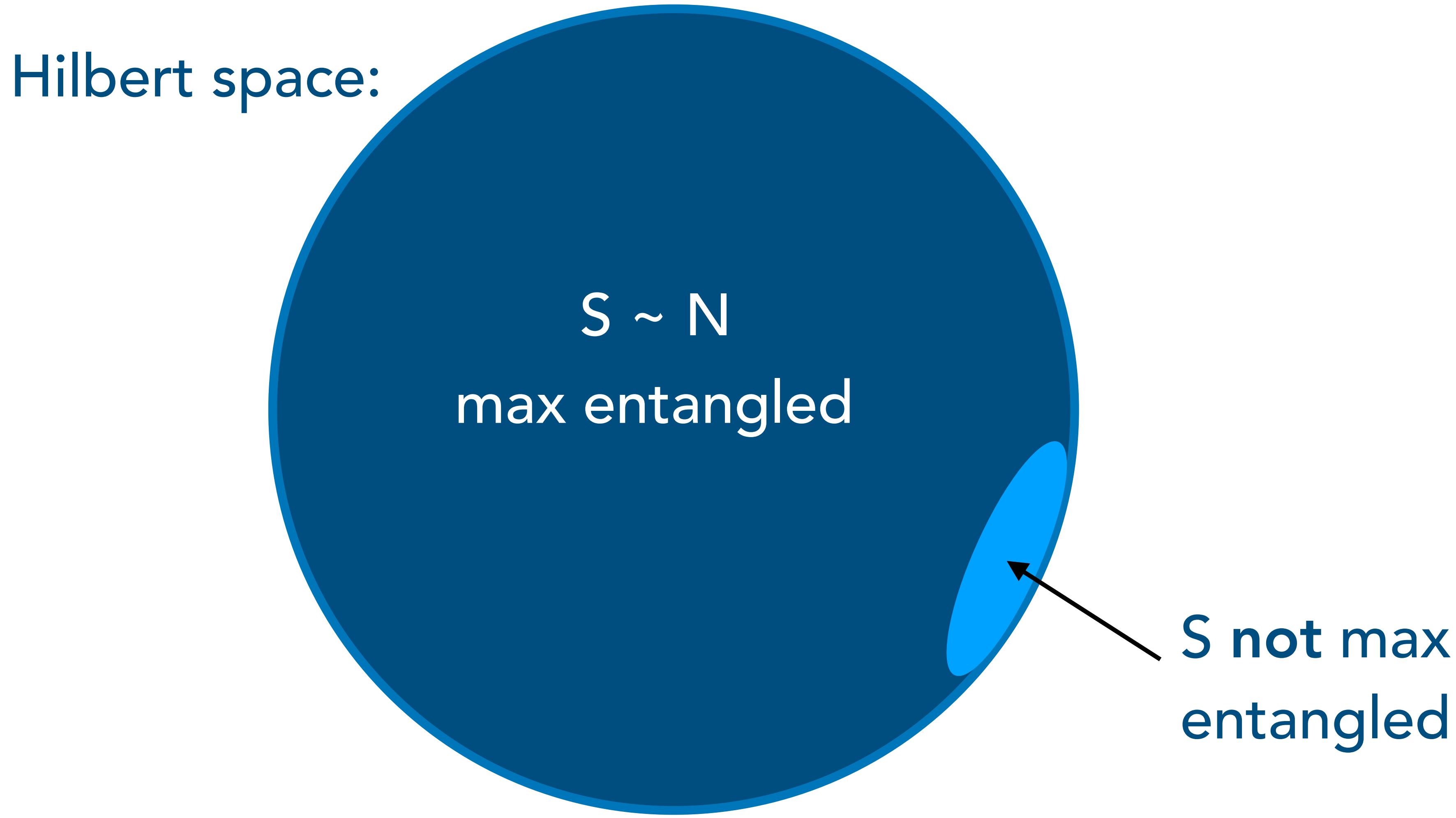
Many-Body Entanglement

Fact: randomly chosen wavefunctions have maximum entropy with probability 1.0



Many-Body Entanglement

Which wavefunctions live in the special region that is not maximally entangled?



Consider ***ground states*** of 1D Hamiltonians

Heisenberg spin chain:

$$H = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

Hubbard chain:

$$H = -t \sum_{j,\sigma} (c^\dagger_{j,\sigma} c_{j+1,\sigma} + c^\dagger_{j+1,\sigma} c_{j,\sigma}) + \sum_j U n_{j\uparrow} n_{j\downarrow}$$

1D "electronic structure" Hamiltonian:

$$H = \int_x \psi^\dagger(x) \Big[-\frac{1}{2}\partial_x^2 + v(x) \Big] \psi(x) + \int_{x,x'} u(x-x') n(x) n(x')$$

By ***ground state*** we mean

$$H|\Psi_n\rangle = E_n|\Psi_n\rangle \qquad E_0 \leq E_1 \leq E_2 \leq \ldots$$

Then the ground state is $|\Psi_0\rangle$

(May be degenerate, meaning $|E_1 - E_0| \sim e^{-aN}$)

Special cases of ground states

Case #1: Heisenberg ferromagnet

$$H = -\sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

$$|\Psi_0\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = |\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle$$

Special cases of ground states

Case #1: Heisenberg ferromagnet

$$H = -\sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1}$$

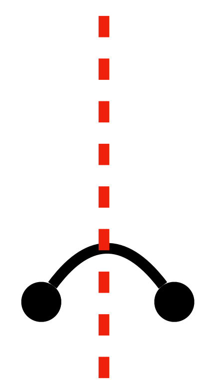
$$|\Psi_0\rangle = |\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\rangle = |\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle|\uparrow\rangle$$

zero entanglement

How typical are these cases?

As system size N increases, is following possible?

$$|\Psi_0\rangle =$$



$$S = \ln(2)$$

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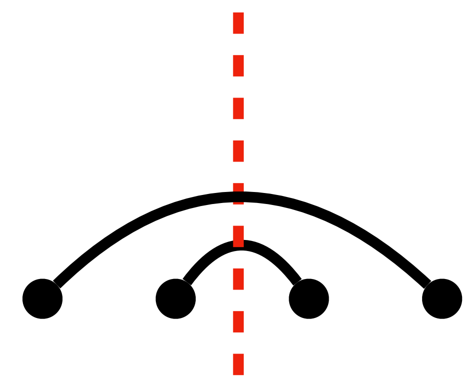
As system size N increases, is following possible?

$$|\Psi_0\rangle =$$

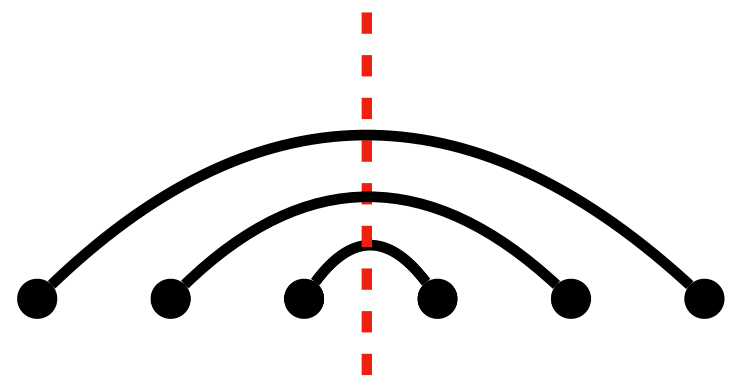


$$S = 2\ln(2)$$

How typical are these cases?

As system size N increases, is following possible?

$$|\Psi_0\rangle =$$

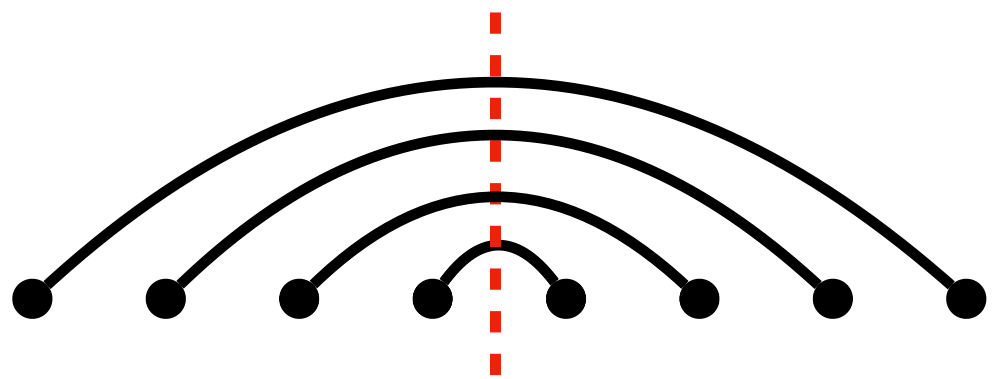


$$S = 3\ln(2)$$

How typical are these cases?

As system size N increases, is following possible?

$$|\Psi_0\rangle =$$



$$S = 4\ln(2)$$

Would give a "**volume law**" of entanglement: $S \sim N$

But Hamiltonian would be non-local:

$$H = \mathbf{S}_1 \cdot \mathbf{S}_8 + \mathbf{S}_2 \cdot \mathbf{S}_7 + \mathbf{S}_3 \cdot \mathbf{S}_6 + \ldots$$

What is the case for *local* Hamiltonians?

Around 2000-2005 many researchers observed for 1D systems, that $S_{\rm vN} \sim {\rm const.} \sim N^0$ for the ground state

But logarithmic violations also observed (Vidal, 2003)

What is the case for *local* Hamiltonians?

Around 2000-2005 many researchers observed for 1D systems, that $S_{\mathrm{vN}} \sim \mathrm{const.} \sim N^0$ for the ground state

But logarithmic violations also observed (Vidal, 2003)

Then in 2007, M. Hastings proved:

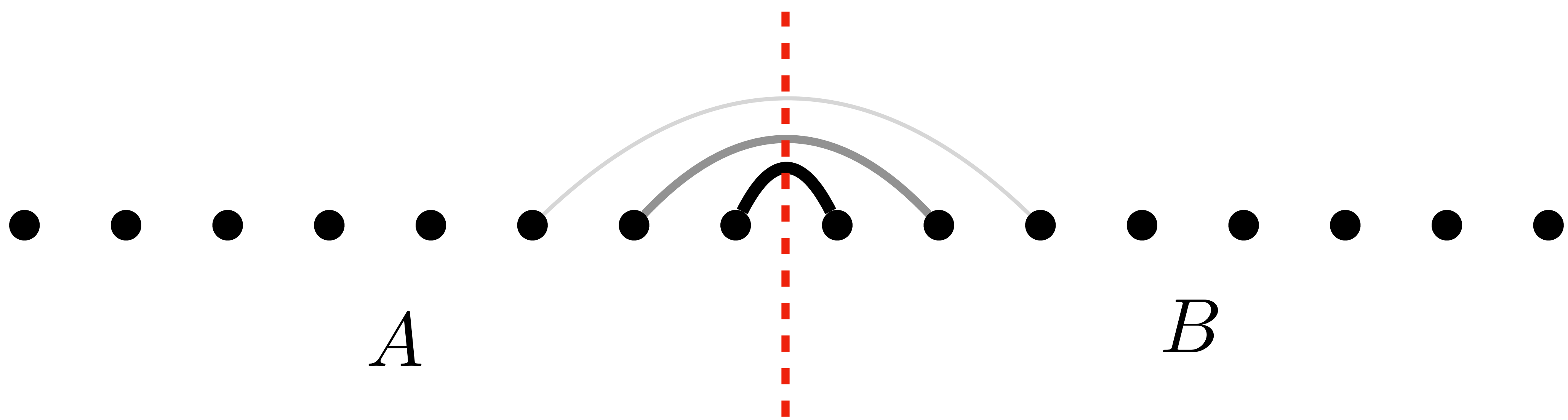
> For 1D, **local** Hamiltonians with a **gap** between ground and excited states, the entanglement entropy of a bipartition is independent of system size as $N \to \infty$

this is the "**area law**" or "**boundary law**"

Hastings, J. Stat. Mech. P08024 (2007)

Intuition of **boundary law**

All entanglement between A and B due to entangled spins near their boundary



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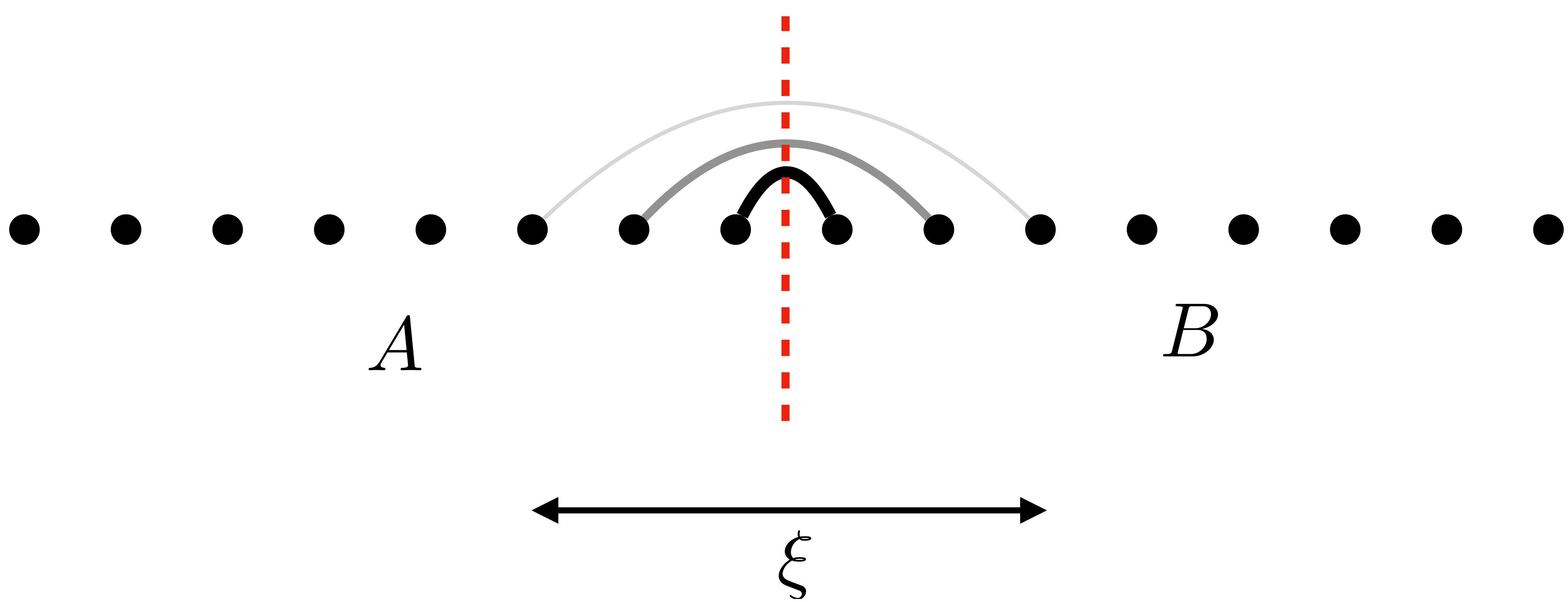

Local H and **gap** required implies a correlation length ξ

Takeaway

- MPS guaranteed to obey boundary law, as do all 1D ground states (of gapped, local Hamiltonians)

- MPS can capture certain interesting states exactly

- maybe they are a useful class of wavefunction to optimize!

Future seminar/lecture (?)

- Matrix Product Operators.
- DMRG in the MPS language.
- Can it be extended to 2D?

  “2D-DMRG” (cylinders)

  PEPS, MERA,...

What is the **scaling** of calculations with MPS?

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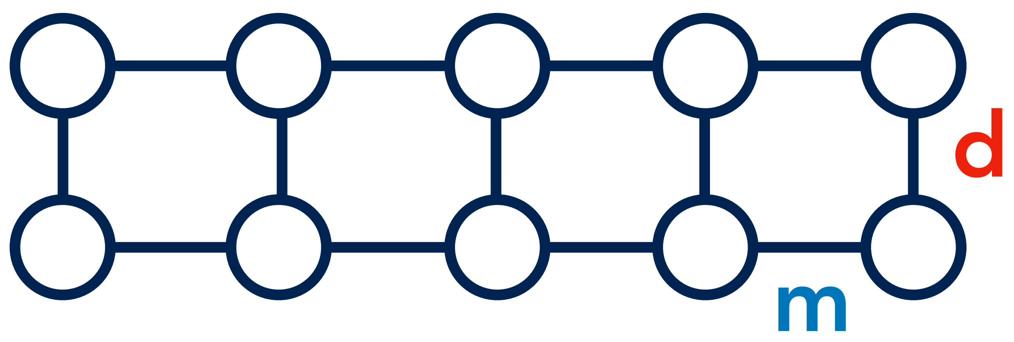
Consider norm of MPS bond dimension **m**, site dimension **d**

$$\langle \Psi | \Psi \rangle =$$



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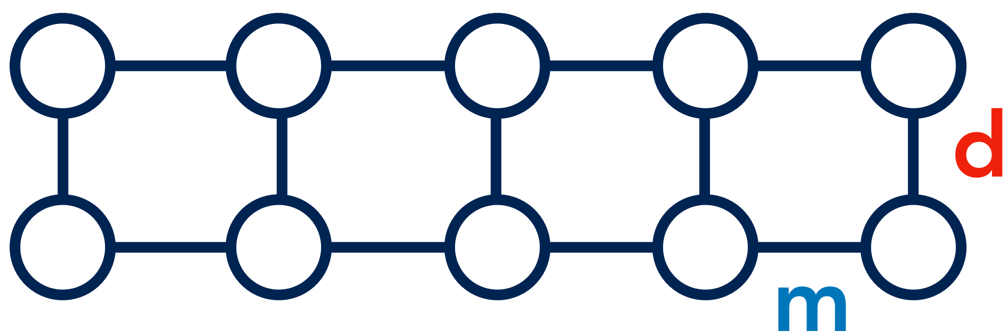

Two key operations

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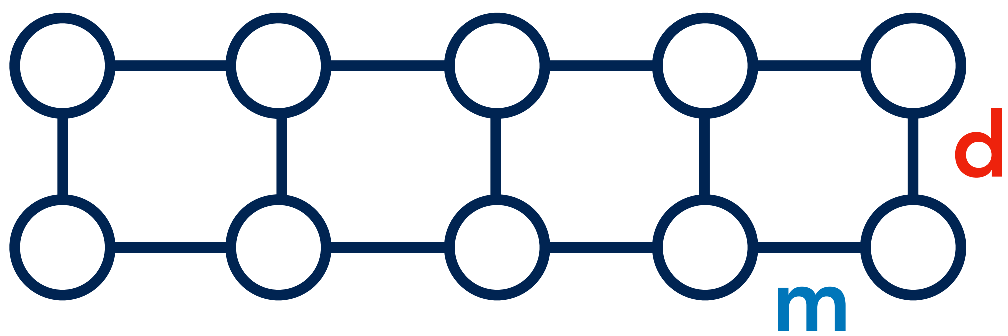
$$\langle \Psi | \Psi \rangle =$$ 

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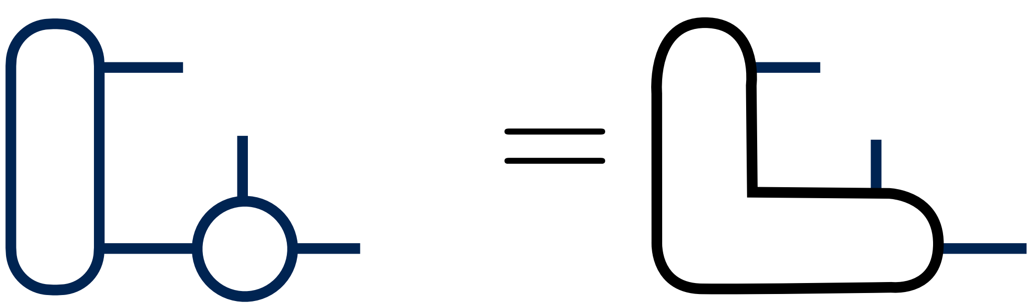
(1) 

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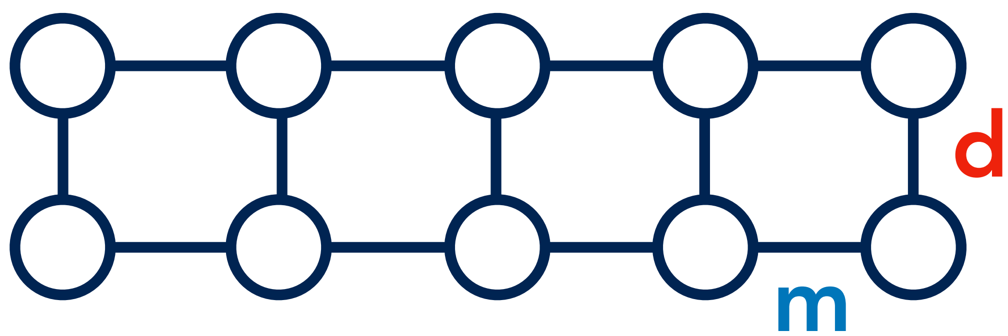

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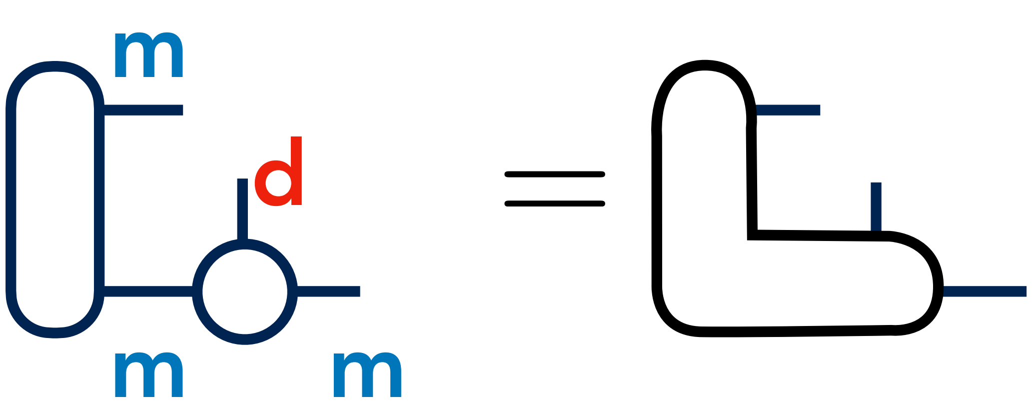

scaling is $m^3\, d$

What is the **scaling** of the computational cost ?

Consider norm calculation, MPS bond dimension **m**,
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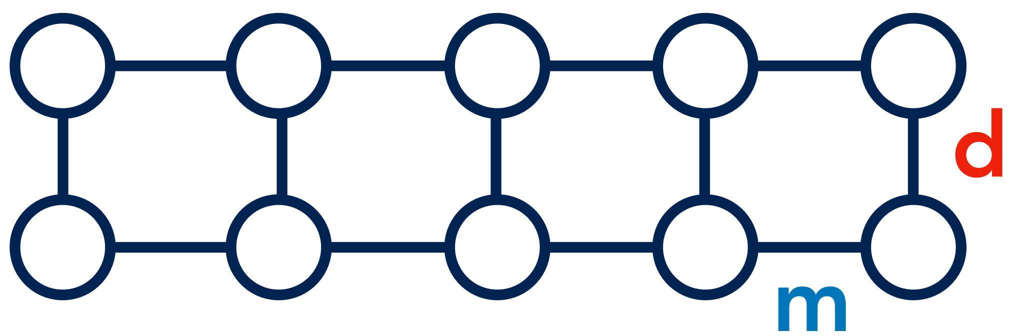
$\langle \Psi | \Psi \rangle =$ 

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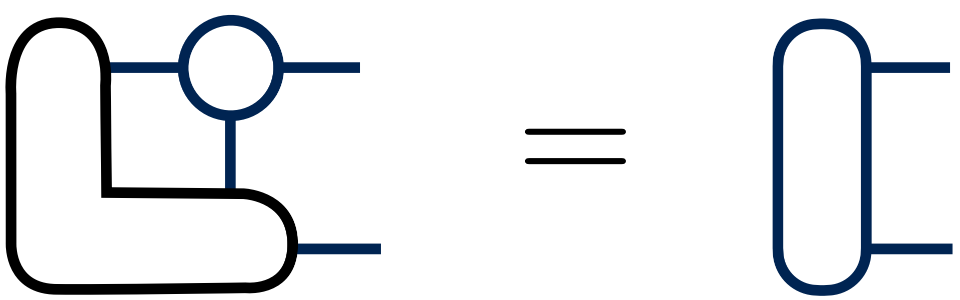
(2) 

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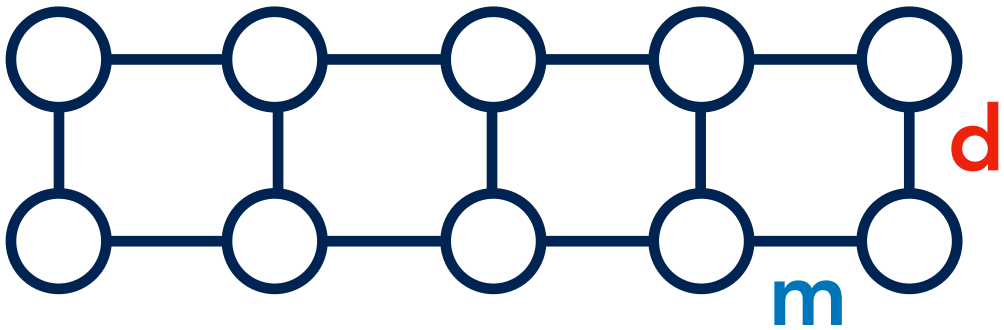
$\langle\Psi|\Psi\rangle =$ 

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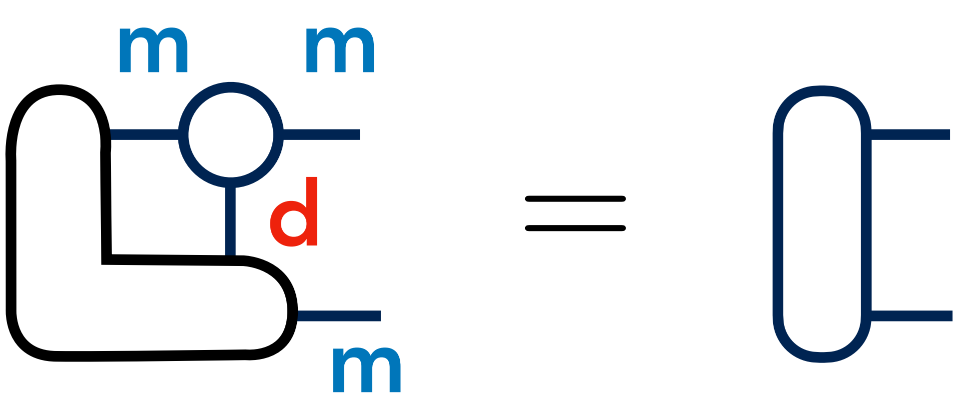
(2) 

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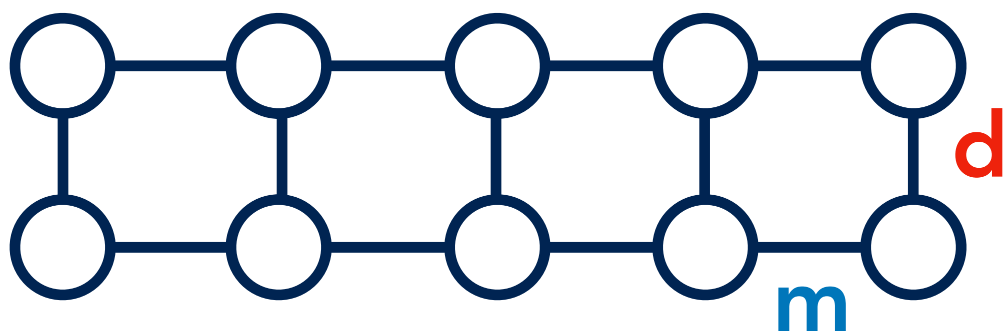
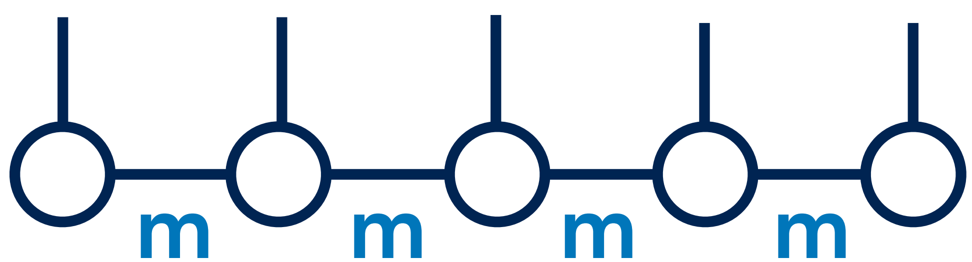


So overall scaling of norm calculation is

$$m^3 \, d$$

Rule of thumb: most every operation needed to manipulate MPS can be made to scale as

$$m^3$$



Intuition: MPS involves multiplying **m**x**m** matrices

Scaling of **m**x**m** matrix multiplication is m^3