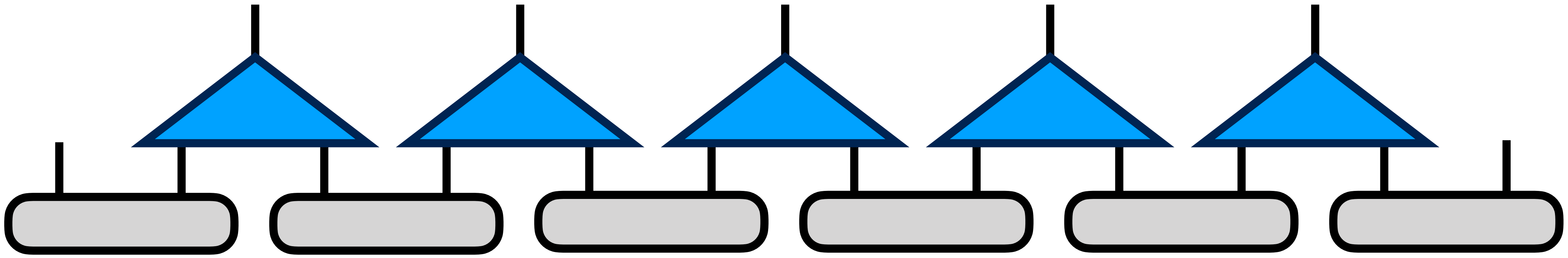
Tensor Networks and Applications



E.M. Stoudenmire

Apr 2018 - Sao Paulo

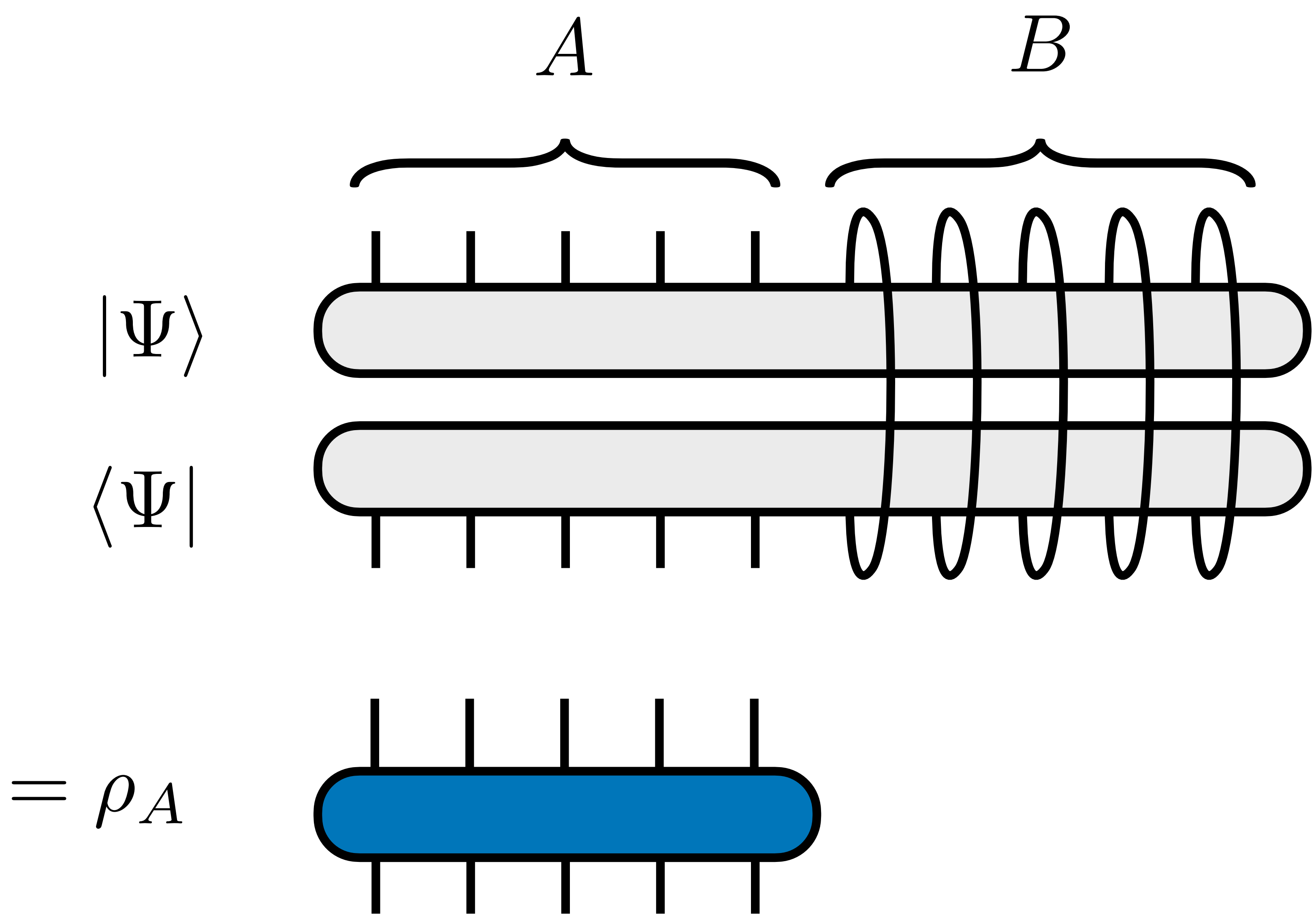
FLATIRON INSTITUTE

SIMONS FOUNDATION

Review of Previous Lecture

Reduced density matrix

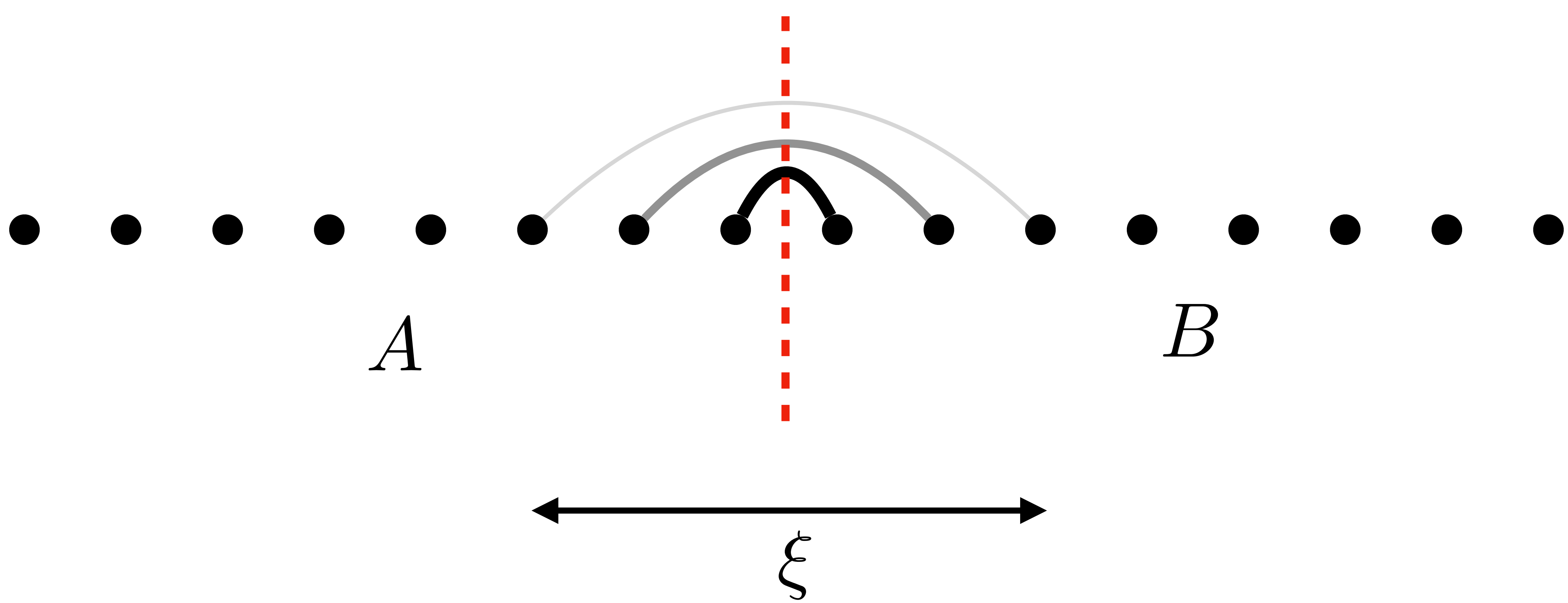
Trace over region B to get reduced density matrix of A



Eigenvalues of ρ_A define entanglement between A and B

Boundary law implies limited entanglement of ground states

Entanglement between A and B due to spins near boundary (for ground state of gapped, local Hamiltonian)



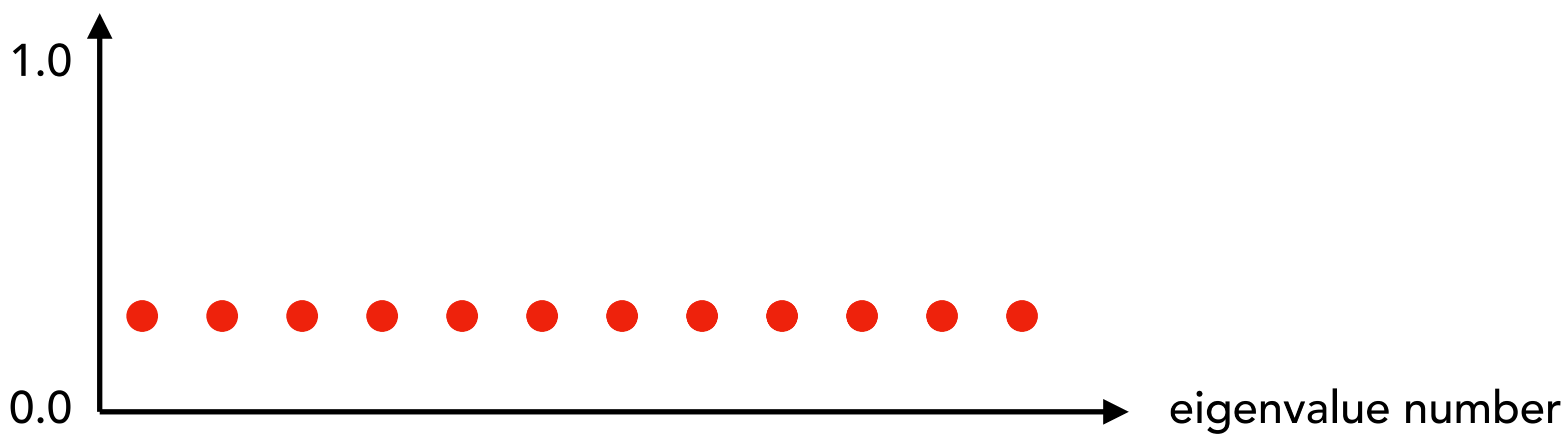
Local H and **gap** implies a correlation length ξ

Truncating Wavefunctions

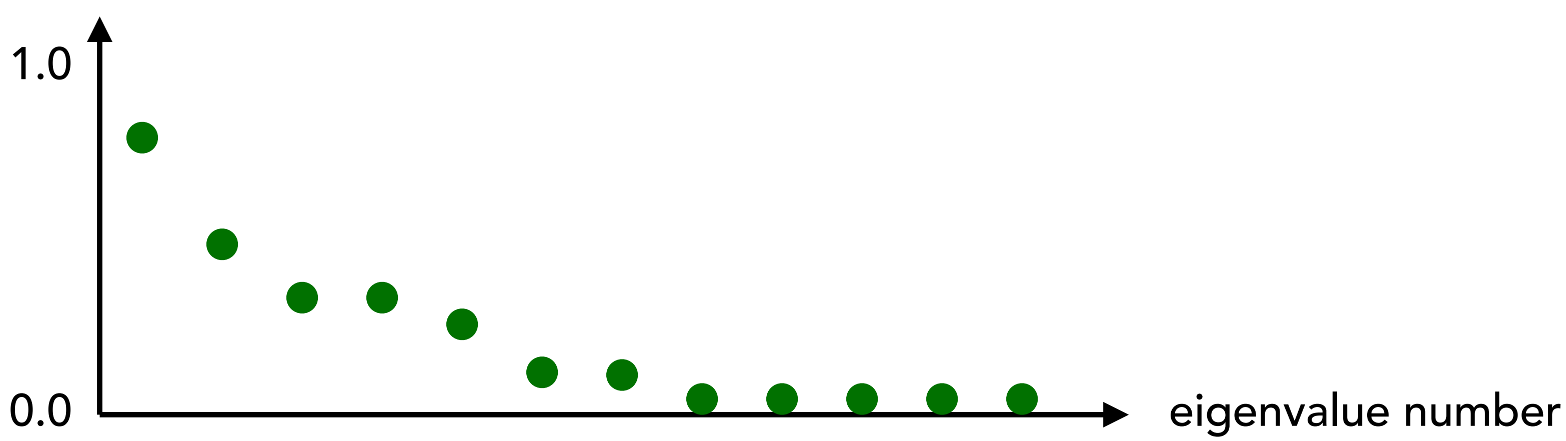
Boundary law means entanglement much less than it could be

So density matrix eigenvalues fall quickly...

Random state:

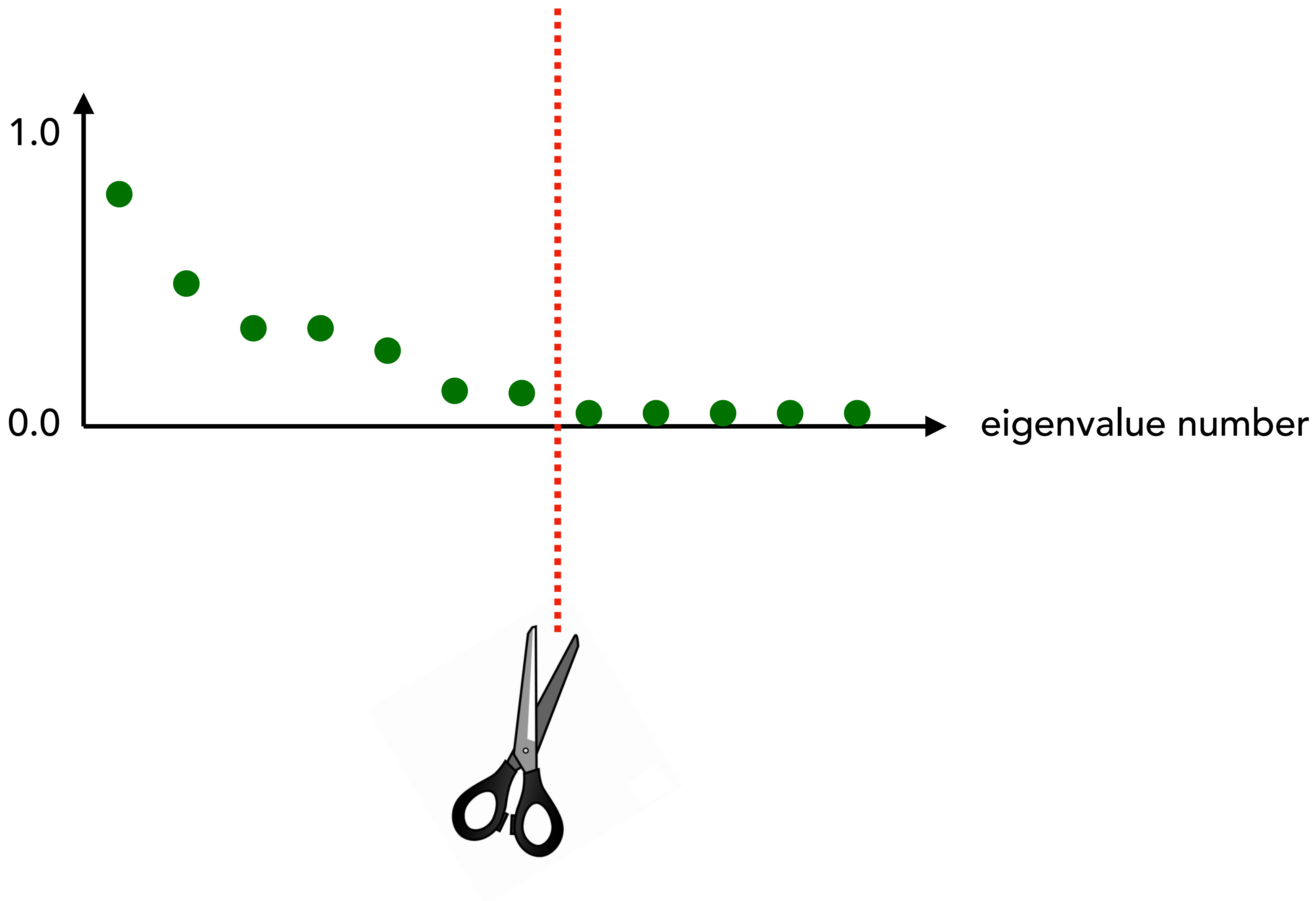


Ground state:



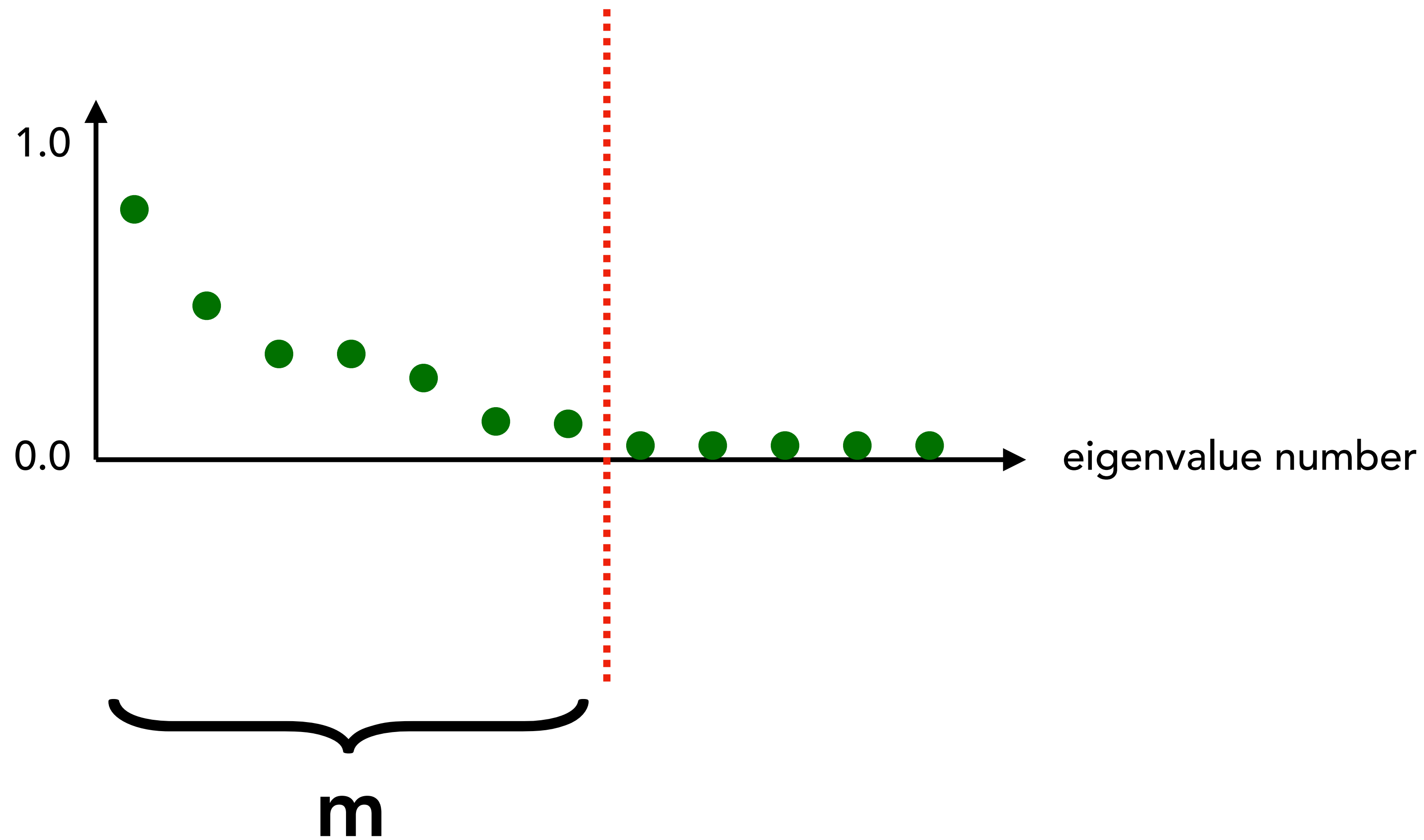
Suggests an approximation

Idea of **truncating** density matrix spectrum



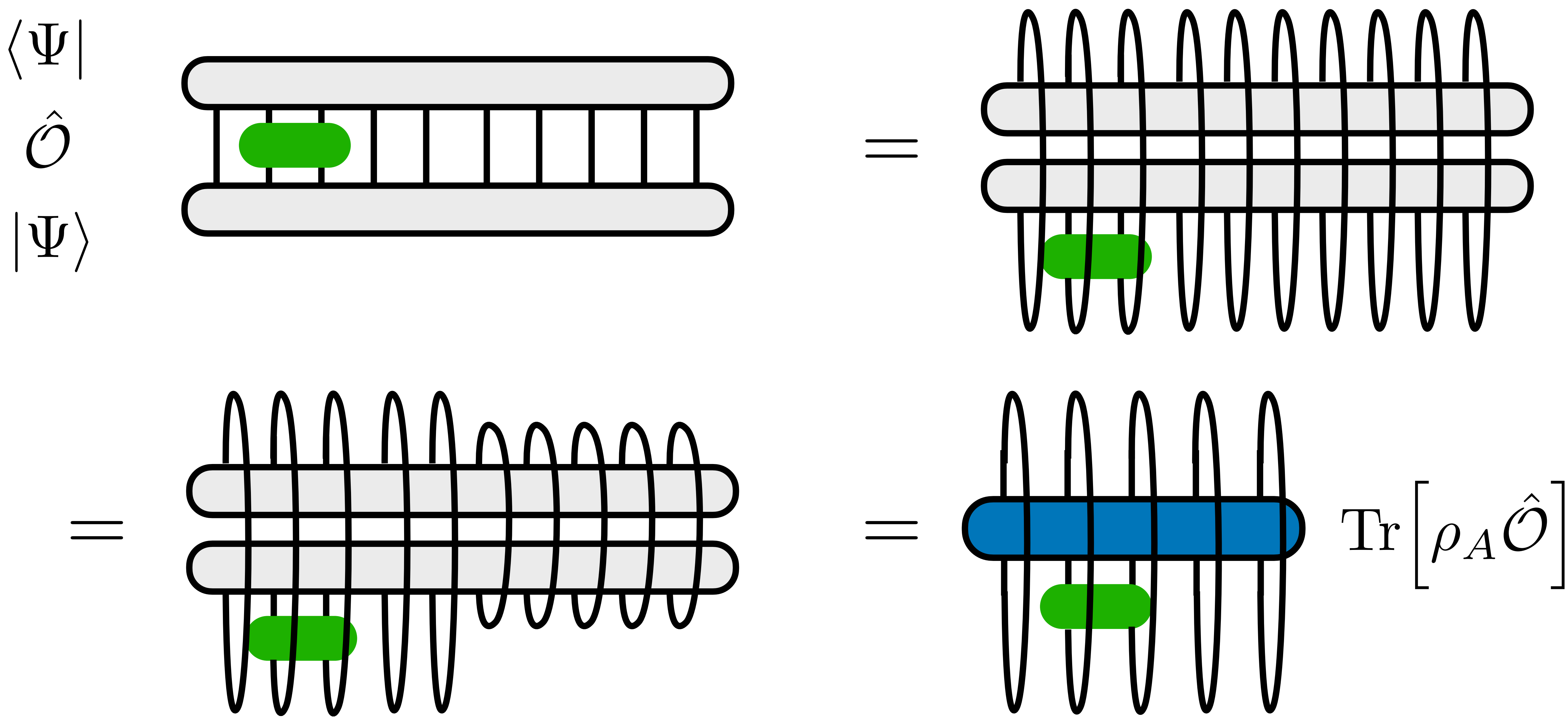
Implication of **boundary law** (= area law):

Number of eig. vals **m** needed for accuracy doesn't grow with N



Why approximate density matrix?

Reduced density matrix determines **all** observables in region A



Any observable in region A can be written as

$$\langle \hat{\mathcal{O}} \rangle = \langle \Psi | \hat{\mathcal{O}} | \Psi \rangle = \mathrm{Tr}\left[\rho_A \hat{\mathcal{O}} \right]$$

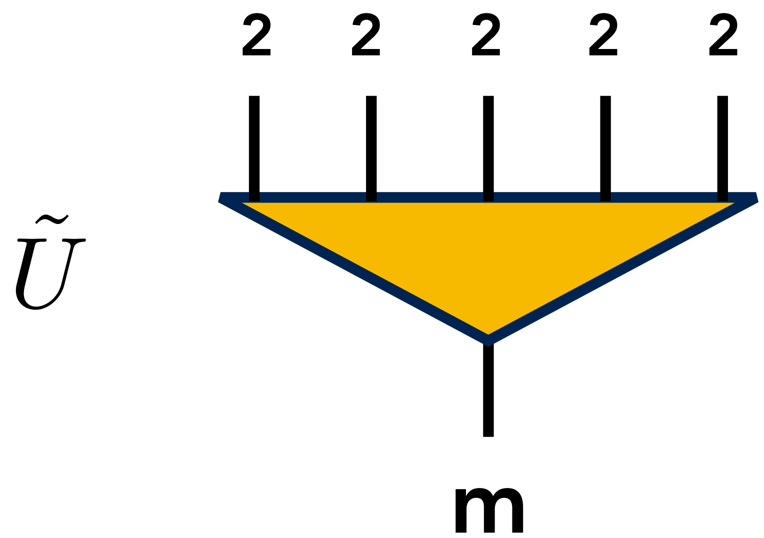
If we diagonalize $\rho_A = \sum_n p_n |n\rangle\langle n|$

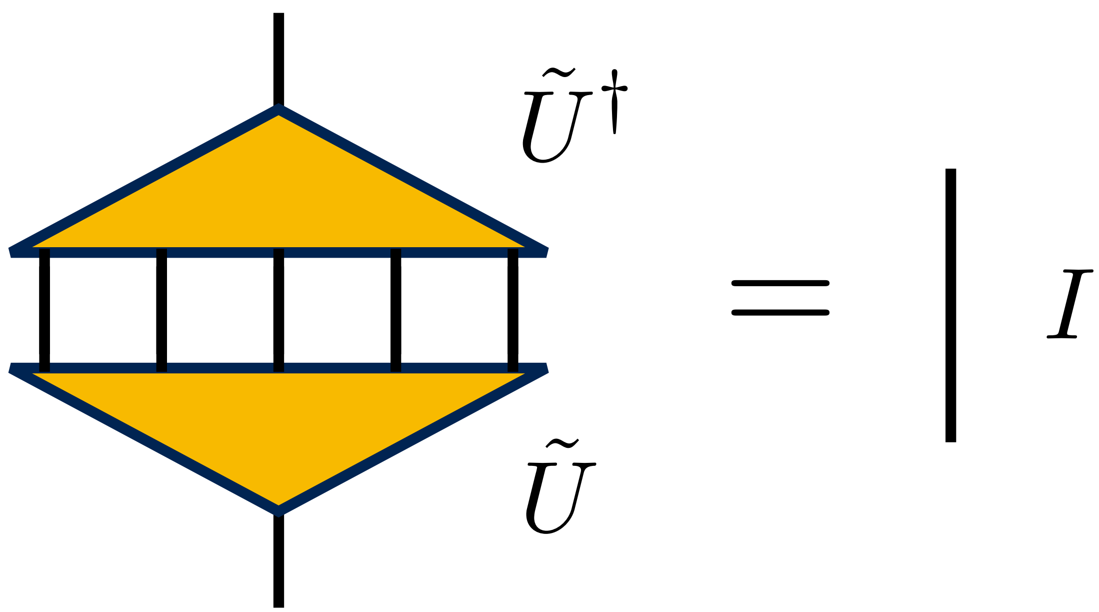
$$\langle \hat{\mathcal{O}} \rangle = \mathrm{Tr}\left[\rho_A \hat{\mathcal{O}} \right] = \sum_n p_n \langle n | \hat{\mathcal{O}} | n \rangle$$

discarding small p_n *means small error in* $\langle \hat{\mathcal{O}} \rangle$

Ability to truncate ρ_A means the following

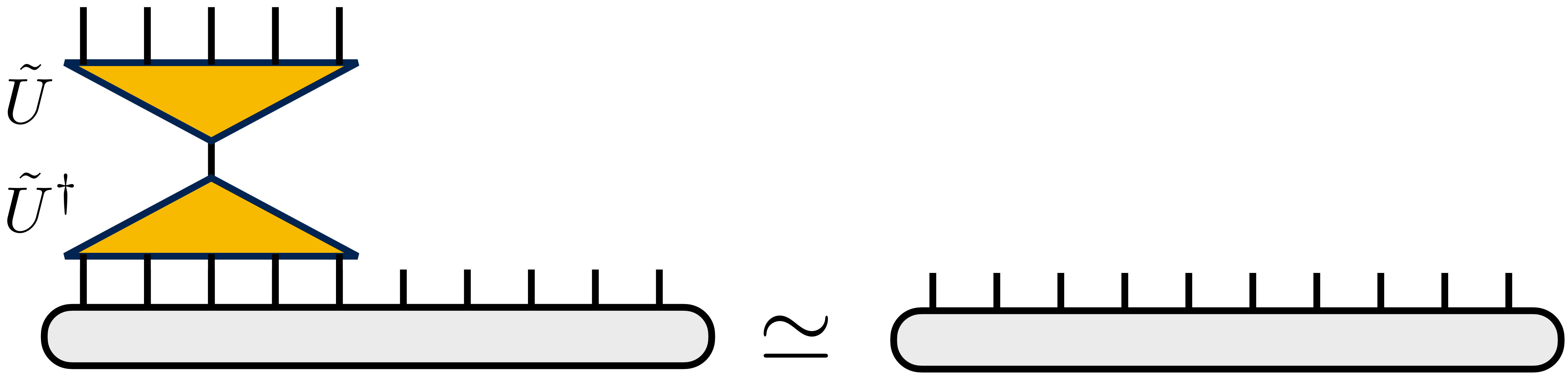
There is an isometry (rotation + projection) from sites of A to truncated basis of ρ_A





$\tilde{U}$ is first **m** columns of unitary diagonalizing ρ_A

Proposition: following approximation holds

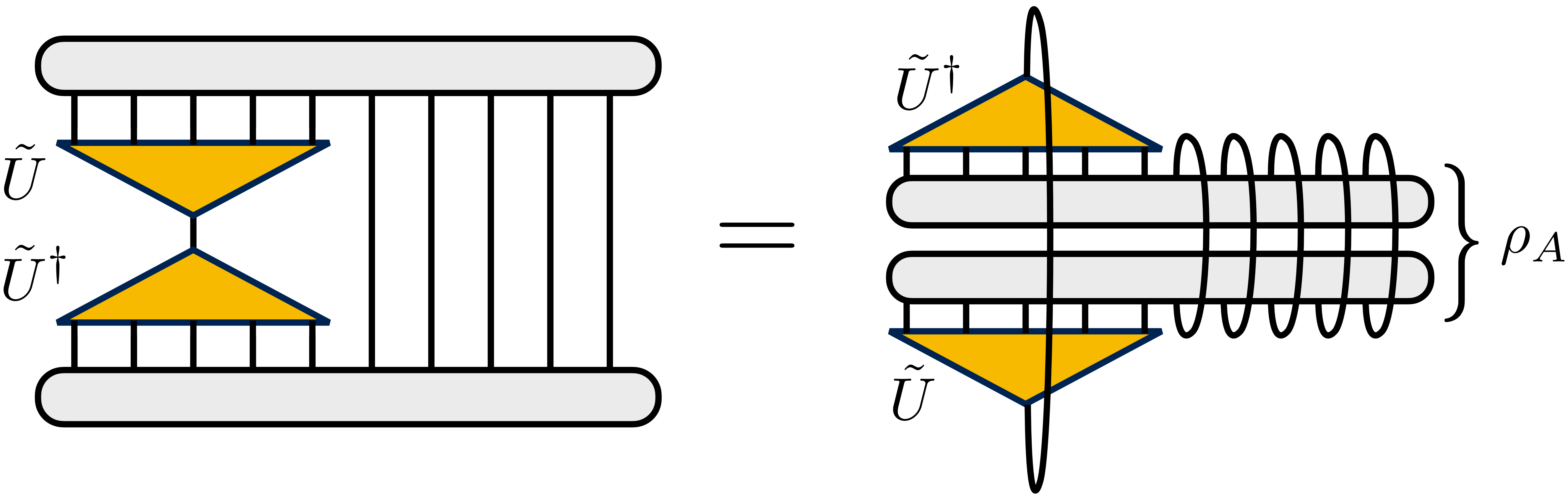


$$\tilde{U}\tilde{U}^\dagger|\Psi\rangle \simeq |\Psi\rangle + \mathcal{O}(\epsilon)$$

Where $\epsilon = \sum_{n=m+1}^{d_A} p_n$ is the sum of discarded eigenvalues of ρ_A

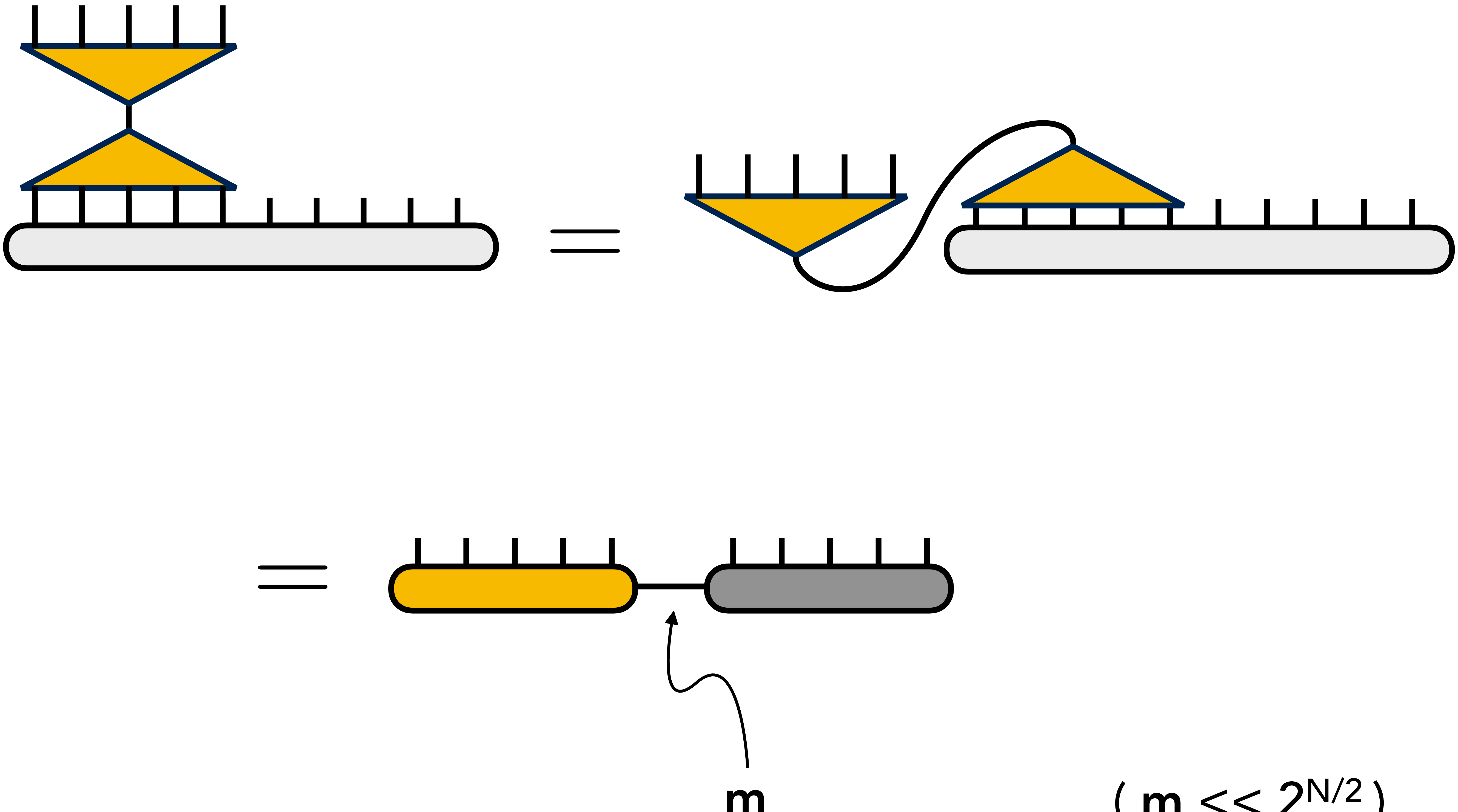
Why?

To prove, compute overlap $\langle\Psi|\left(\tilde{U}\tilde{U}^\dagger|\Psi\rangle\right)$



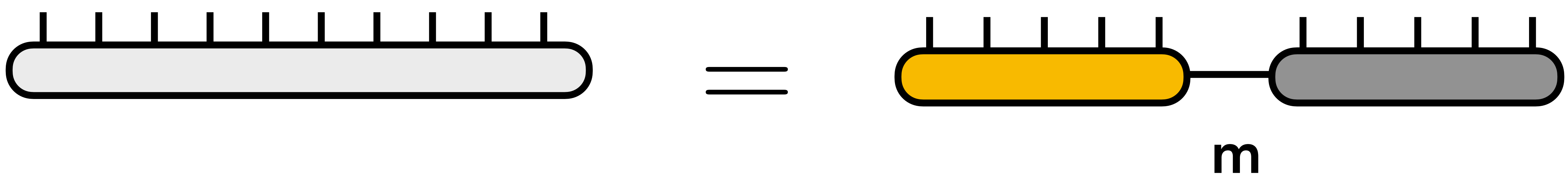
$$= \tilde{U}^\dagger \rho_A \tilde{U} = \sum_{n=1}^{m} p_n = \boxed{1-\epsilon}$$

Can approximately rewrite $|\Psi\rangle$ as follows



$(m << 2^{N/2})$

The upshot is we can factorize any ground state



2^N dimensional 'vector'

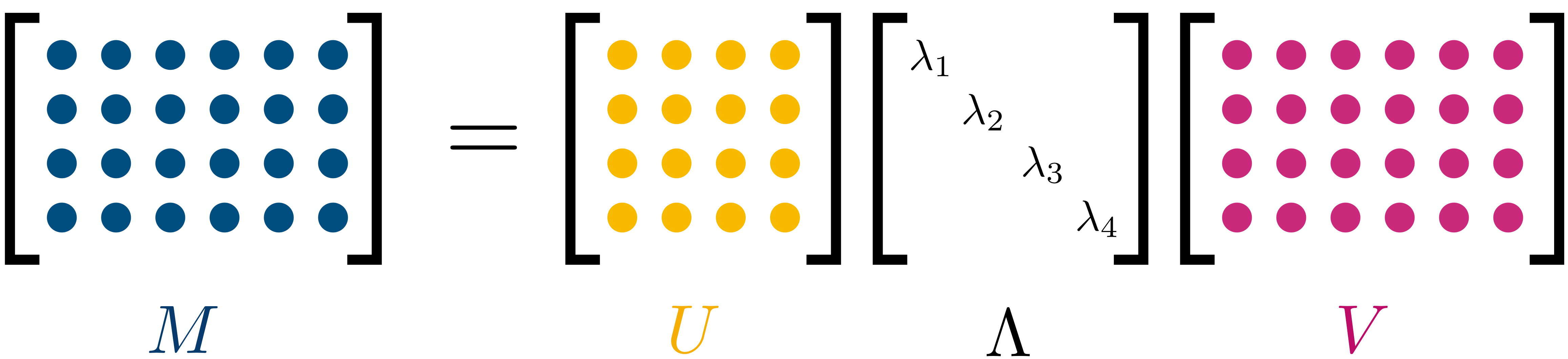
two ($2^{N/2}$ x **m**) 'matrices'

huge reduction in parameters!

Density matrix approach is "roundabout" however

Simpler approach is singular value decomposition (SVD)

Recall, for any rectangular matrix:



U and V are unitary, and singular values λ_n are real & positive

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:

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

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

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

Keep fewer and fewer singular values:

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

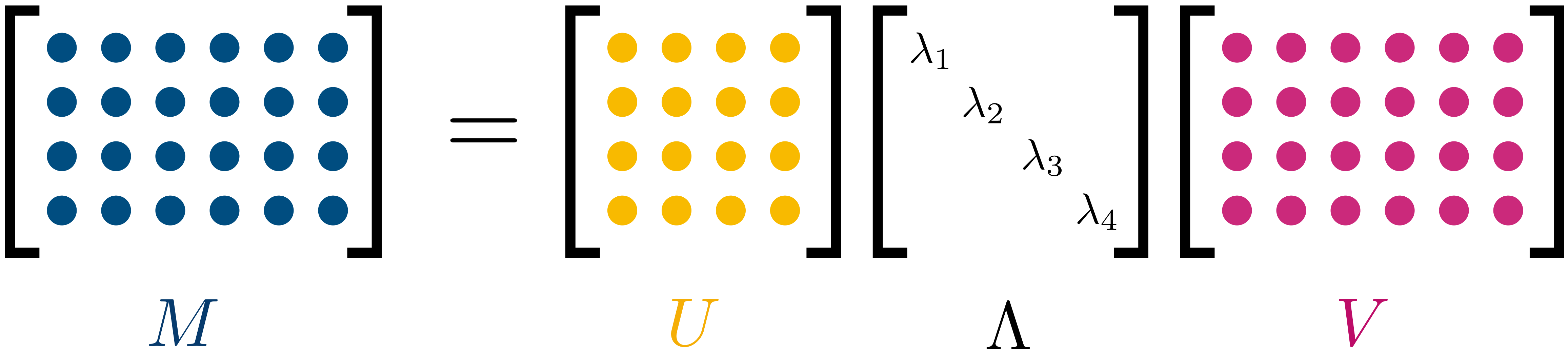
$$= M_3 = \begin{bmatrix} 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \\ 0.329773 & 0.329773 & 0 \end{bmatrix}$$

Truncating SVD =

Controlled approximation for M

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

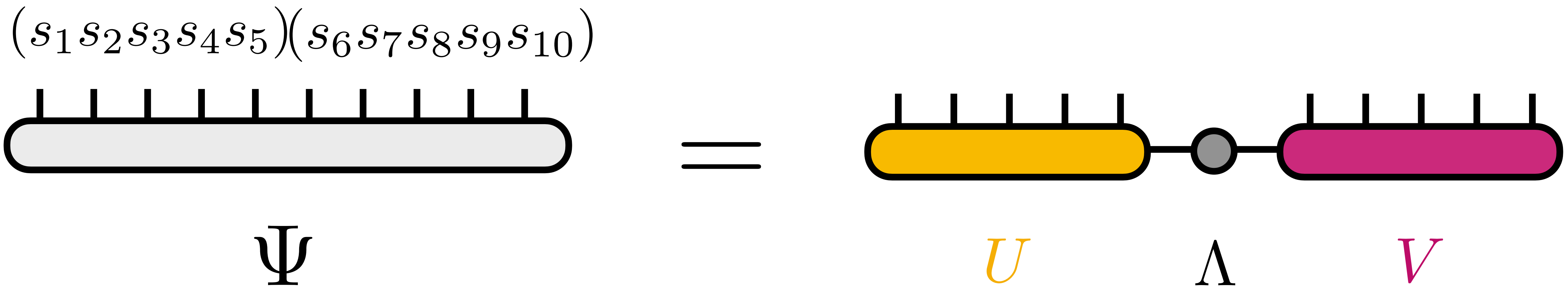
Diagrammatically, SVD looks like:



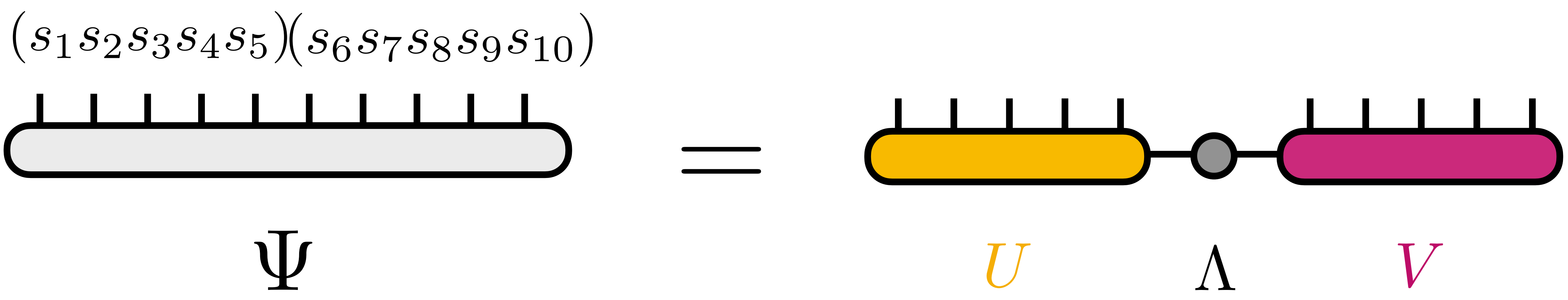
Let's apply it to our wavefunction

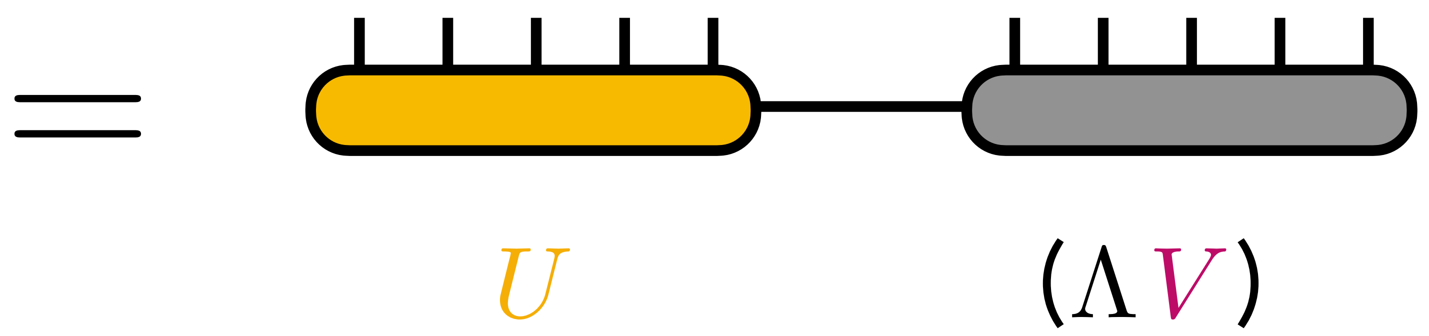
Treat wavefunction as matrix by grouping indices

$$\Psi^{(s_1 s_2 s_3 s_4 s_5)(s_6 s_7 s_8 s_9 s_{10})} = \sum_n U_n^{(s_1 s_2 s_3 s_4 s_5)} \Lambda_n V_n^{(s_6 s_7 s_8 s_9 s_{10})}$$



Multiplying singular vals into V, get same factorization as before



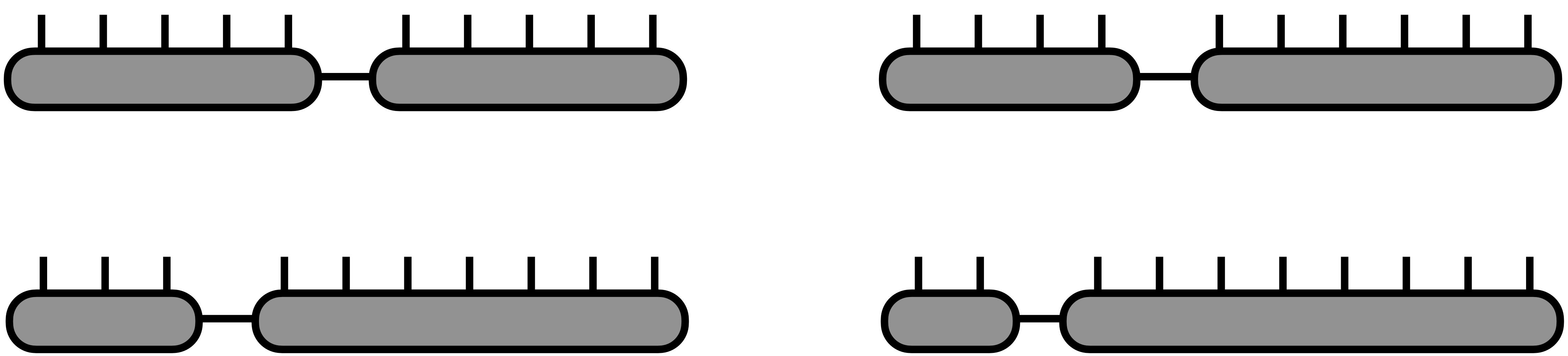


Matrix U is the *same* as from diagonalizing density matrix

Central idea of tensor networks:

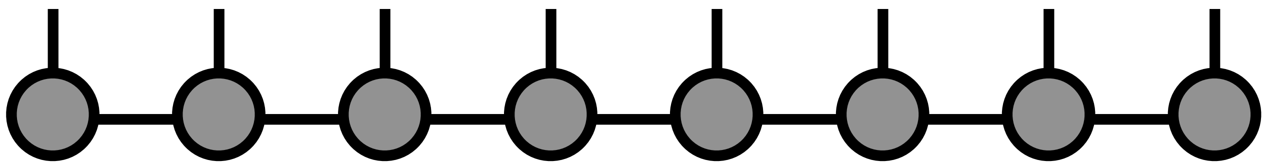
can factorize (s_1 s_2 s_3) (s_4 s_5 s_6), but what is special about this bond or partition?

why not factorize all partitions at once?



etc.

Motivates following factorization



Known as *matrix product state*

Key example of a tensor network

Matrix Product States

Wavefunction just a rule to map spin configurations to numbers $\Psi^{s_1 s_2 s_3 s_4 s_5 s_6 s_7 s_8}$

$$\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow \longrightarrow \Psi^{\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow}$$

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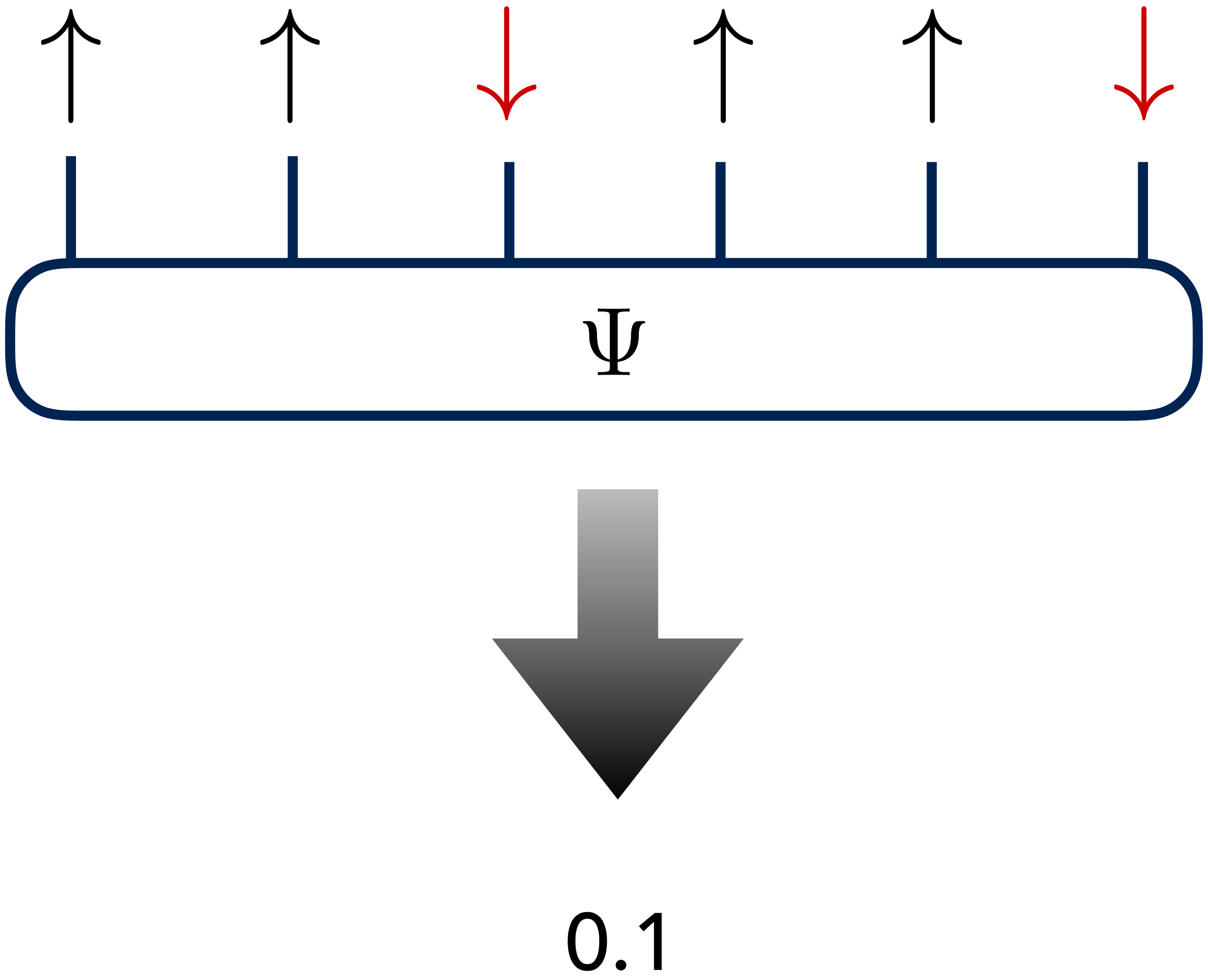
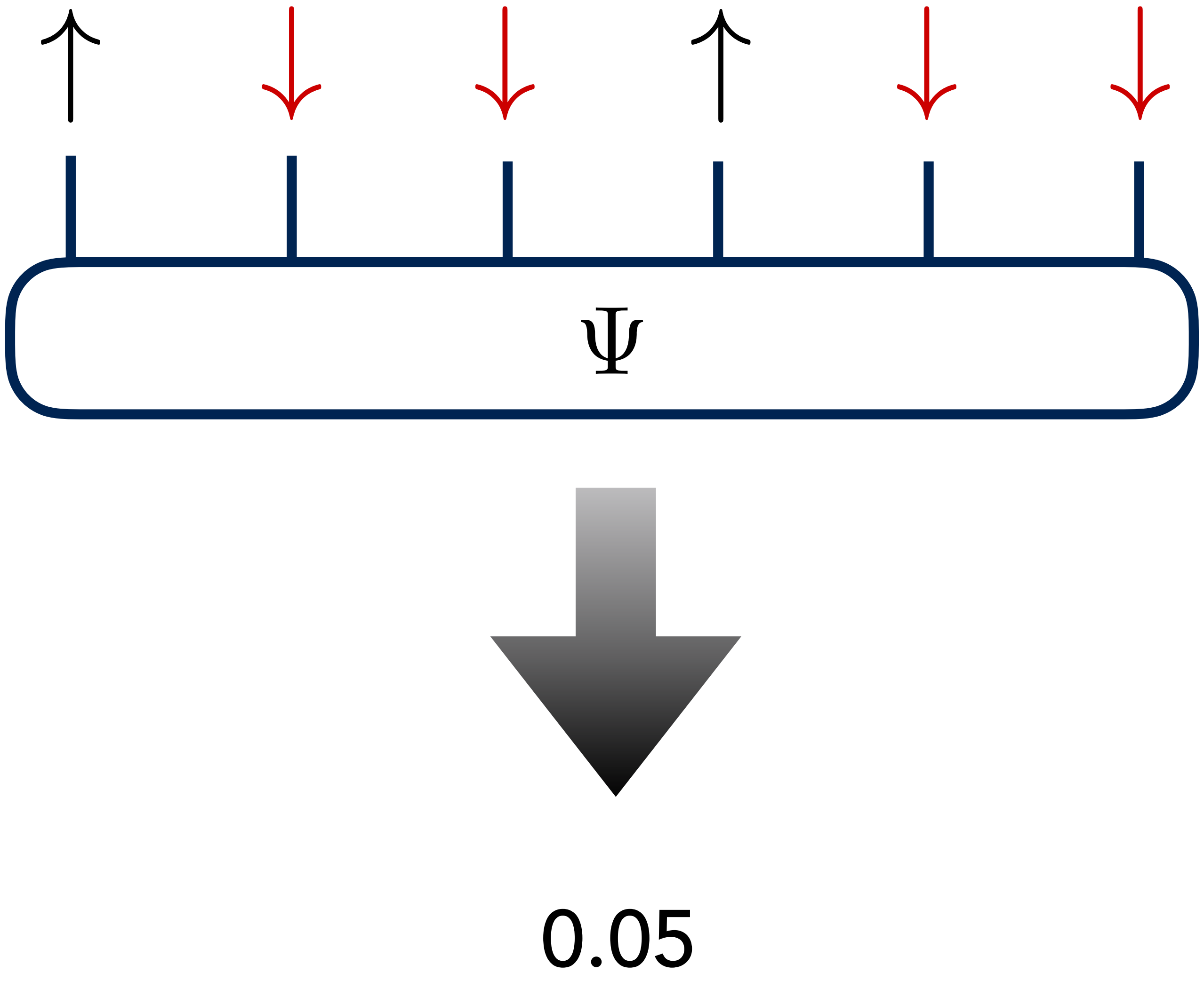
Simplest rule: store every amplitude separately

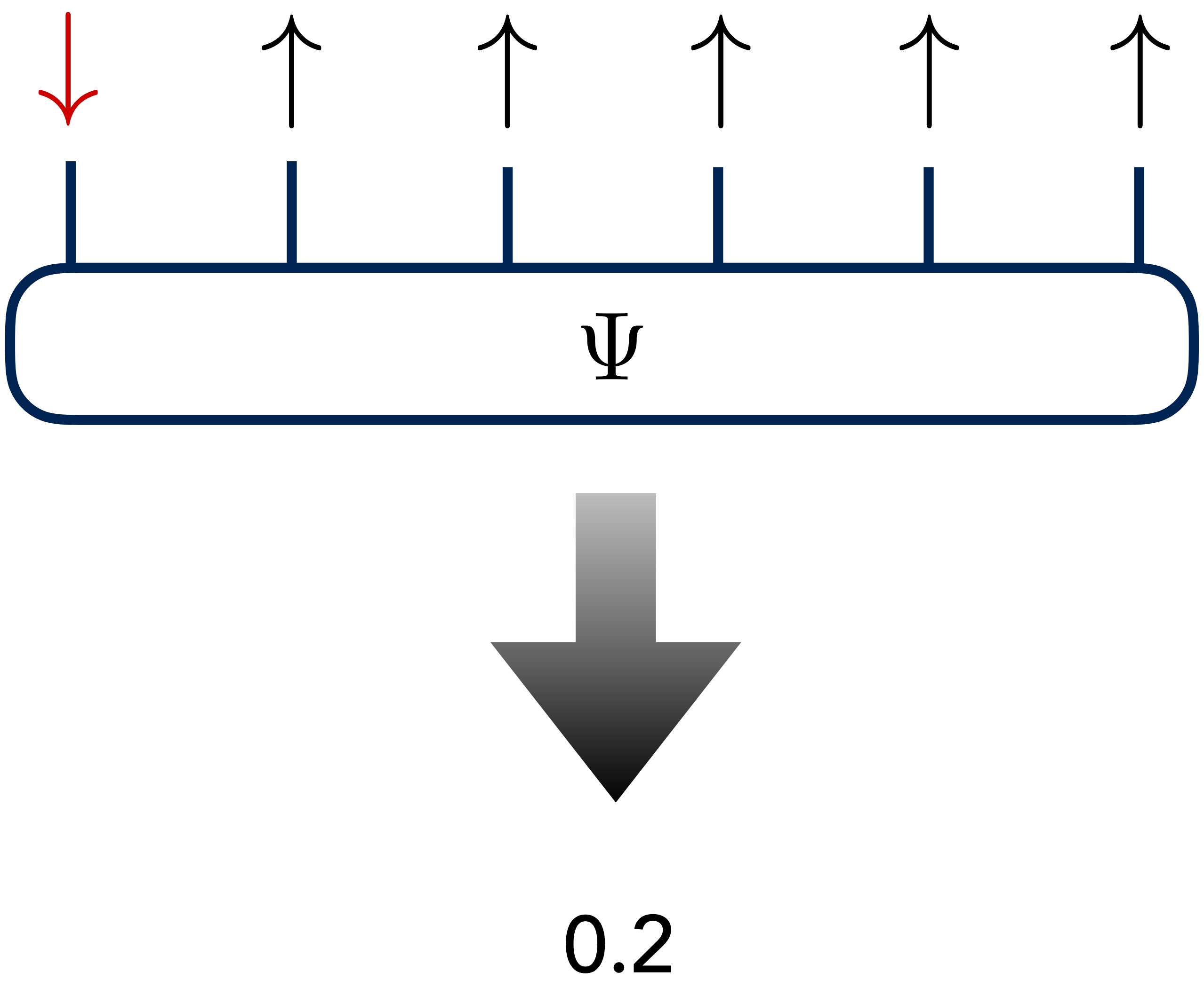
Wavefunction a "machine" mapping configurations to numbers



Wavefunction a "machine" mapping configurations to numbers



Can make up any rule assigning patterns to numbers



How about this rule:

- to each spin state (up, down) associate a matrix
- multiply matrices to get the probability

Pictorially:

$\uparrow$

$\downarrow$

Pictorially:

$$\uparrow \quad \longrightarrow \quad M^{\uparrow} = \begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix}$$

$$\downarrow \quad \longrightarrow \quad M^{\downarrow} = \begin{bmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{bmatrix}$$

Compute wavefunction by multiplying matrices together

$$\Psi^{\uparrow\downarrow\uparrow\uparrow\downarrow} \approx$$

Compute wavefunction by multiplying matrices together

$$\Psi^{\uparrow\downarrow\uparrow\uparrow\downarrow} \approx M_1^{\uparrow}$$

Compute wavefunction by multiplying matrices together

$$\Psi^{\uparrow\downarrow\uparrow\uparrow\downarrow} \approx M_1^{\uparrow} M_2^{\downarrow}$$

Compute wavefunction by multiplying matrices together

$$\Psi^{\uparrow\downarrow\uparrow\uparrow\downarrow} \approx M_1^{\uparrow} M_2^{\downarrow} M_3^{\uparrow}$$

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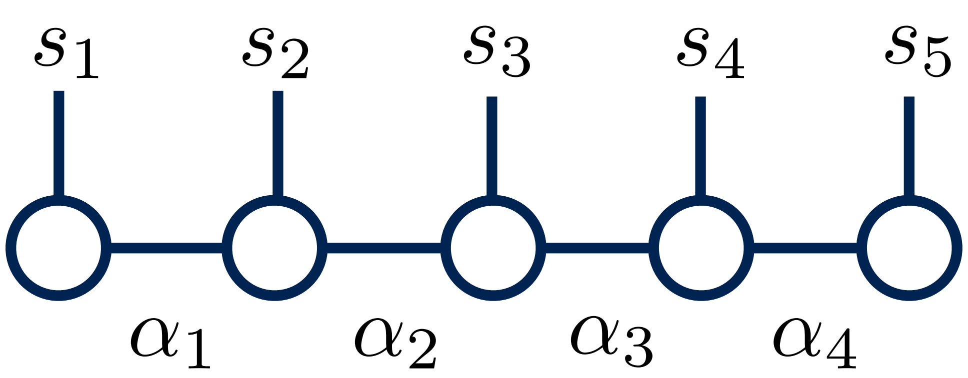
Ansatz known as ***matrix product state***

$$\Psi^{s_1 s_2 s_3 s_4 s_5} = M_1^{s_1} M_2^{s_2} M_3^{s_3} M_4^{s_4} M_5^{s_5}$$

More detail & diagrammatic form

$$\Psi^{s_1 s_2 s_3 s_4 s_5} = M_1^{s_1} M_2^{s_2} M_3^{s_3} M_4^{s_4} M_5^{s_5}$$

$$= \sum_{\{\alpha\}} M_{\alpha_1}^{s_1} M_{\alpha_1 \alpha_2}^{s_2} M_{\alpha_2 \alpha_3}^{s_3} M_{\alpha_3 \alpha_4}^{s_4} M_{\alpha_4}^{s_5}$$

$=$ 

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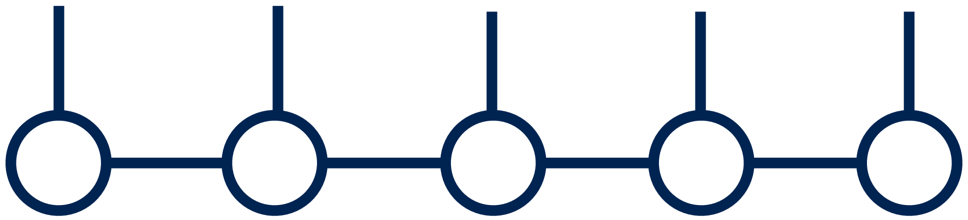
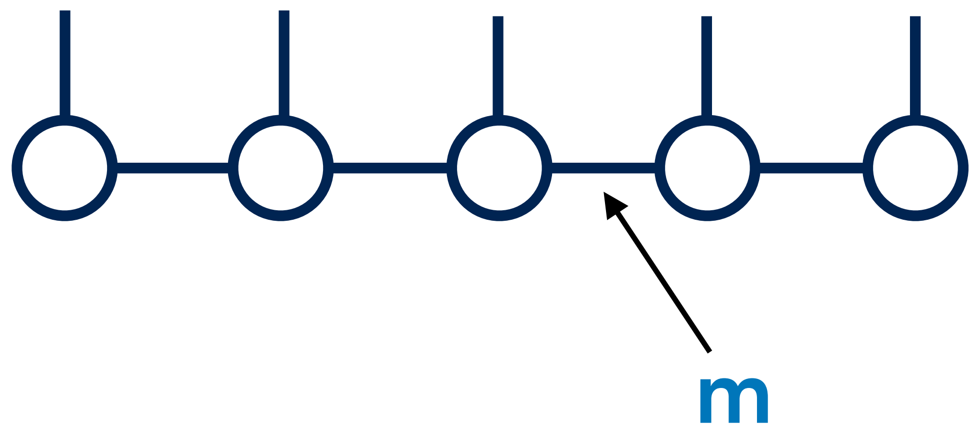
$$=$$



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

Computations with Matrix Product States

Key reason to use matrix product states (MPS) is many computations become *efficient*

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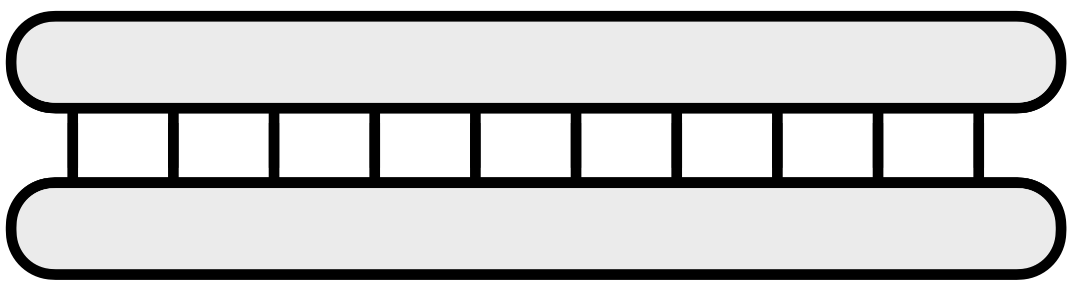
Consider computing norm of full wavefunction

$\langle \Psi | \Psi \rangle$ 

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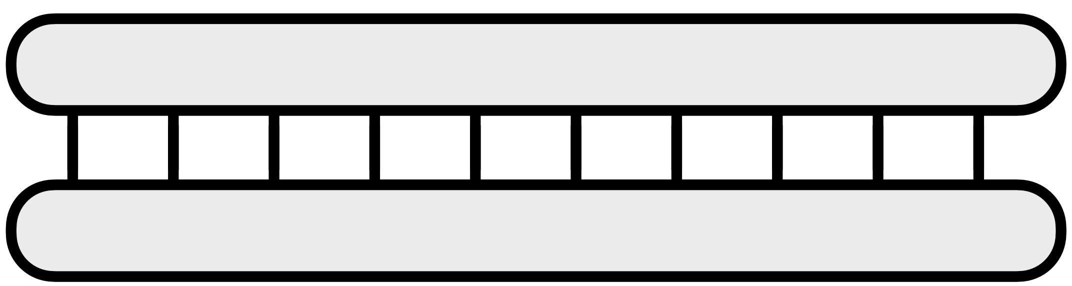
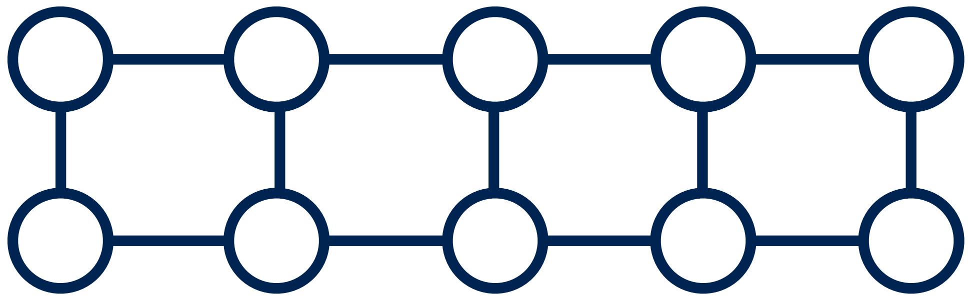
$\langle \Psi | \Psi \rangle$ 

$$= \sum_{\{s\}} \Psi^{s_1 s_2 s_3 s_4 s_5 s_6 s_7 s_8 s_9 s_{10}} \bar{\Psi}_{s_1 s_2 s_3 s_4 s_5 s_6 s_7 s_8 s_9 s_{10}}$$

Requires summing 2^{10} terms

Is there a more efficient strategy to compute norm of MPS?

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



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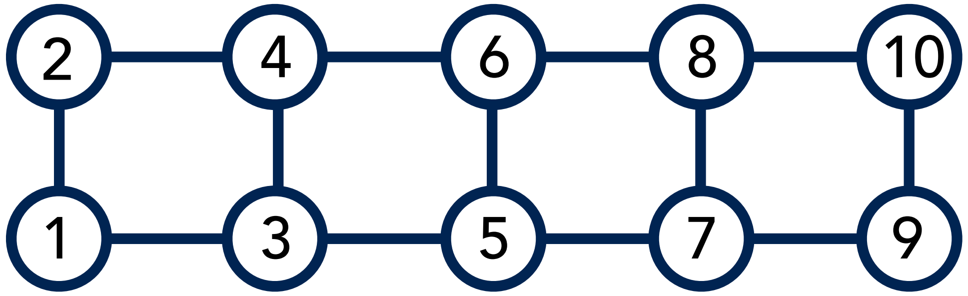

Yes!

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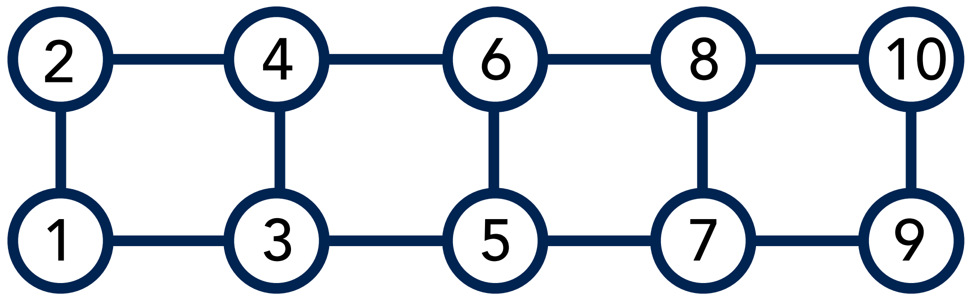
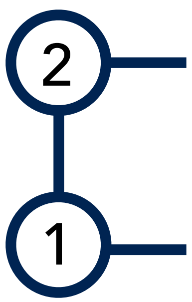


Yes!

(1)



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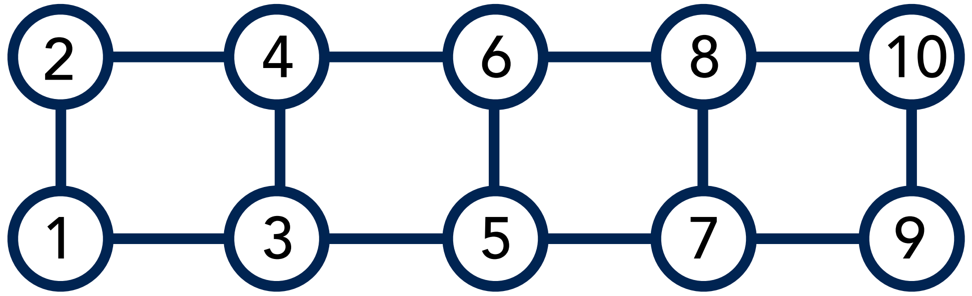
$\langle \Psi | \Psi \rangle =$ 

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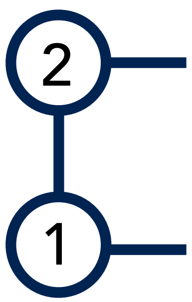
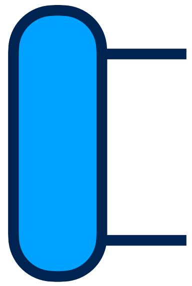
(1) 

$=$ 

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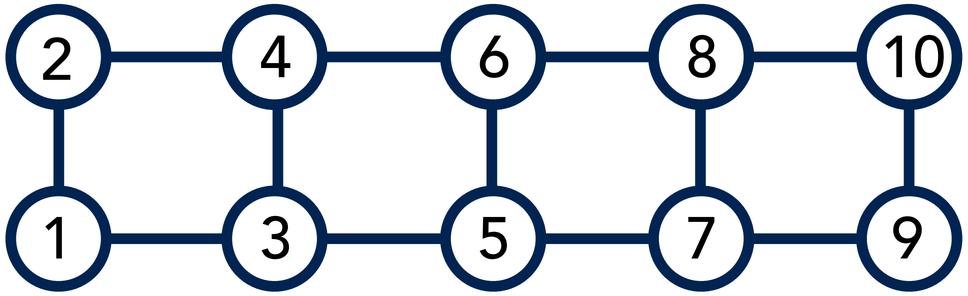

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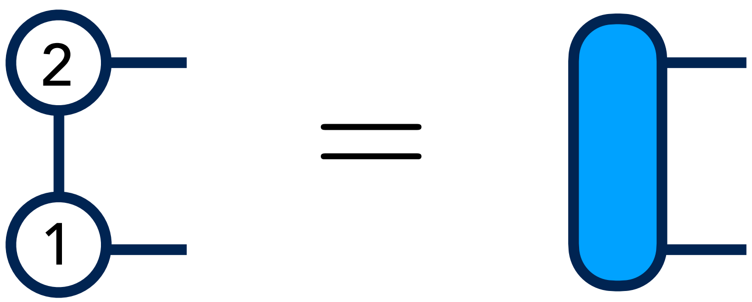
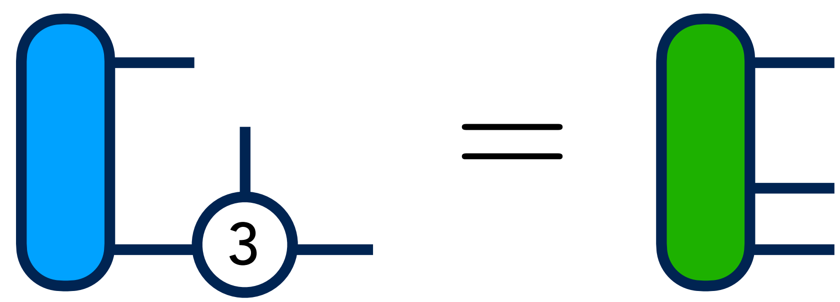
(1) 

(2) 

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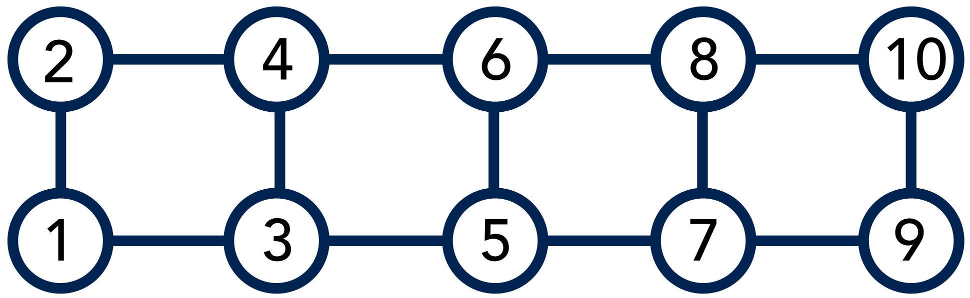
$\langle \Psi | \Psi \rangle =$ 

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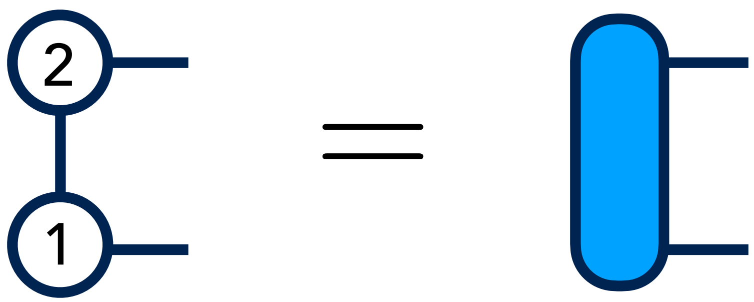
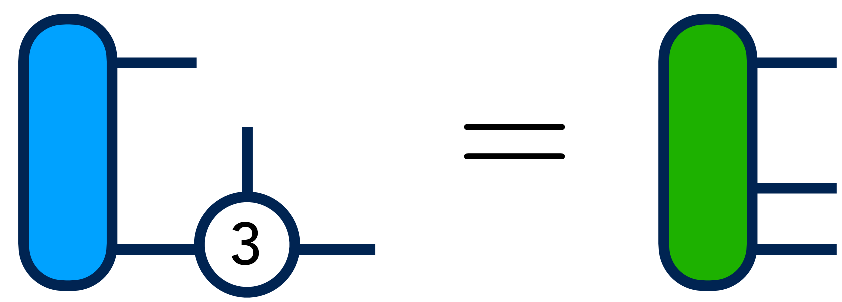
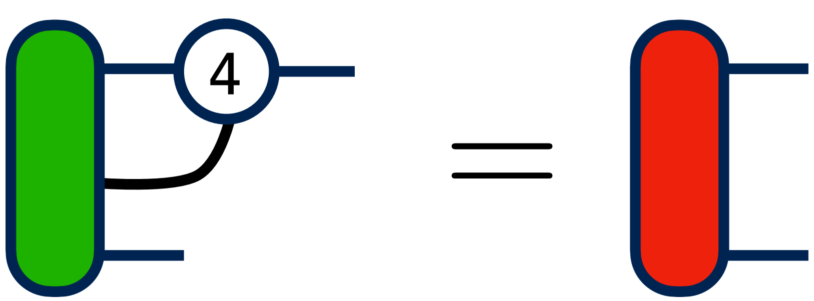
(1) 

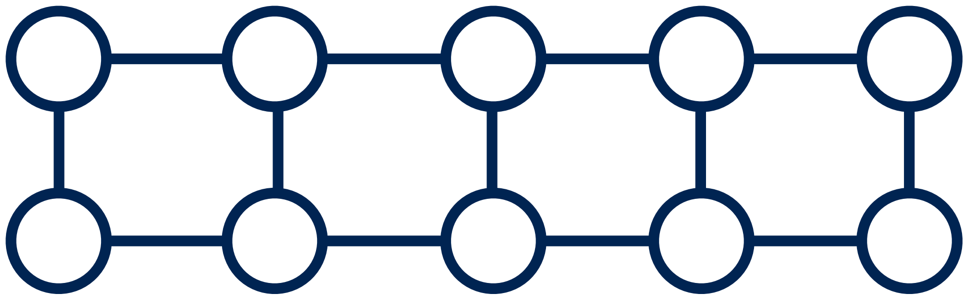
(2) 

(3) 

etc. until all tensors are contracted

Full contraction process:

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



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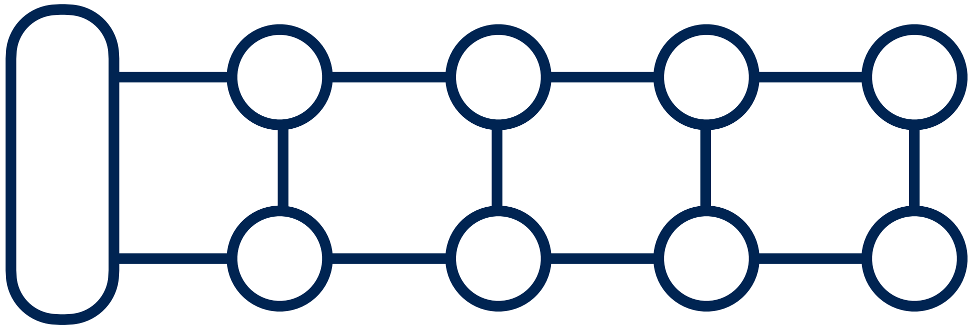

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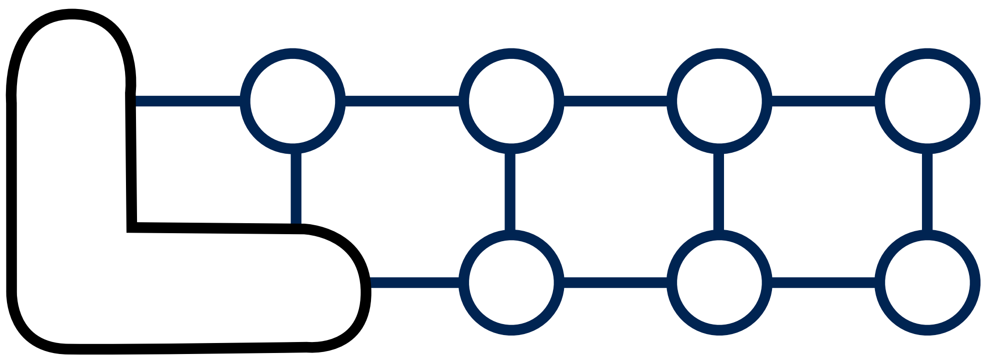

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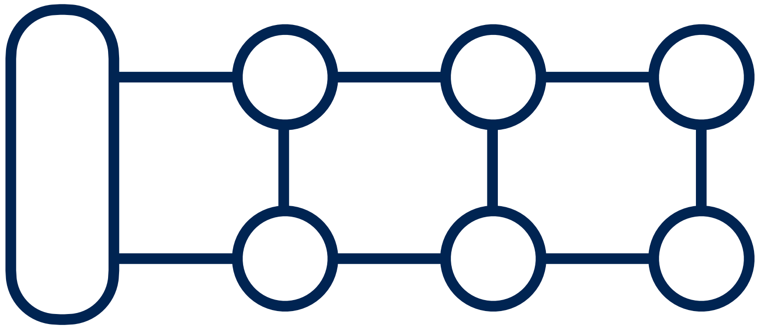

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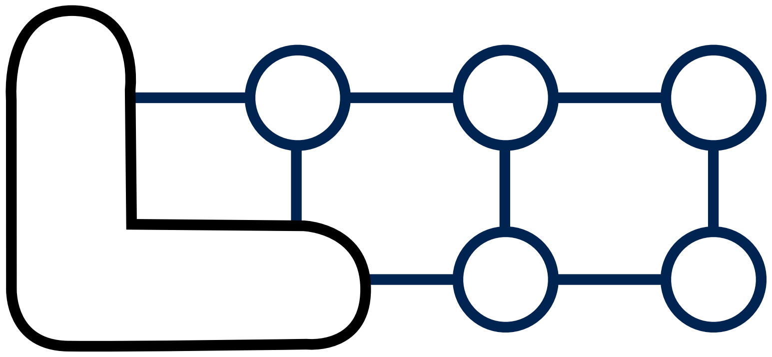

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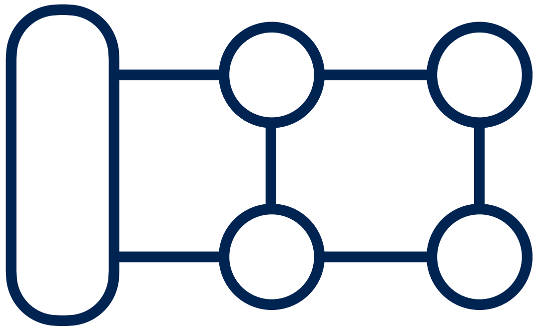
$$\langle\Psi|\Psi\rangle =$$



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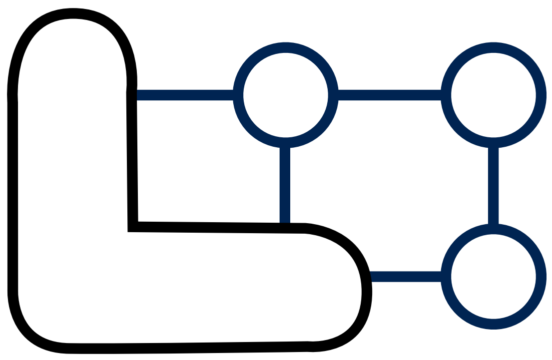

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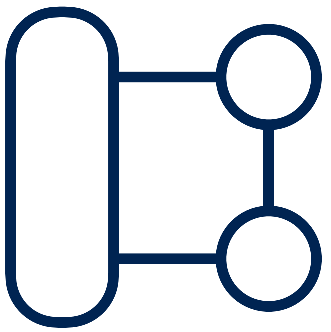

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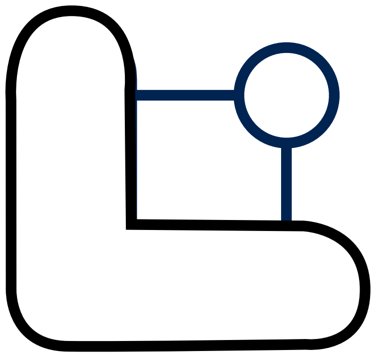
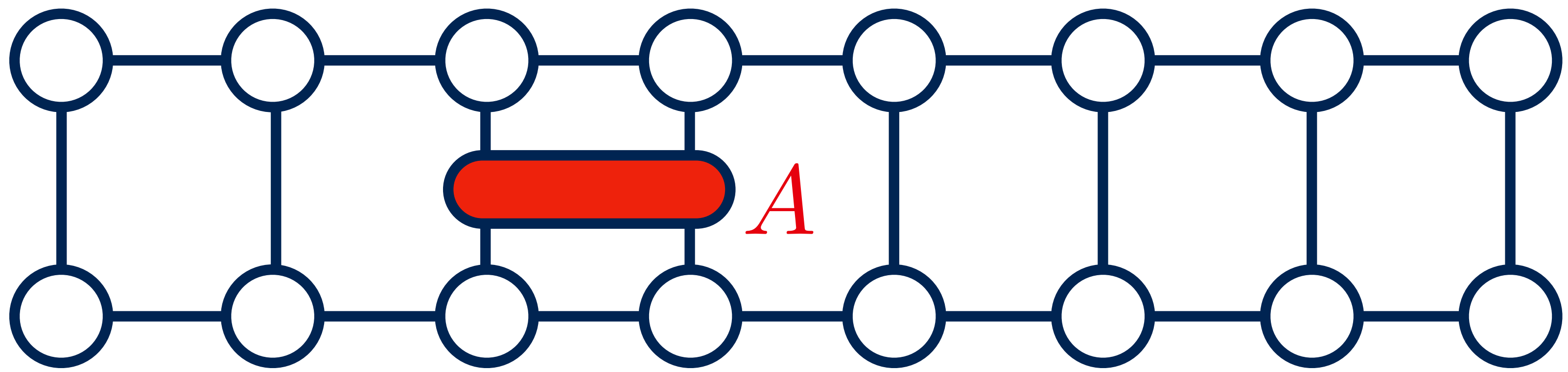


equals a scalar (**why?**)

Another key computation is an **expectation value**

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



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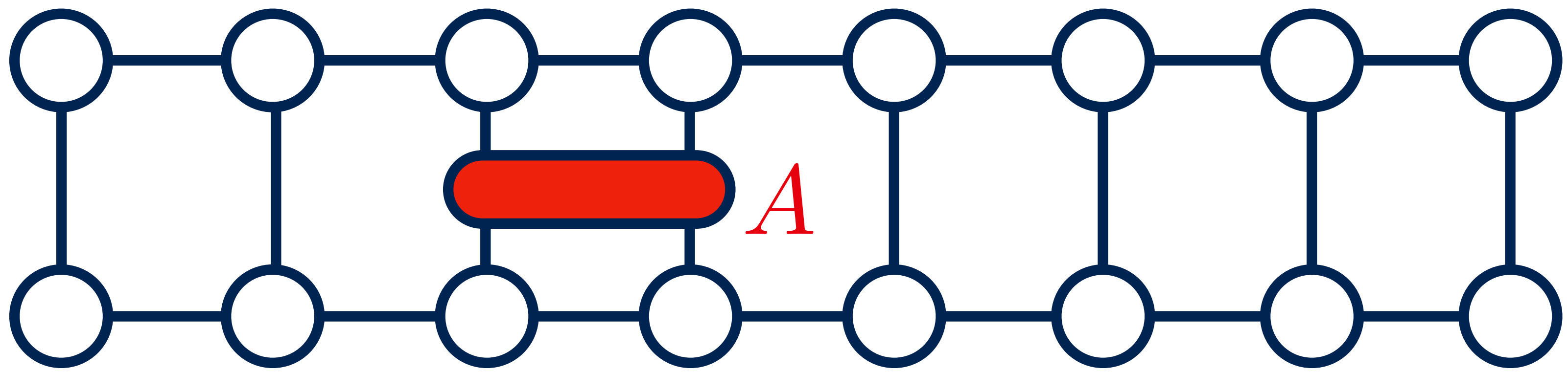
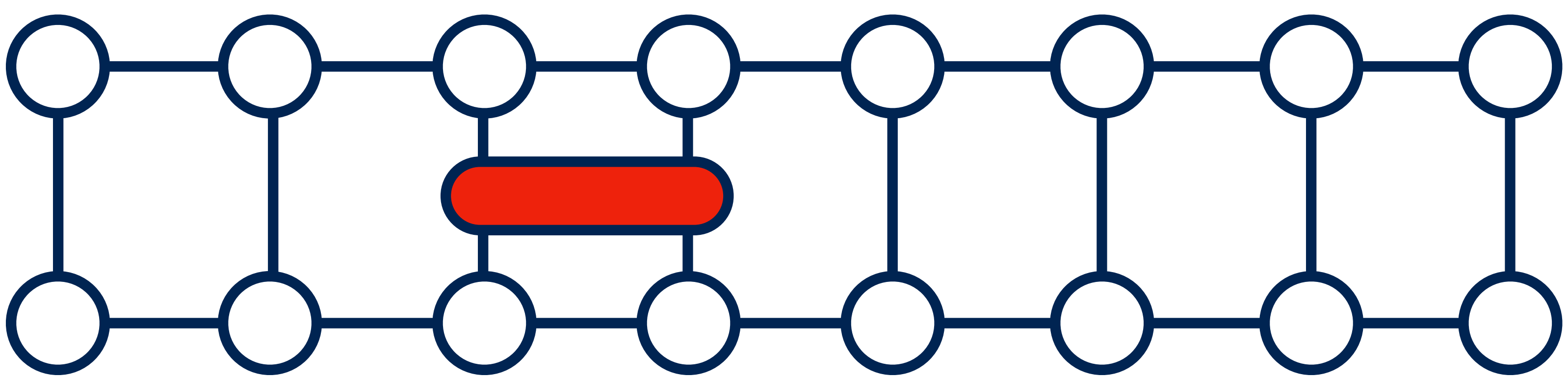


Using similar procedure as norm:



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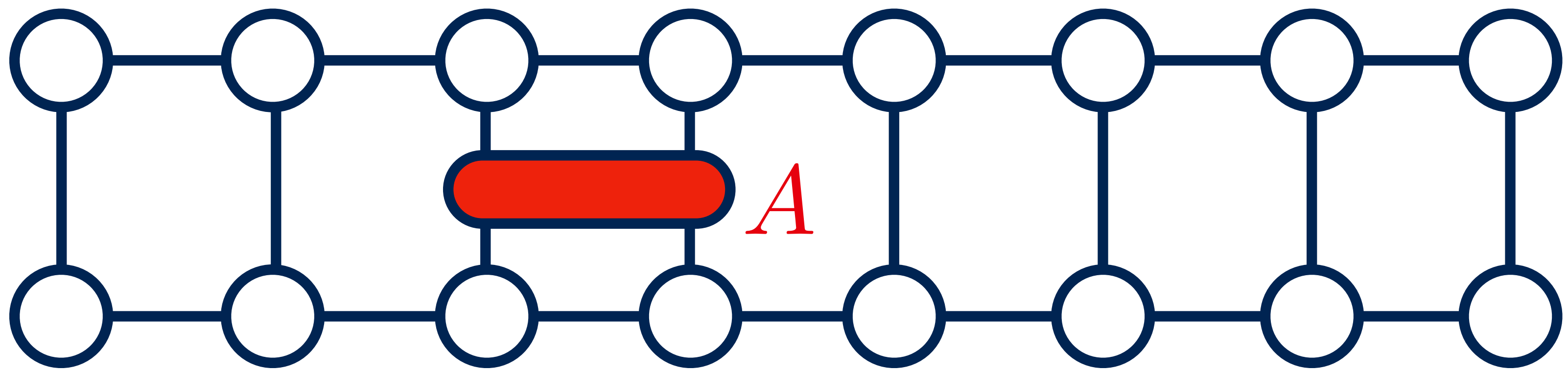

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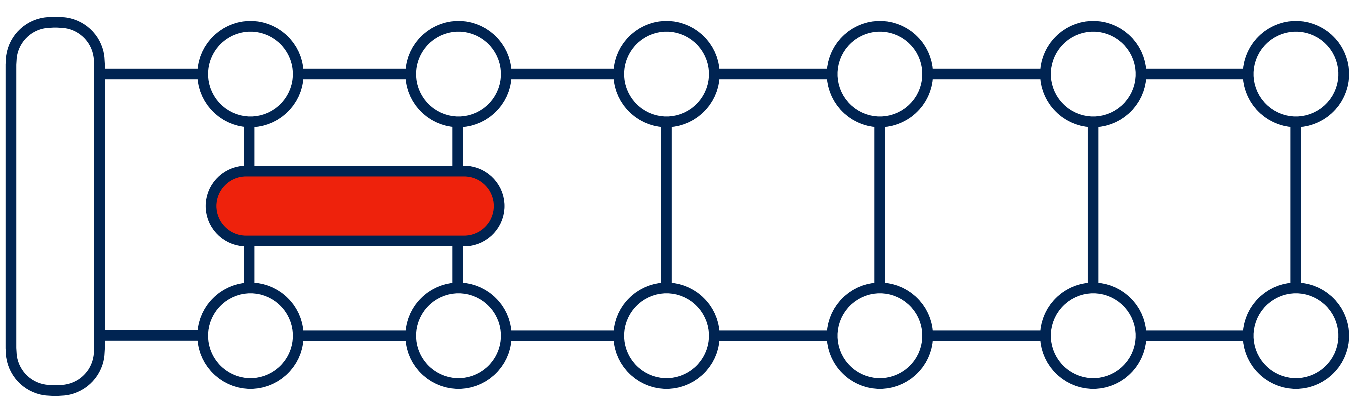

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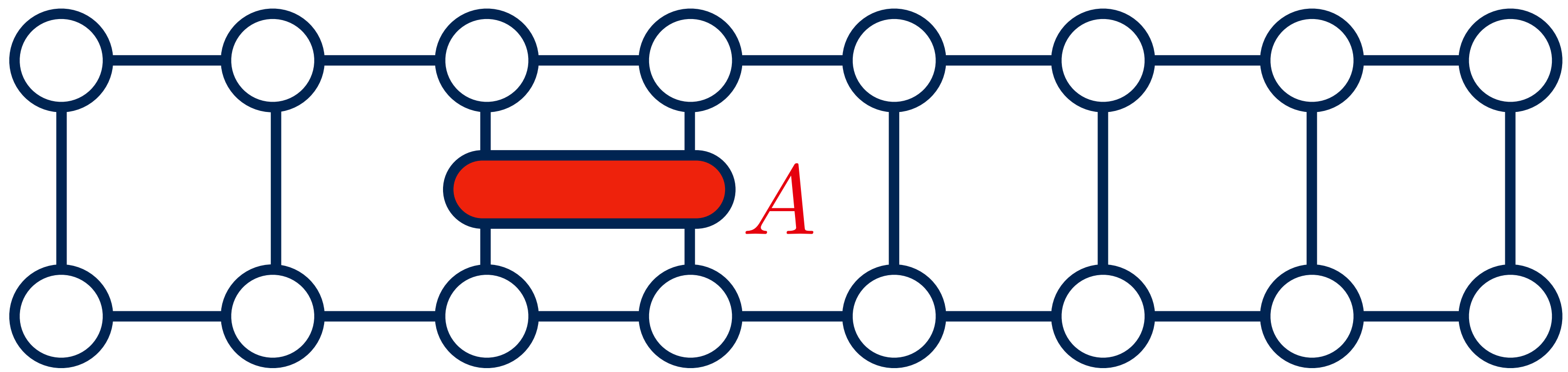

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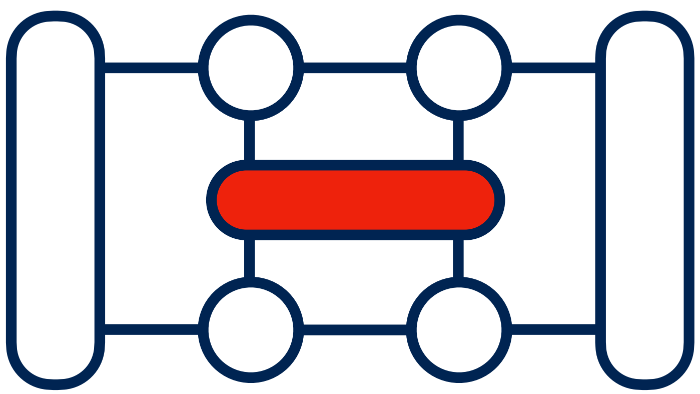
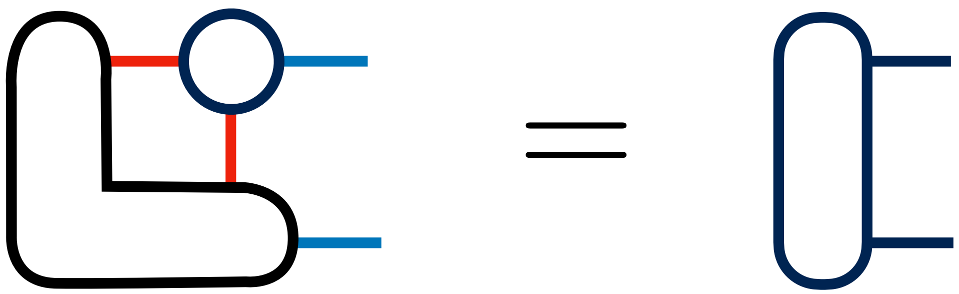


What is the **scaling** of the computational cost ?

To calculate, break computation into separate steps, such as:

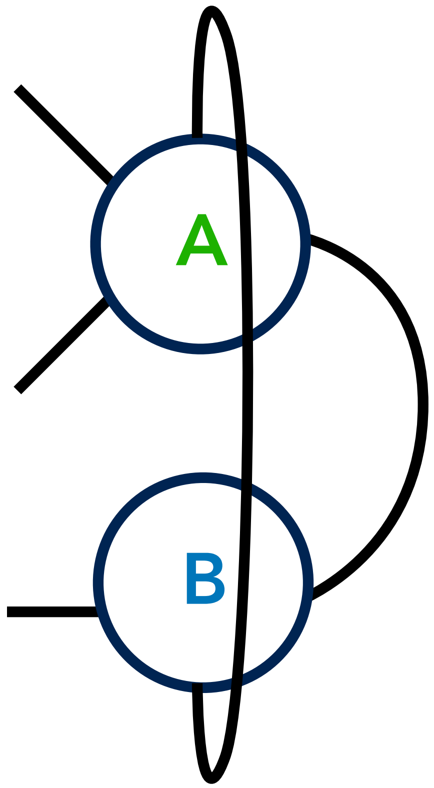


Then use rule for cost of tensor contraction:

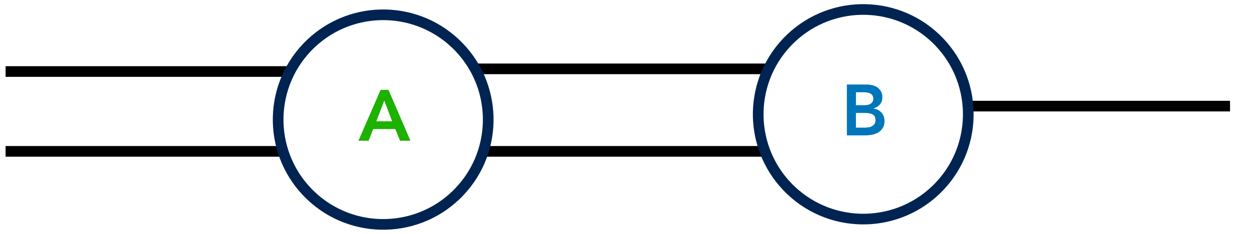
(**dimension of contracted indices**)

x (**dimension of uncontracted indices**)

Complicated tensor contraction



Can always be written as matrix mult. with grouped indices



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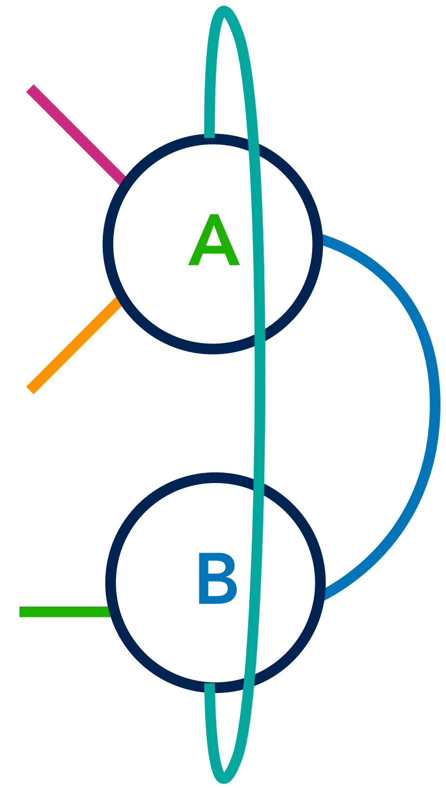
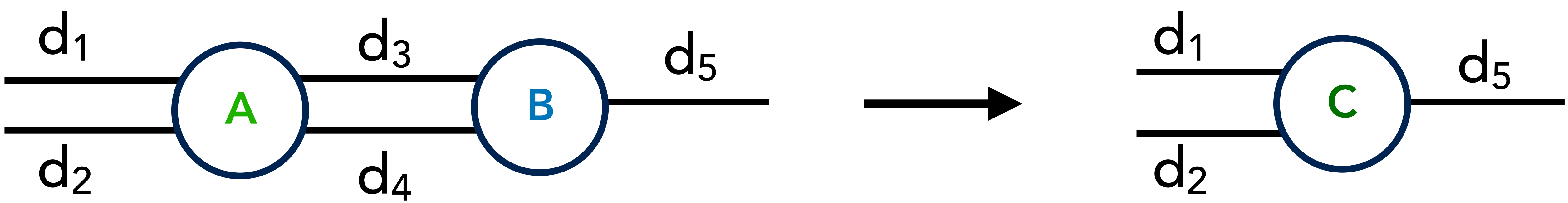


Can always be written as matrix mult. with grouped indices

To compute scaling, consider index dimensions



Computation of C equivalent to:

```
for i₁=1:d₁, i₂=1:d₂, i₅=1:d₅
    for i₃=1:d₃, i₄=1:d₄
        C[i₁,i₂,i₅] = A[i₁,i₂,i₃,i₄]*B[i₃,i₄,i₅]
    end
end
```

Computation of C:

```
for i1=1:d1, i2=1:d2, i5=1:d5
    for i3=1:d3, i4=1:d4
        C[i1,i2,i5] = A[i1,i2,i3,i4]*B[i3,i4,i5]
    end
end
```

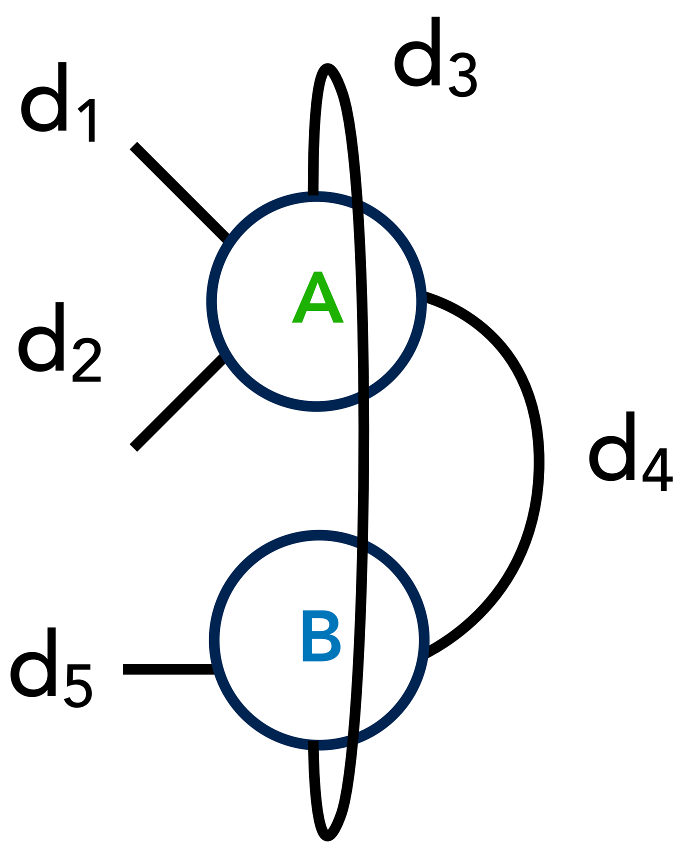
Each i_n loop takes d_n operations to complete

Overall scaling: $$(d_1 d_2 d_5) \times (d_3 d_4)$$

(dim. contracted indices) x (dim. uncontracted indices)

Summary of **scaling rule**

Whenever you see a tensor contraction



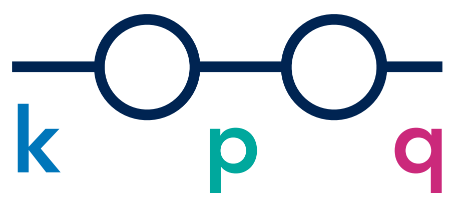
Multiply dimension of every index (just once)

$$\text{cost} = (d_1 \cdot d_2 \cdot d_3 \cdot d_4 \cdot d_5)$$

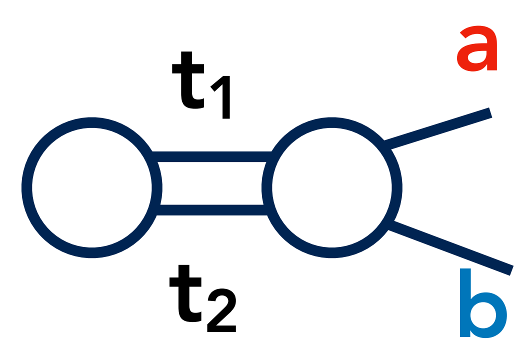
Test Your Knowledge! 🤔

Write down the cost of the following tensor contractions (letters are index dimensions):

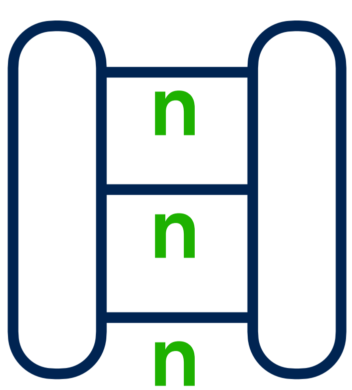
(1)



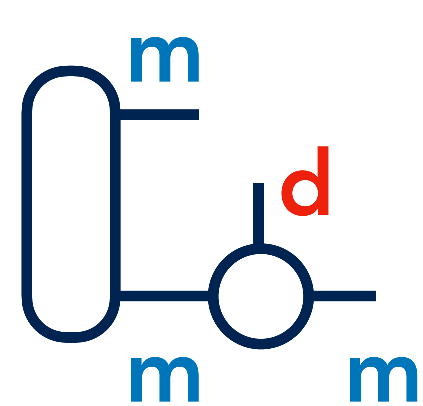
(2)



(3)



(4)



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

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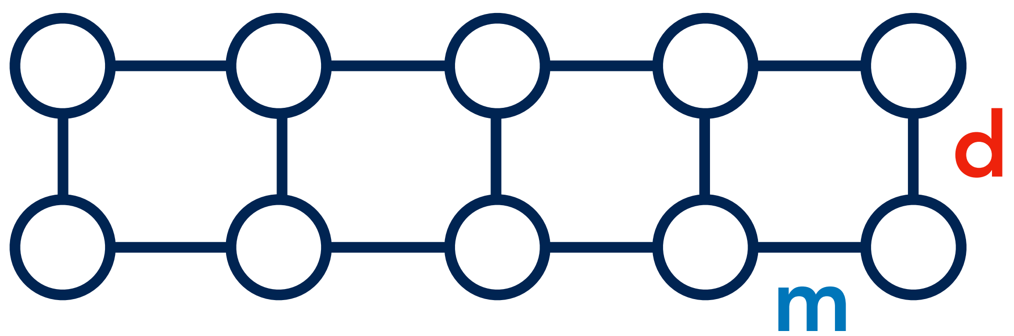
Consider norm of MPS bond dimension **m**, site dimension **d**

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



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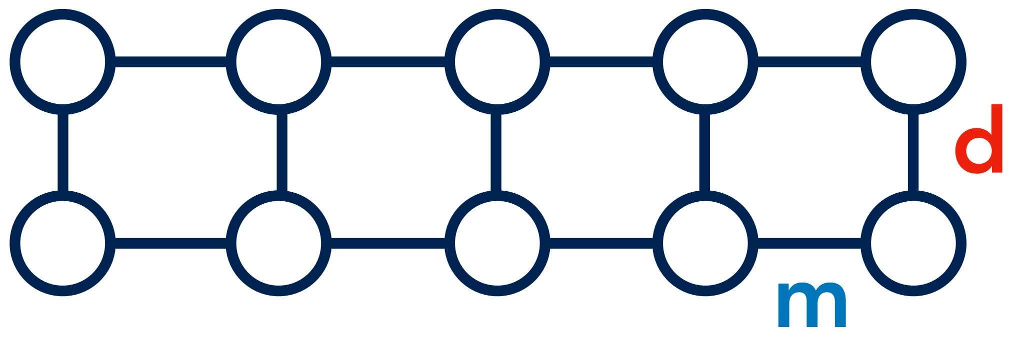

Two key operations

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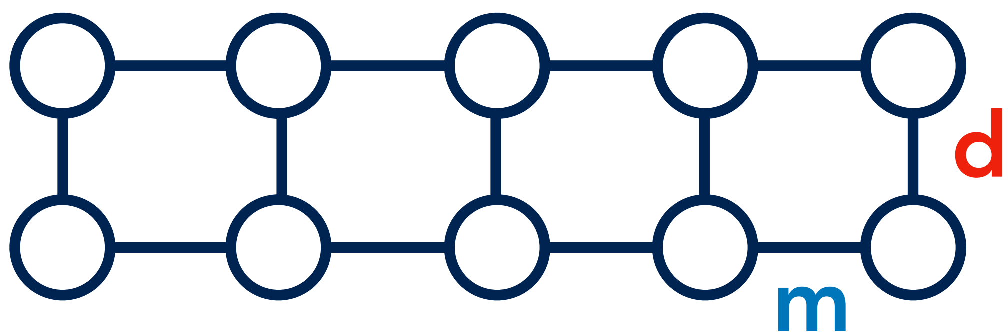
$\langle \Psi | \Psi \rangle =$ 

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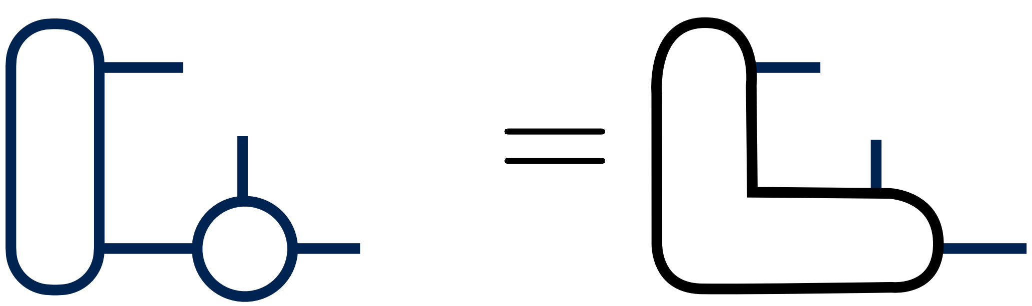
(1) 

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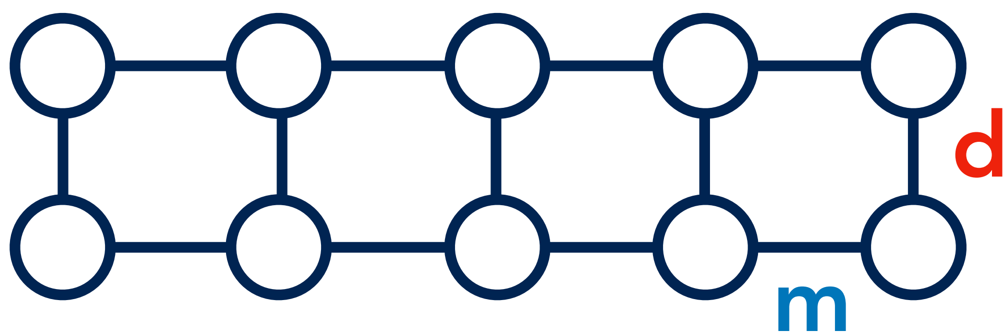
$\langle \Psi | \Psi \rangle =$ 

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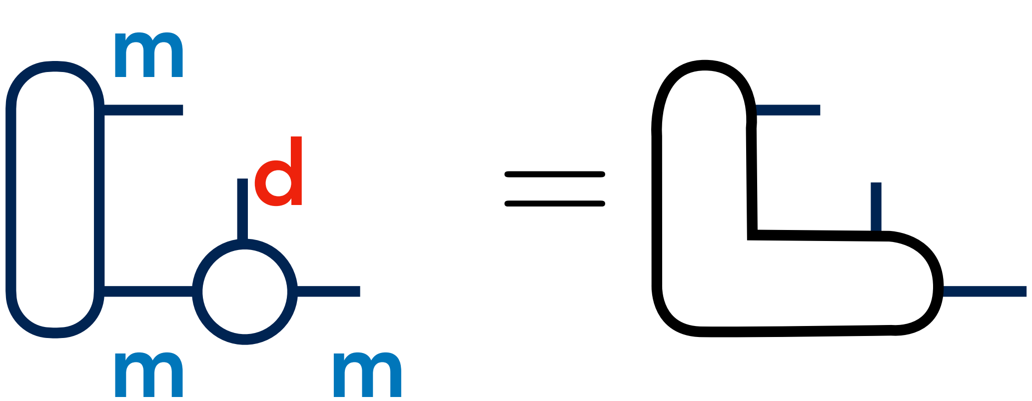
(1) 

scaling is $m^3 d$

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

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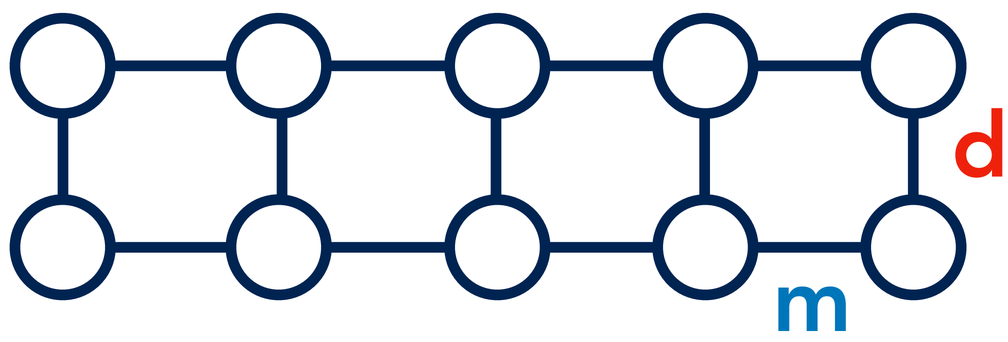
$\langle \Psi | \Psi \rangle =$ 

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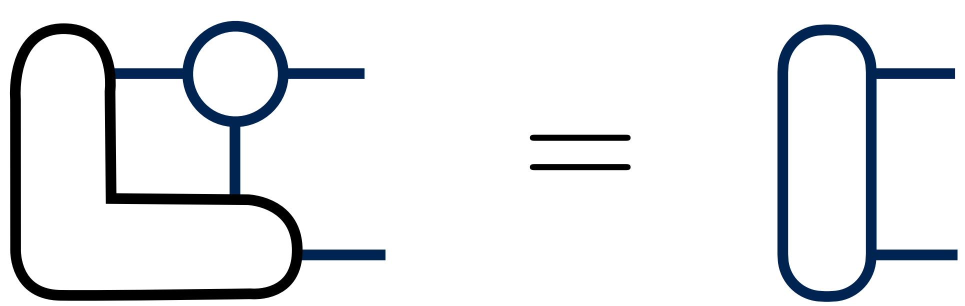
(2) 

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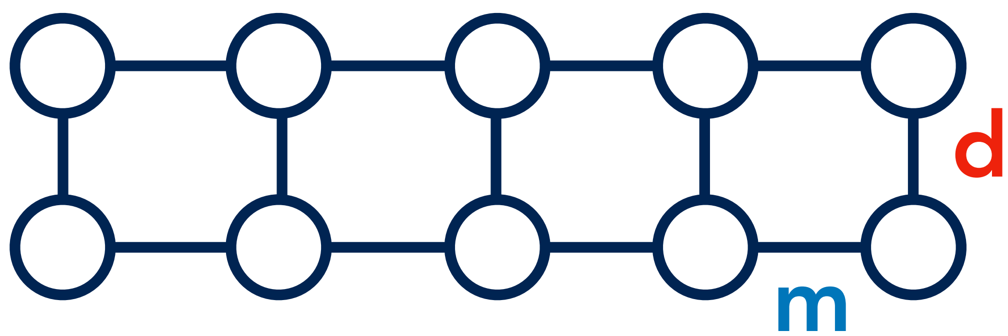
$\langle \Psi | \Psi \rangle =$ 

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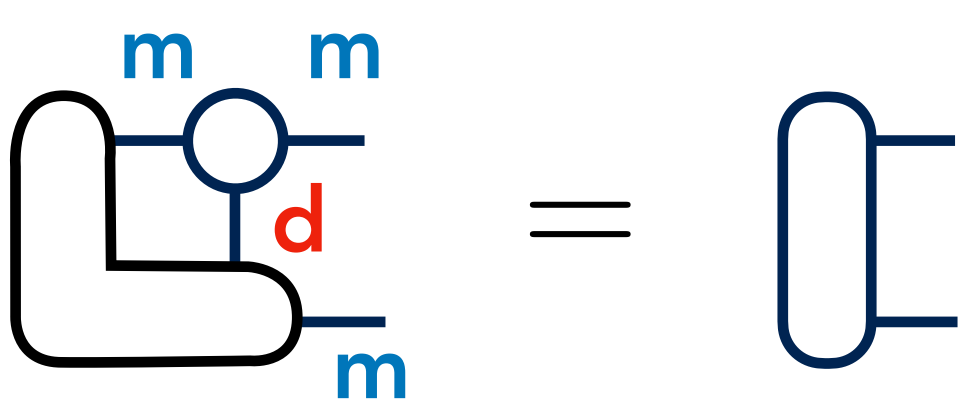
(2) 

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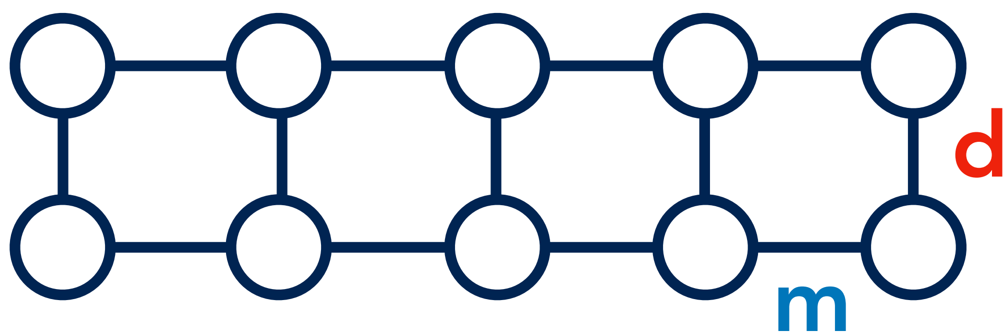
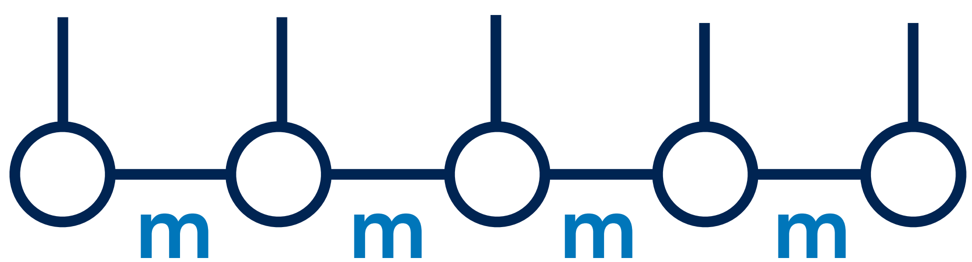
$$\langle\Psi|\Psi\rangle =$$ 

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 mxm matrices

Scaling of mxm matrix multiplication is m^3

Examples of Matrix Product States

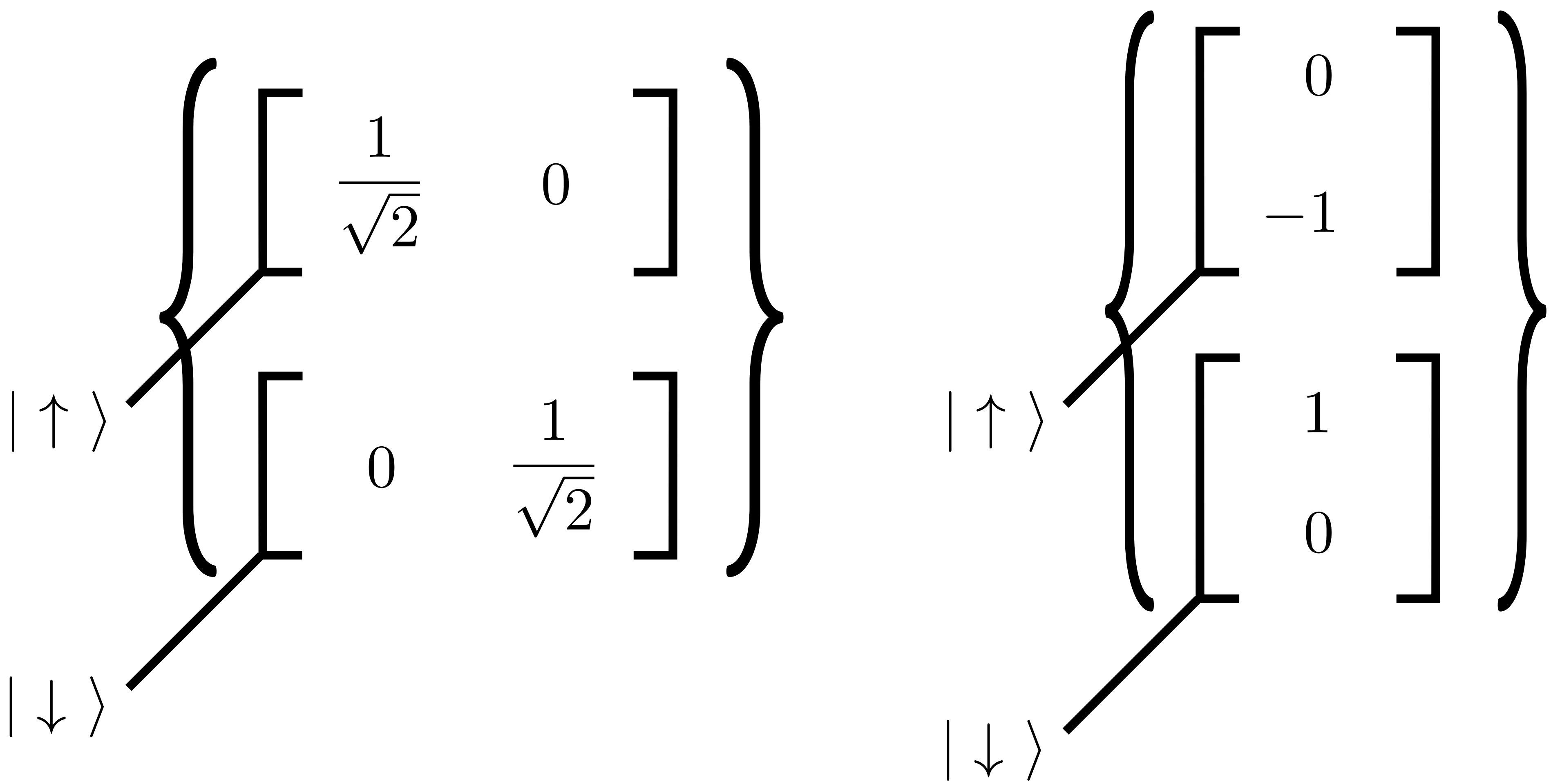
Example #1: singlet state

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

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

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

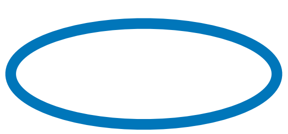
Can construct AKLT wavefunction as follows

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



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

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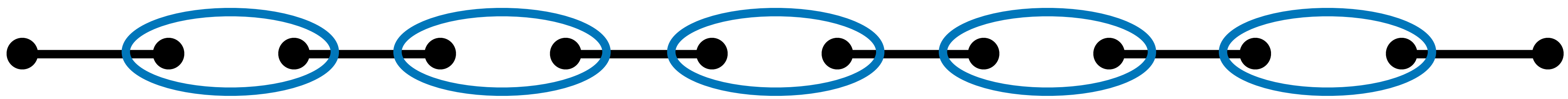

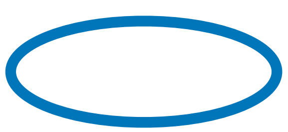

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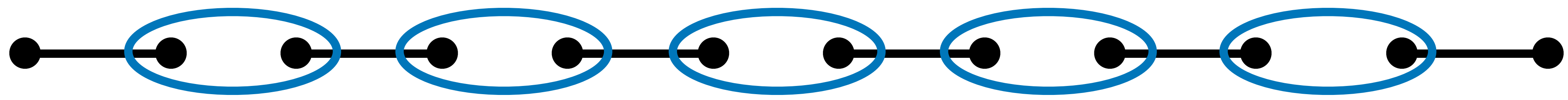
Can construct AKLT wavefunction as follows

After projection, blue ovals are S=1 spins



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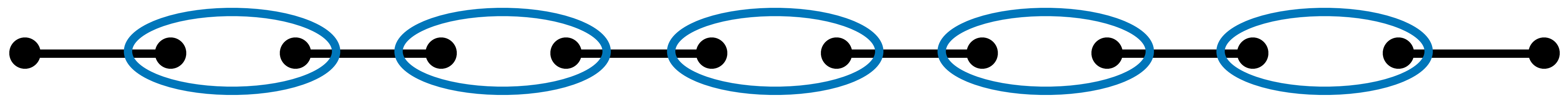
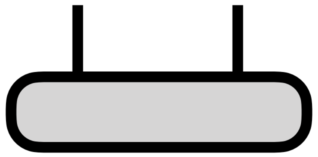


Can predict interesting properties:

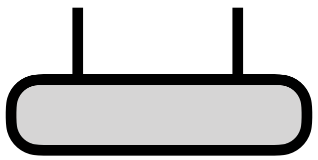
- doubly degenerate entanglement spectrum
- emergent S=1/2 edge spins

Tensor approach to AKLT



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

Tensor approach to AKLT



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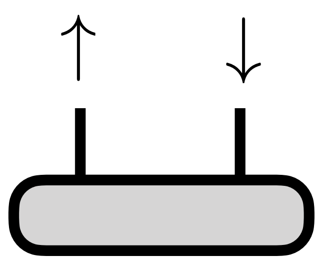
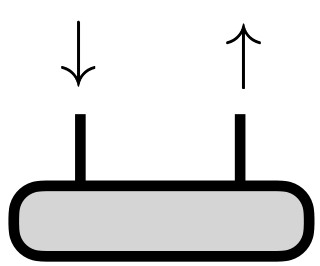
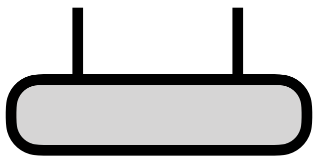


$$= \frac{1}{\sqrt{2}}$$



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

Tensor approach to AKLT



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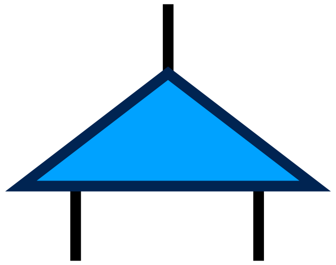
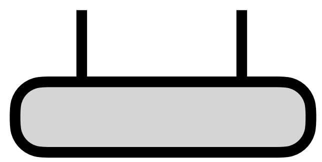


$$= |+\rangle\langle\uparrow\uparrow| + |0\rangle\frac{\langle\uparrow\downarrow| + \langle\downarrow\uparrow|}{\sqrt{2}} + |-\rangle\langle\downarrow\downarrow|$$

Tensor approach to AKLT



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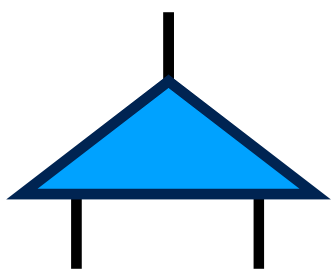

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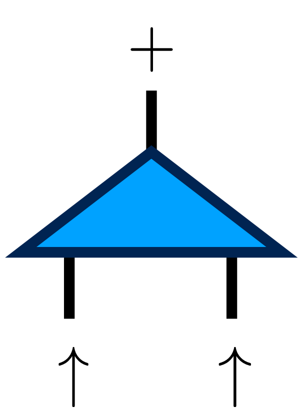
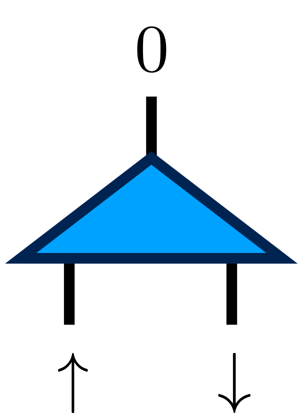
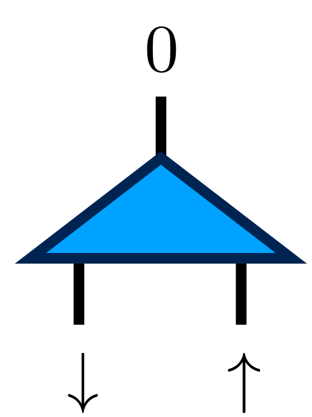


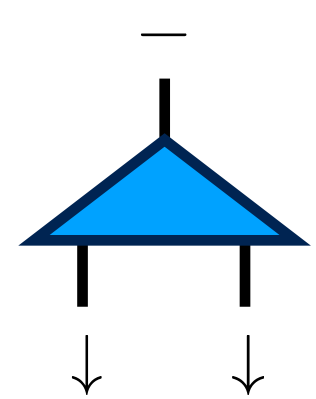
$= 1$



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

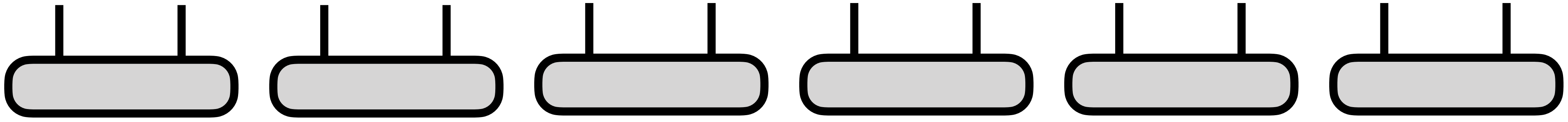


$= \frac{1}{\sqrt{2}}$

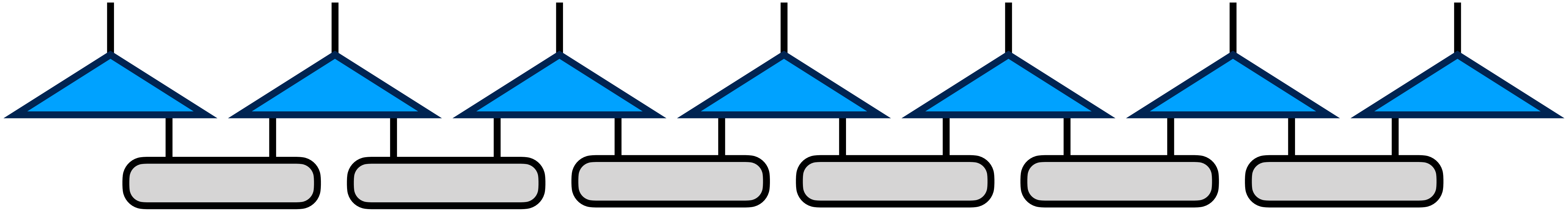


$= 1$

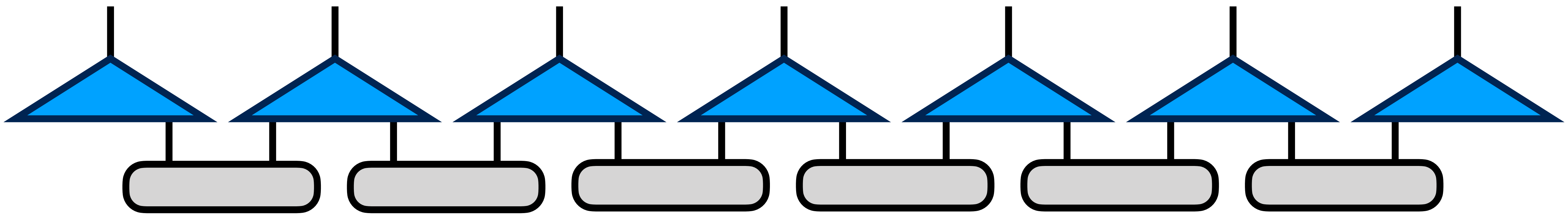
Tensor approach to AKLT



Tensor approach to AKLT

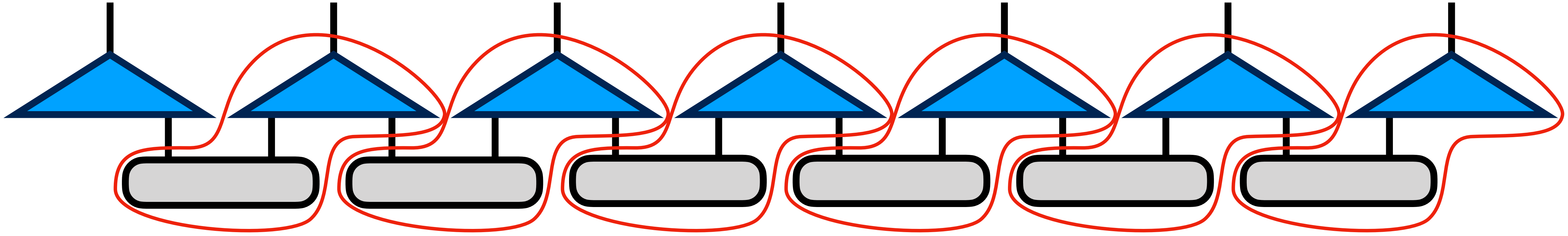


Put into MPS form



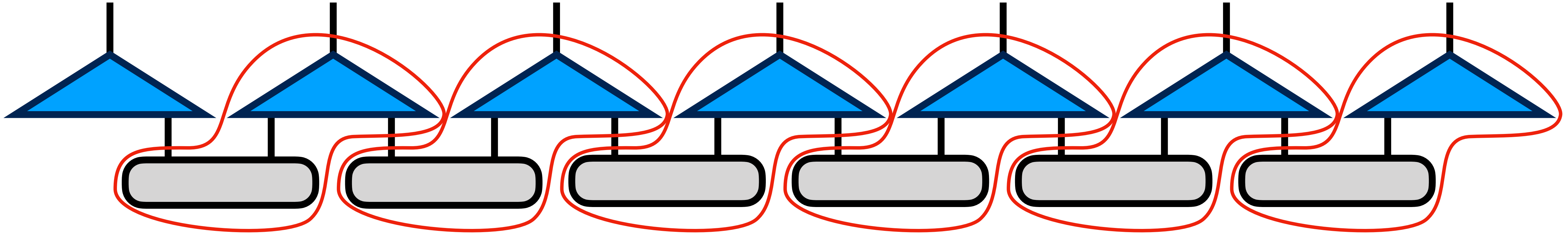
Put into MPS form

Contract pairs of tensors:



Put into MPS form

Contract pairs of tensors:



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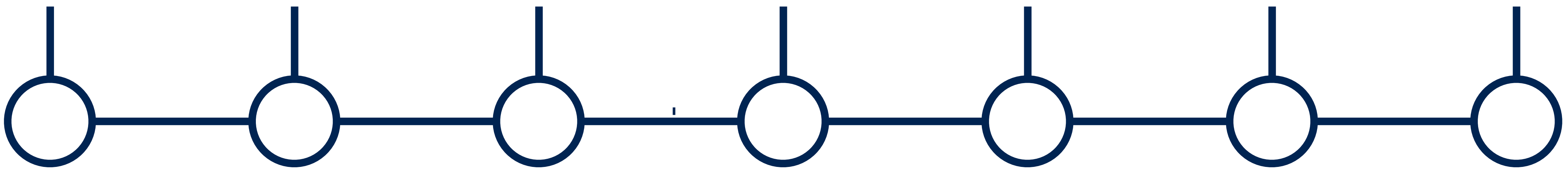

Nice form of AKLT matrix product state with periodic boundary conditions

Can actually show the following:

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

where

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

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

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

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!