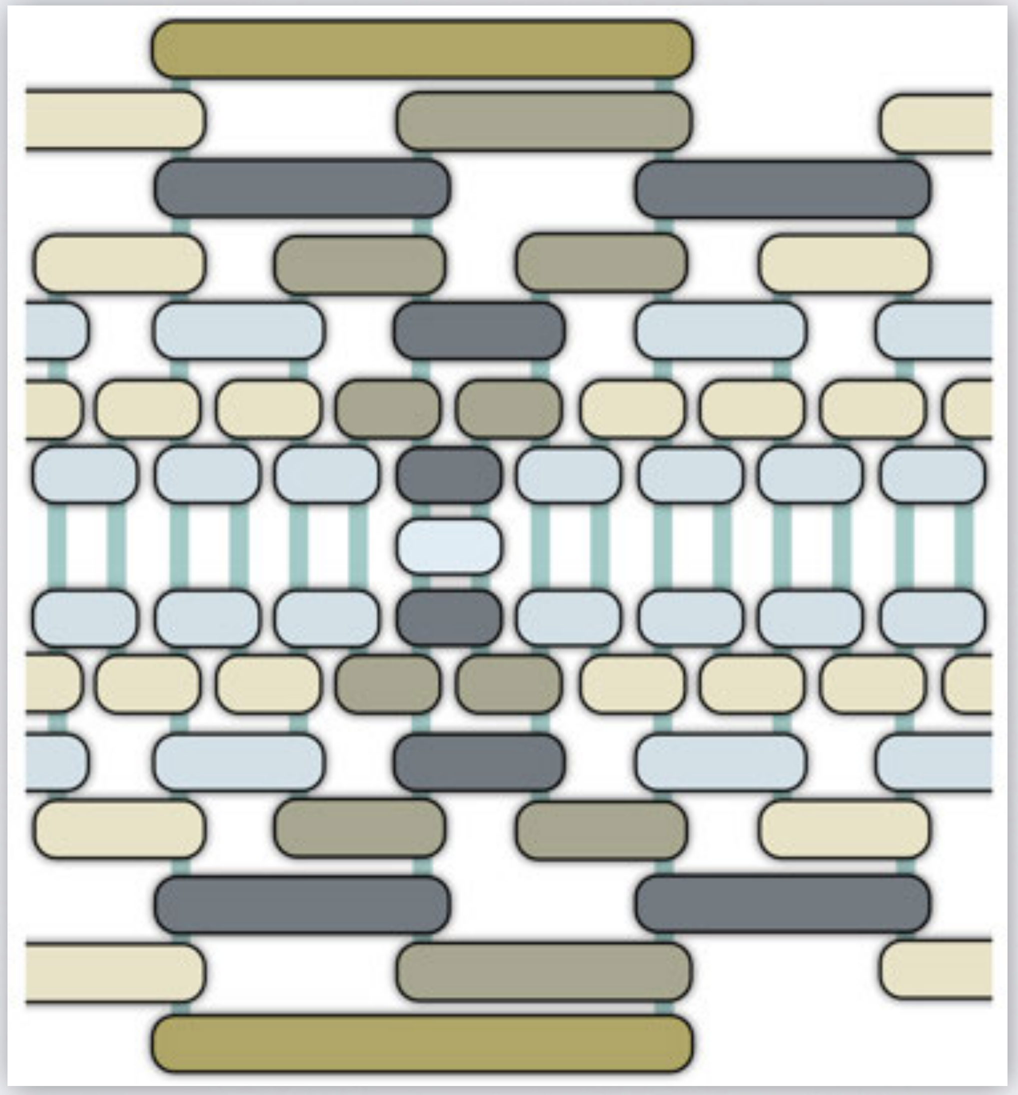
Entanglement and tensor network states



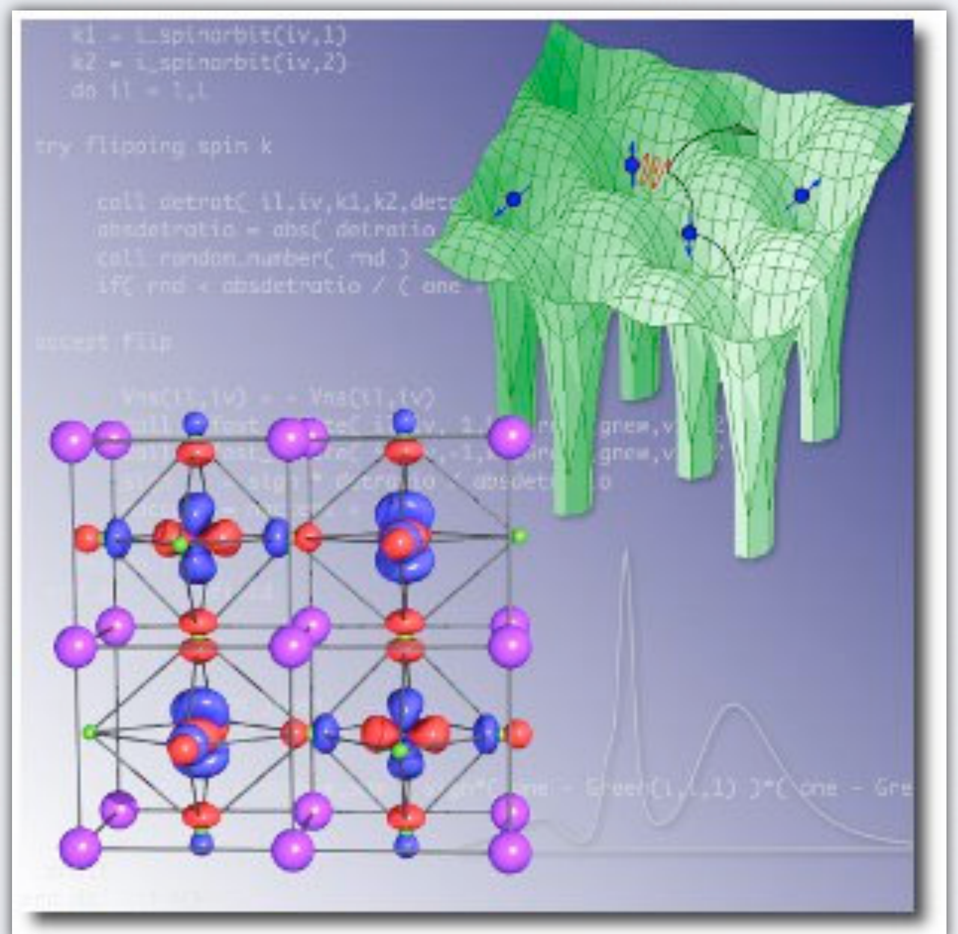
Jens Eisert

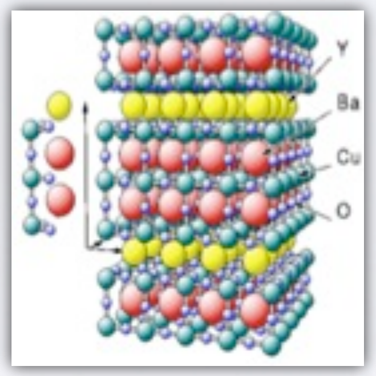
Freie Universität Berlin

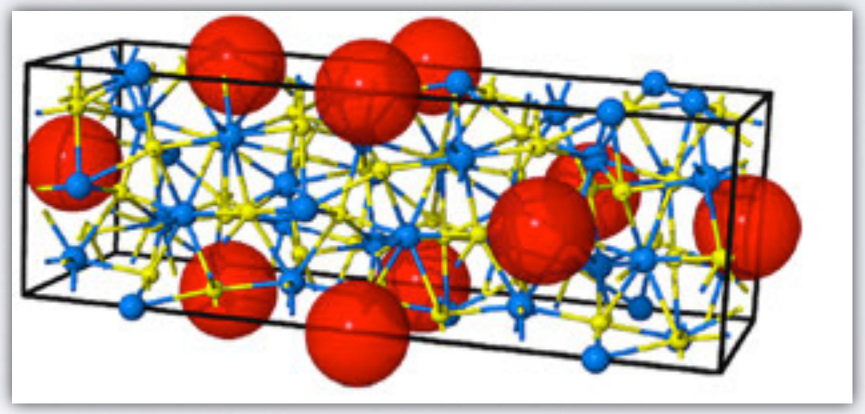
Autumn School on Correlated Electrons: Emergent Phenomena in Correlated Matter
Juelich, September 2013, Organisers: Eva Pavarini, Erik Koch, Uli Schollwoeck

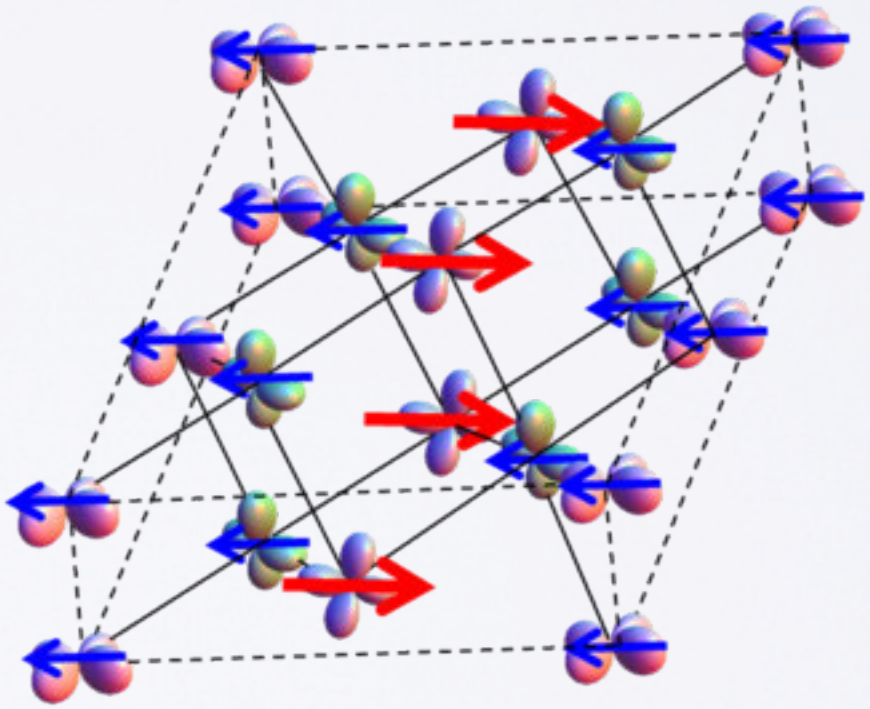
Quantum lattice models

- **Quantum lattice models:** Models for **strongly correlated quantum many-body system**s









- Ubiquitous in **condensed-matter context** and for **cold atoms in optical lattices**

Manifesto of lecture

- **Manifesto :) of lecture**

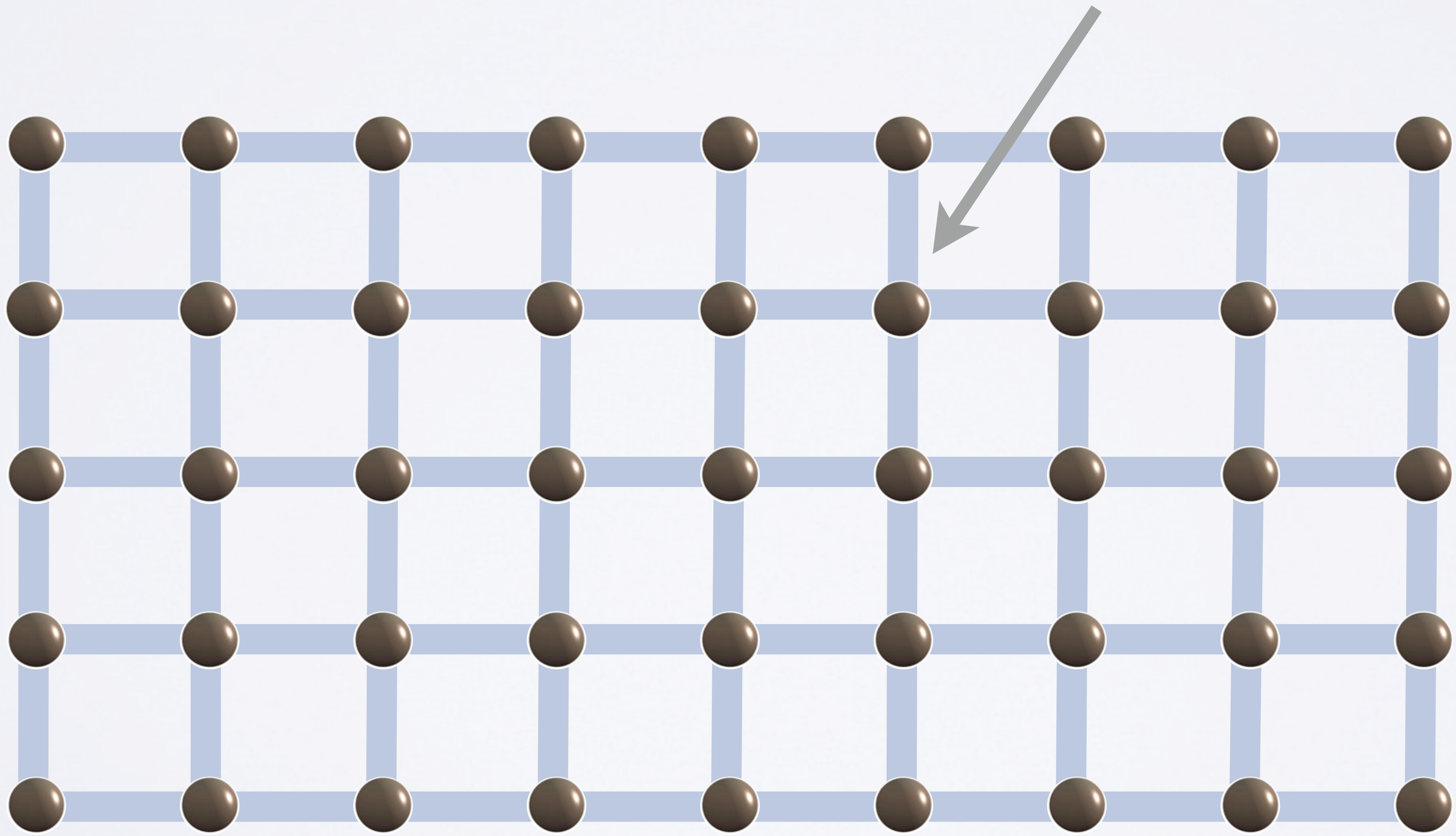
Many natural quantum lattice models have ground states that are little, in fact very little, entangled in a precise sense. This shows that `nature is lurking in some small corner of Hilbert space', one that can be essentially efficiently parametrized. This basic yet fundamental insight allows for a plethora of new methods for the numerical simulation of quantum lattice models using tensor network states, as well as a novel toolbox to analytically study such systems

- **This lecture:** Find out what that means
- Is "double" with subsequent lecture by Uli Schollwoeck
- On slides, will avoid all references (sincere apologies!): For script and references, see http://arxiv.org/abs/1308.3318

Correlations in quantum many-body systems

Quantum lattice models

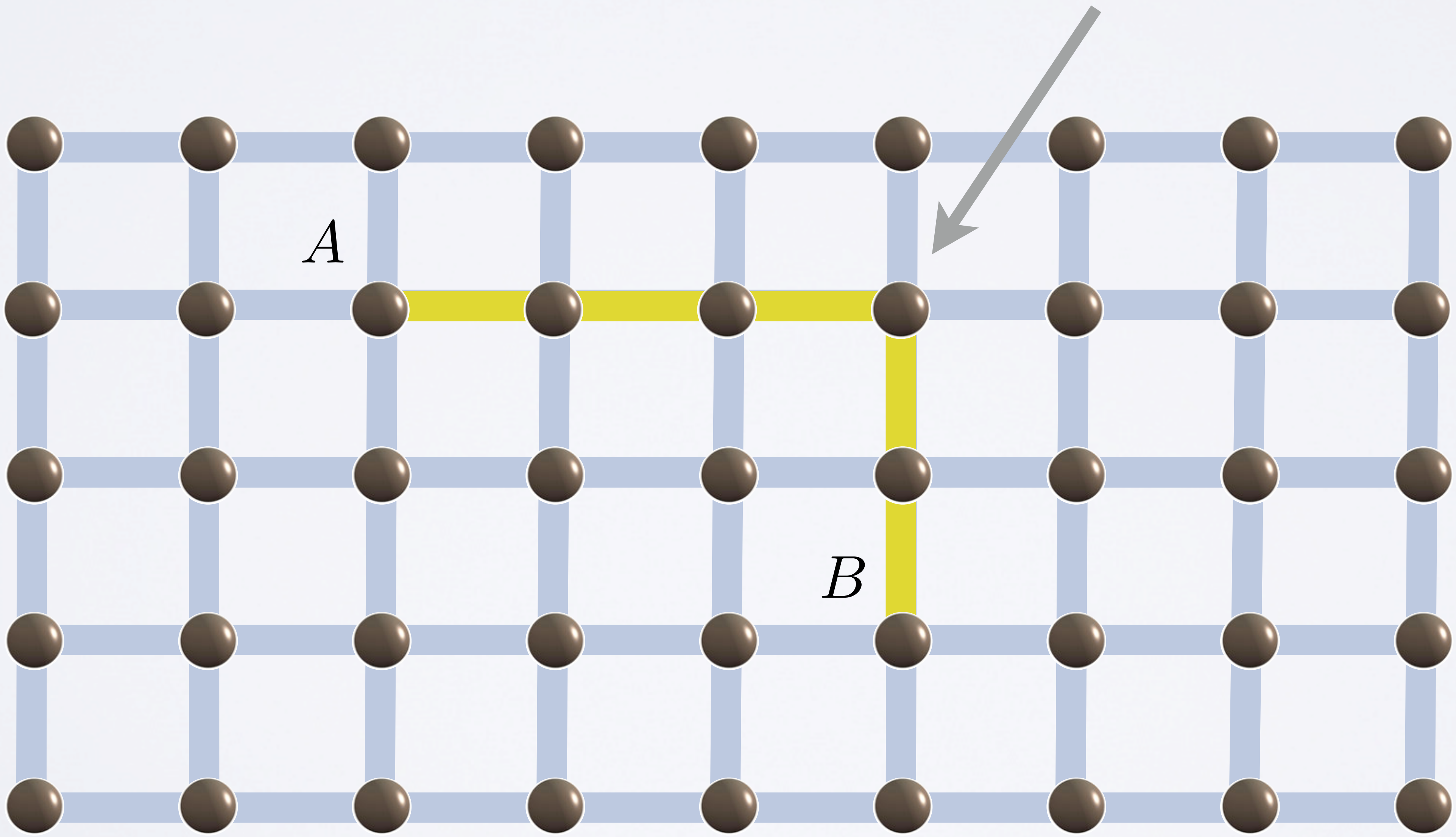
- **Quantum lattice models:** Some lattice $G = (V, E)$, with **quantum degree of freedom** per vertex: Bosonic, fermionic, spin degree of freedom



Quantum lattice models

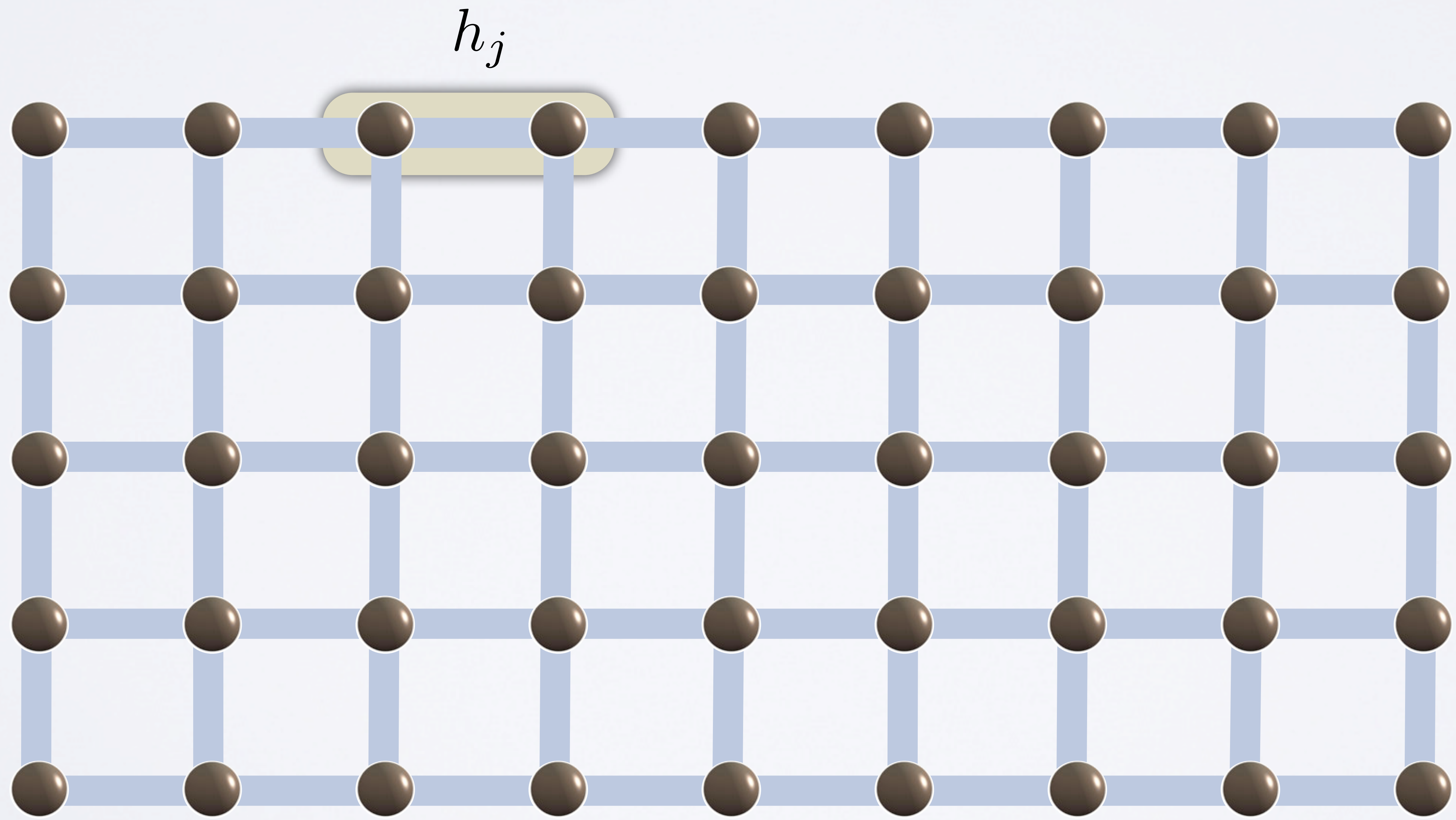
- **Quantum lattice models:** Some lattice $G = (V, E)$, with **quantum degree of freedom** per vertex: Bosonic, fermionic, spin degree of freedom

- **Distance in lattice:** $\mathrm{dist}(A, B)$



Local Hamiltonians

- **Local Hamiltonian** $H = \sum_{j \in V} h_j$, with each h_j supported only on finite neighboring sites, reflecting finite-ranged interactions

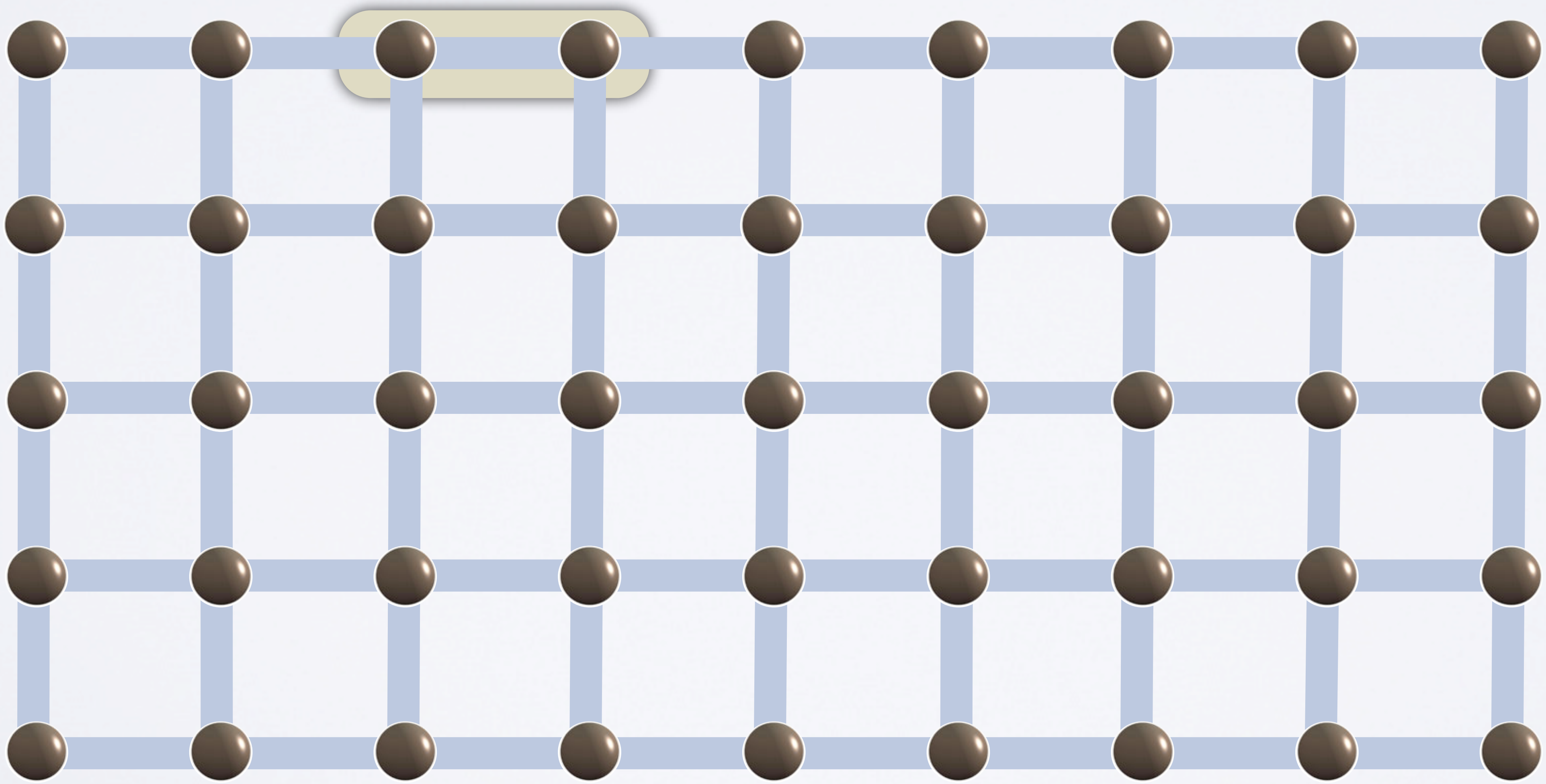


Local Hamiltonians

- **Example:** XY model

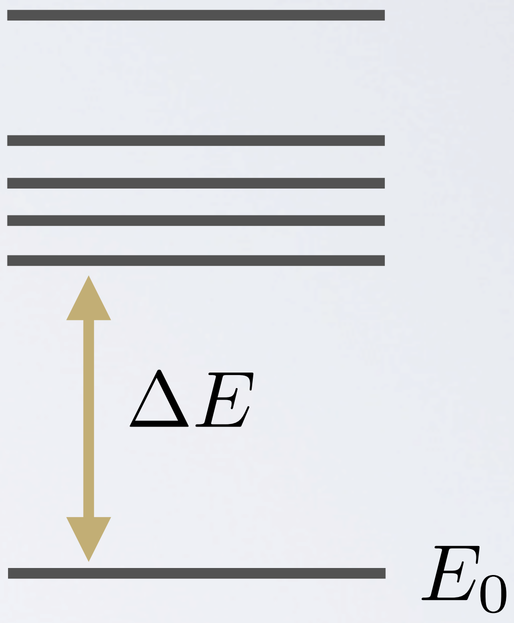
$$H = -\frac{1}{2}\sum_{\langle j,k\rangle}\left(\frac{1+\gamma}{4}X^{(j)}X^{(k)} + \frac{1-\gamma}{4}Y^{(j)}Y^{(k)}\right) - \frac{\lambda}{2}\sum_{j\in V} Z^{(j)},$$

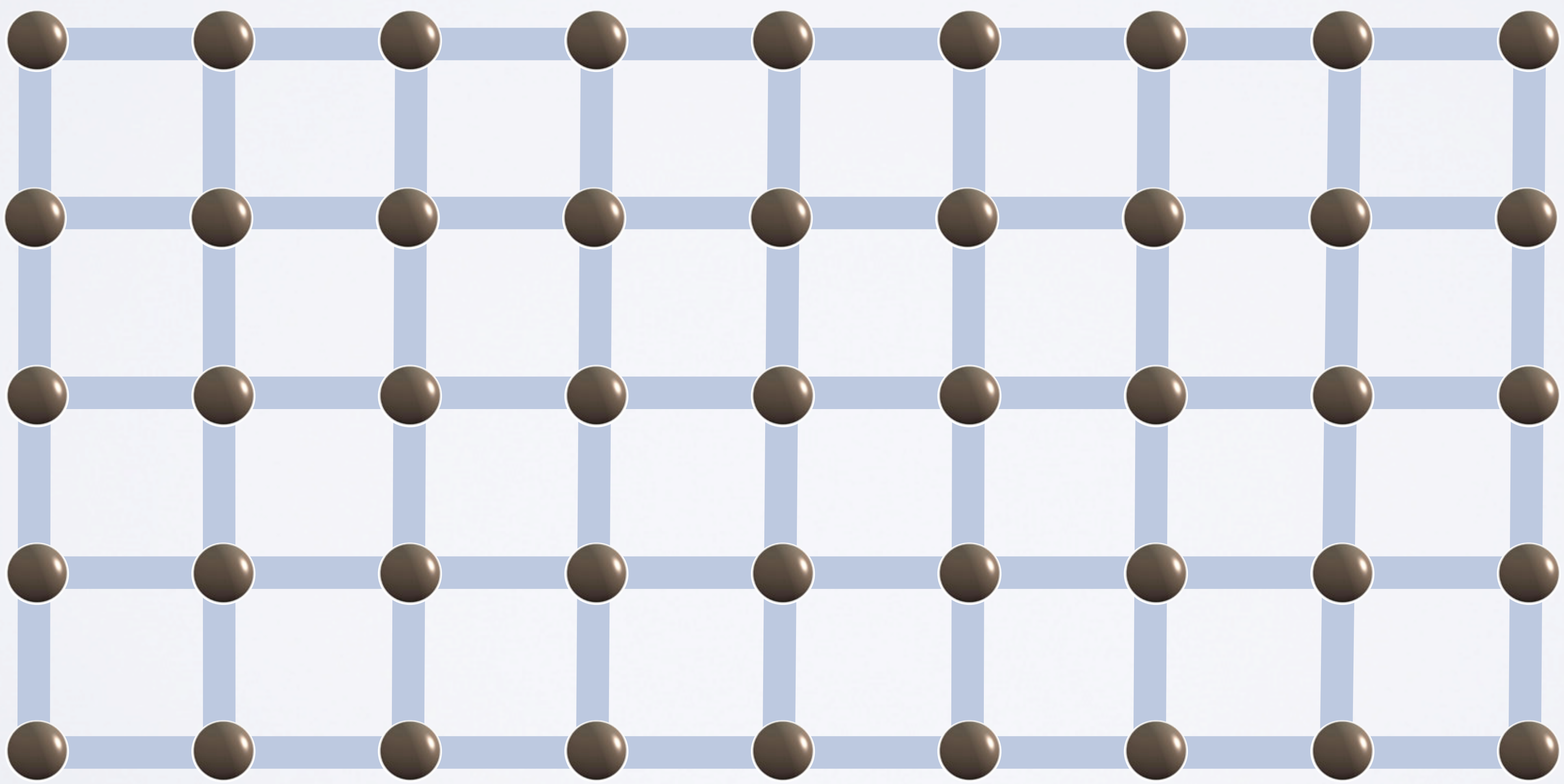
- **Pauli operators** on site j called $X^{(j)}, Y^{(j)}, Z^{(j)}$
- **External field** λ , **anisotropy parameter** γ : Easily exactly solvable in 1d



Ground states and spectral gaps

- **Ground space** $\mathcal{G}$ spanned by vectors minimising $\langle\psi|H|\psi\rangle$
- One-dimensional: Unique, otherwise degenerate
- **Spectral gap:** $\Delta E = \inf_{|\psi\rangle \in \mathcal{H}\setminus\mathcal{G}} \langle\psi|H|\psi\rangle - E_0$





Clustering of correlations in gapped models

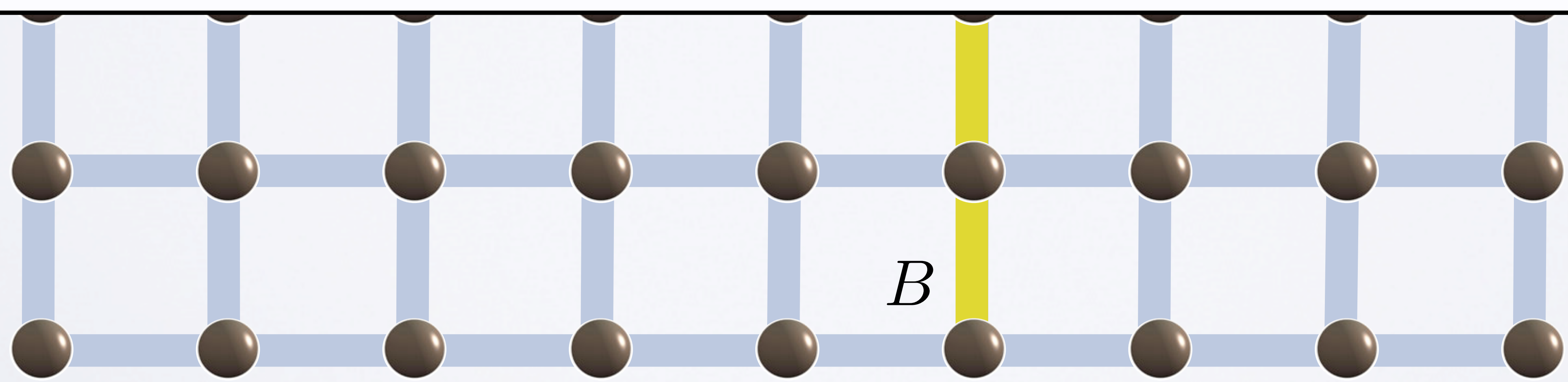
- Gapped models **have short-ranged correlations**
- In fact, they decay, "cluster", exponentially fast

- For $\Delta E > 0$

$$|\langle O_A O_B \rangle - \langle O_A \rangle \langle O_B \rangle| \leq C e^{-\mathrm{dist}(A,B)\Delta E/(2v)} \|O_A\| \, \|O_B\|$$

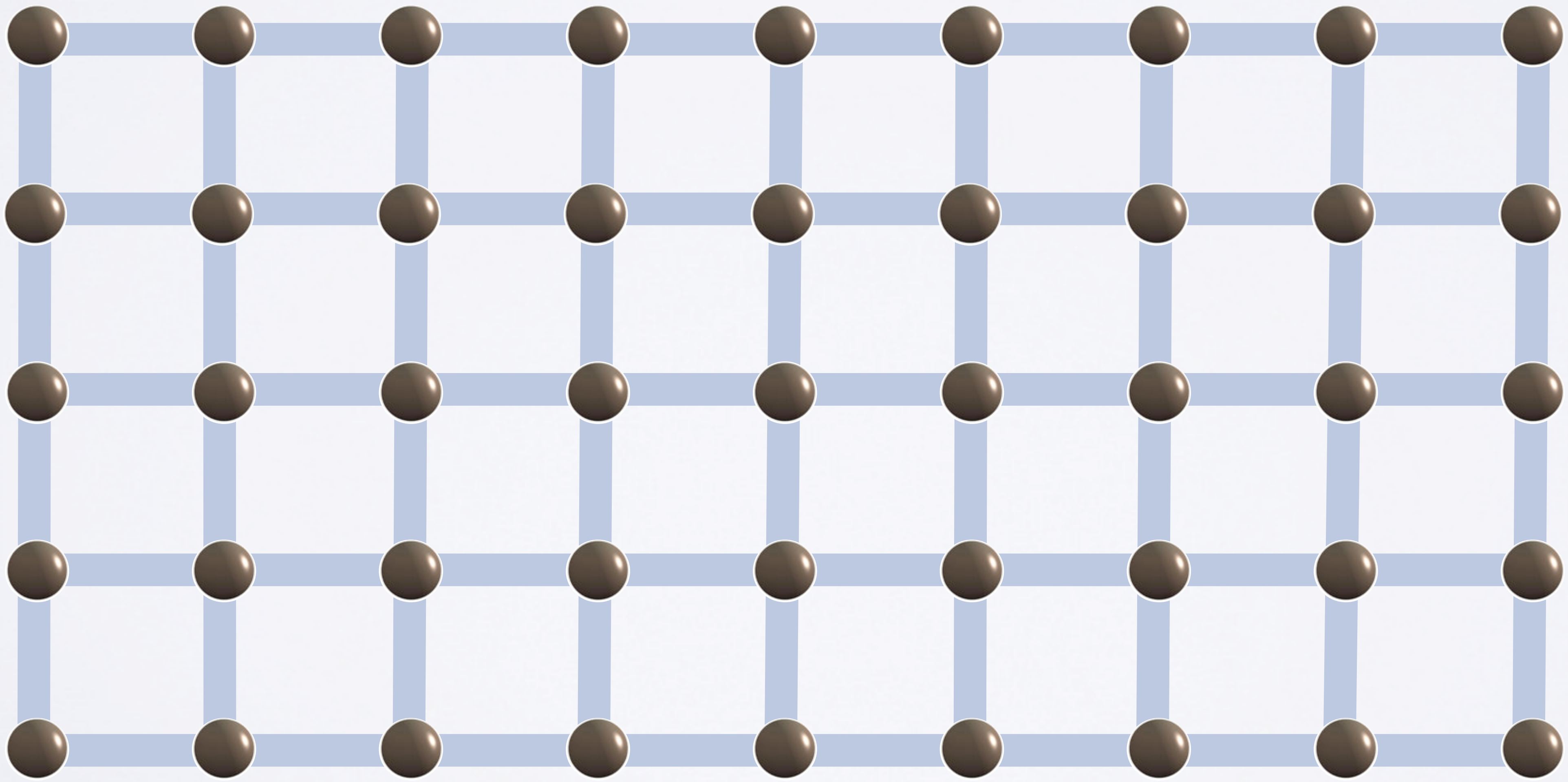
where $C, v > 0$

- Here, $\xi := \dfrac{2v}{\Delta E} > 0$, is the **correlation length**



Entanglement entropies

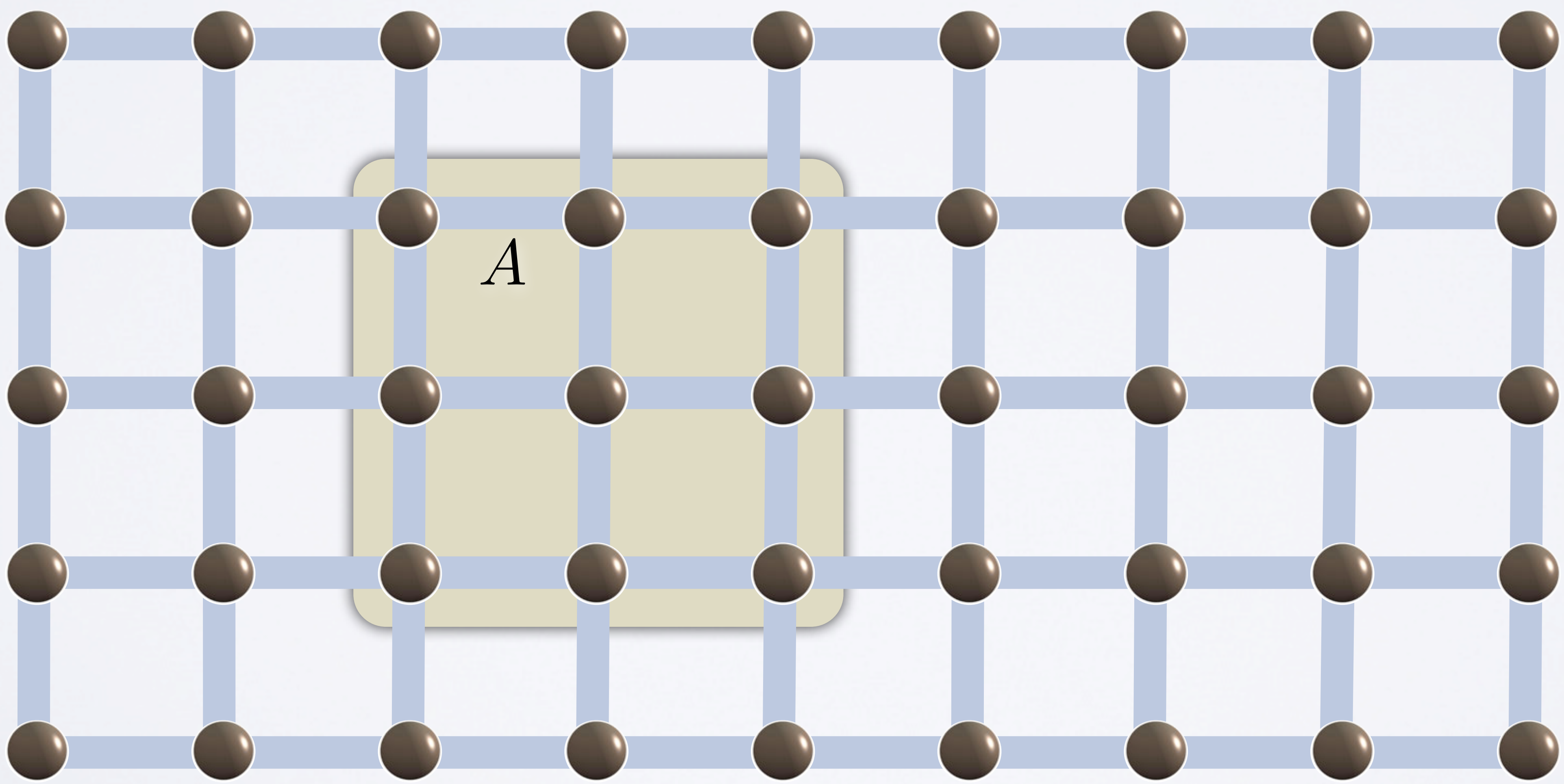
- **Gapless** models have **algebraically decaying correlations** (conformal field theory)
- Locality of interactions inherited by something much stronger?
- Yes, by **entanglement** qualifiers!



Entanglement

Entanglement entropies

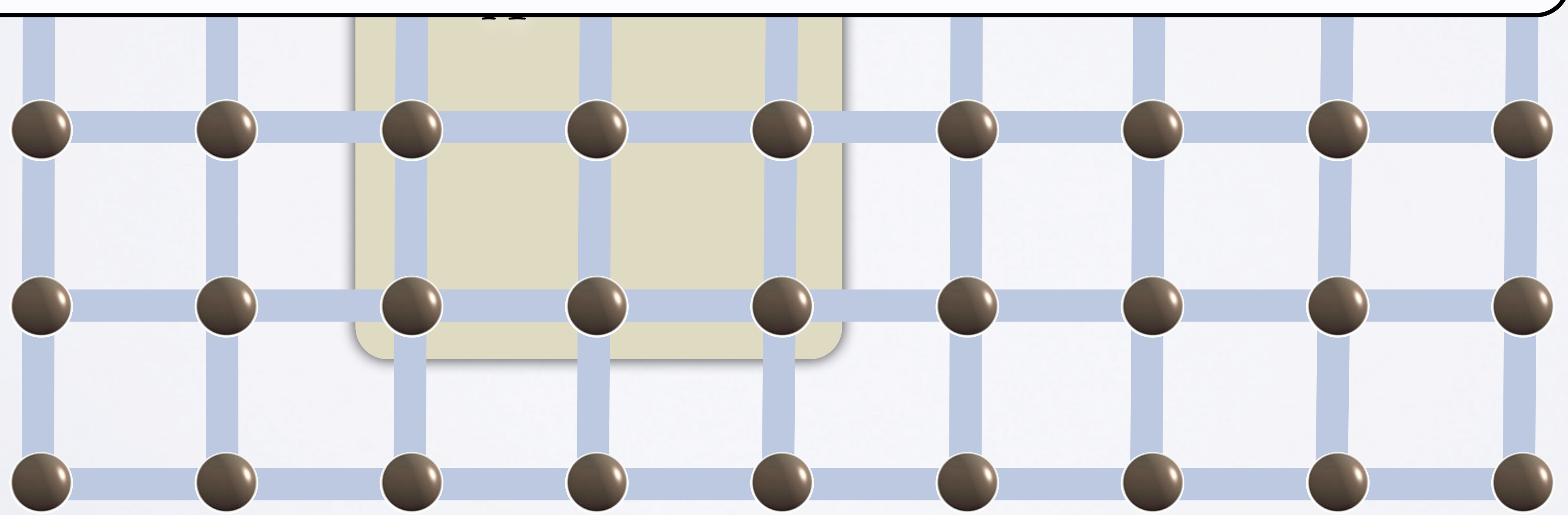
- Assume the entire system is in **pure state**
- Think of some region A of sites, and consider **reduced state** $\rho_A = \mathrm{tr}_B(\rho)$ where $B = V \setminus A$ is complement of region
- All local expectation values in A can be computed using ρ_A only
- In general, ρ_A will be a **mixed state**, even if ρ is pure!



Entanglement entropies

- **Entropy** of ρ_A , $S(\rho_A) = -\mathrm{tr}(\rho_A \log \rho_A)$ will be non-vanishing, even if $S(\rho) = 0$
- Can be computed from eigenvalues of reduced state as $S(\rho_A) = -\sum_k \lambda_k \log \lambda_k$
- Reflects **entanglement** of A with respect to complement: "Unique" measure of entanglement for pure states

- How does the (von-Neumann)-entropy **scale** with the size of A ?
- Like its **volume**, as an **extensive quantity**?

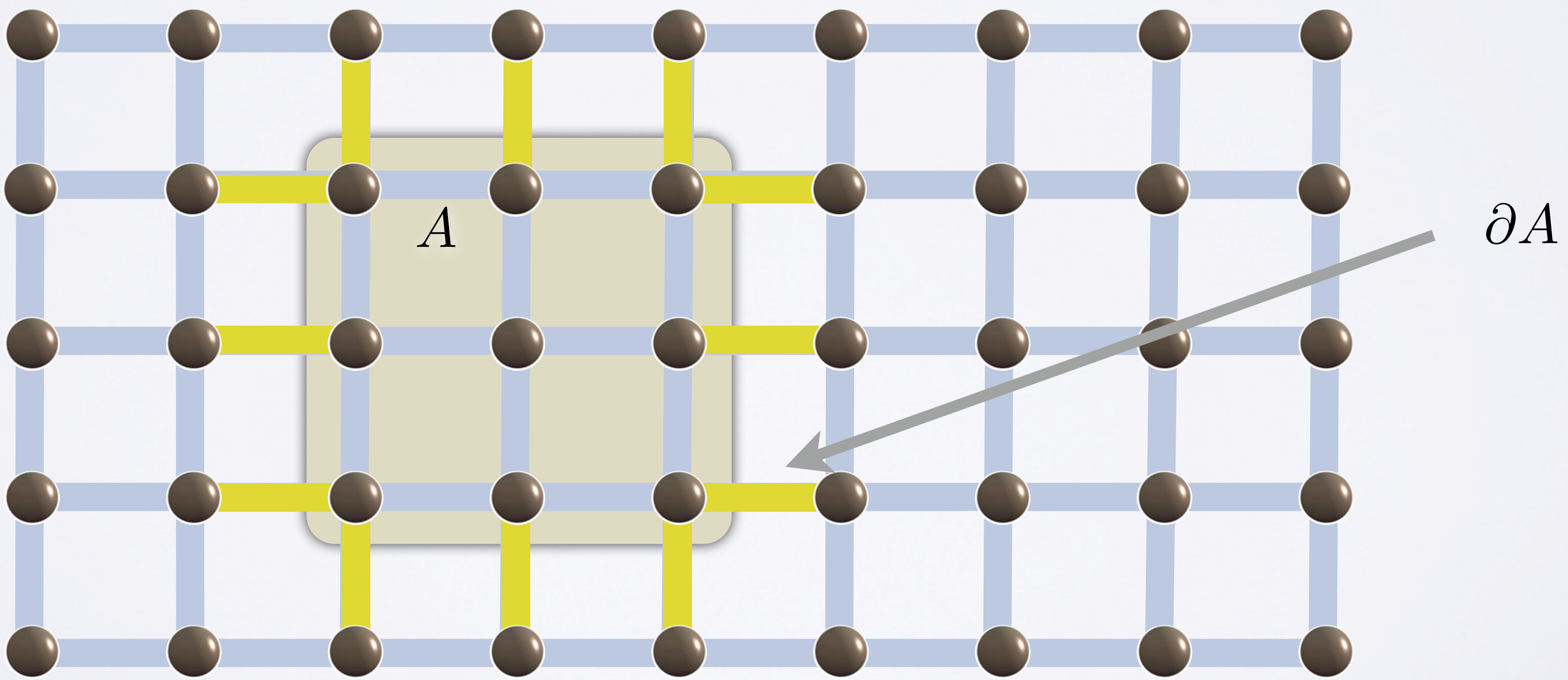


Area laws for the entanglement entropy

- Nope: Entanglement entropies of gapped models generalically scale like the **boundary area of the region**

$$S(\rho_A) = O(|\partial A|)$$

- Entanglement is boundary effect: **Much (!) less** entanglement than there could be



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- **Proven instances of area laws**
  - **1d gapped models**
  - Gapped **free bosonic and fermionic** models in **any dimension**
  - For graph states, projected entangled pair states, matrix-product states, see later
  - Any Hamiltonian that is in the **same gapped phase** as a free model

- Evidence that **gapped models satisfy area laws**

Violation of area laws

- Critical models in 1d are known to **violate area laws**, but only **logarithmically**

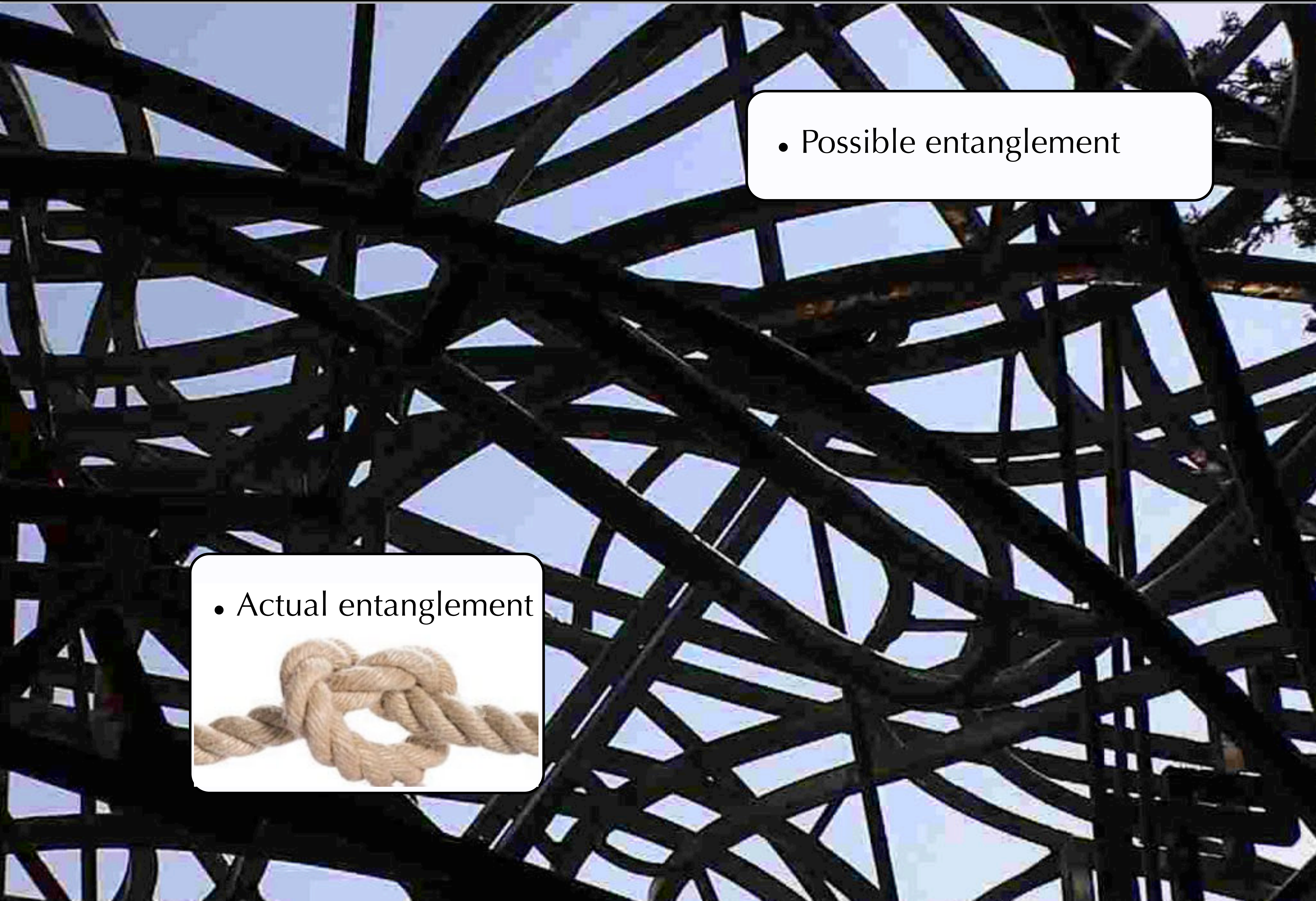
$$S(\rho_A) = \Theta(\log(|A|))$$

- Conformal field theory, conformal charge c , suggests $S(\rho_A) = (c/3)\log(l/a) + C$

- Critical higher-dimensional free models: scaling is different for **bosons** and **fermions**: Bosons **satisfy** an area law, while fermions **violate it**

$$S(\rho_A) = \Theta(L^{\mathcal{D}-1}\log L)$$

Lesson



- Possible entanglement

- Actual entanglement

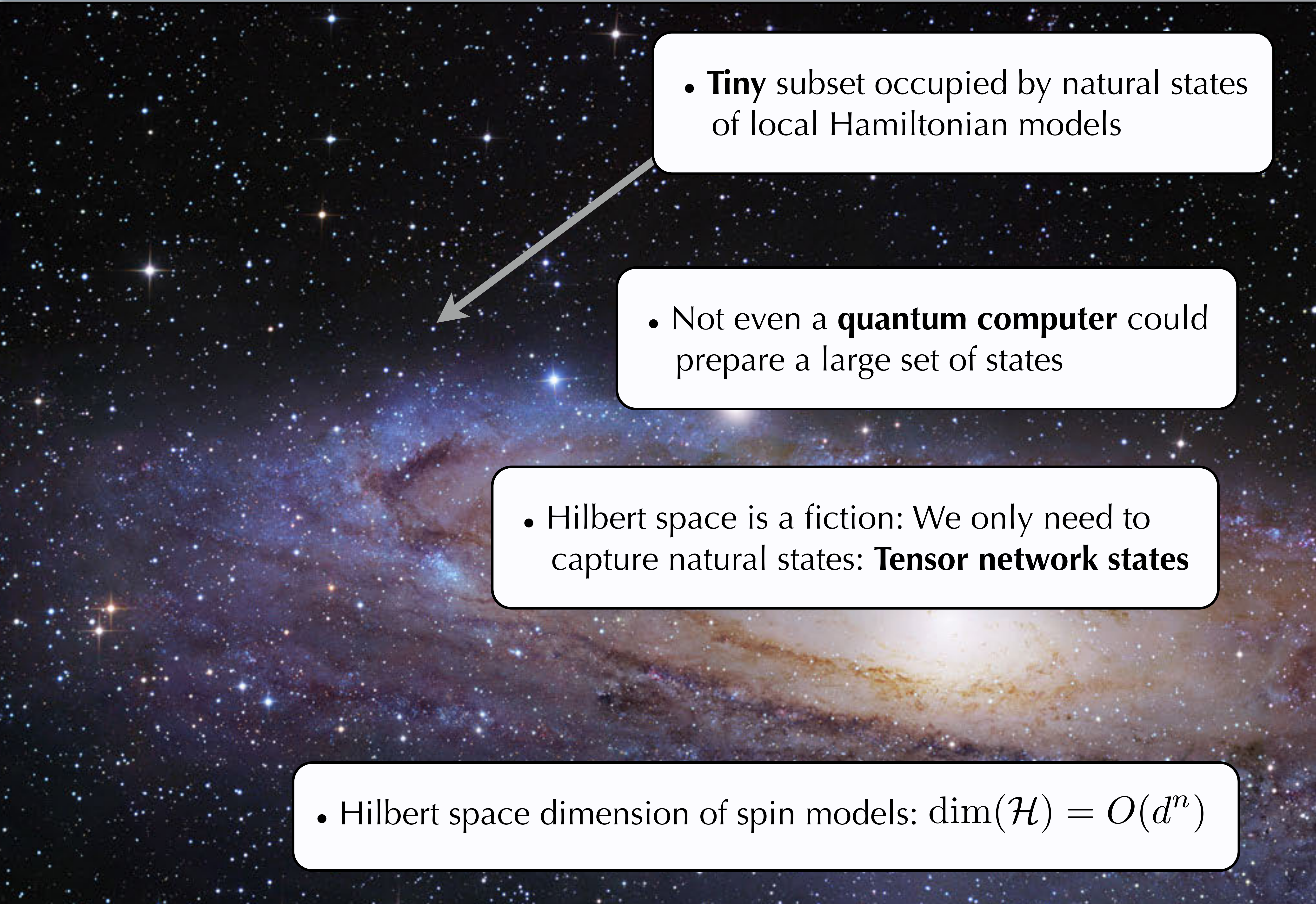
Other measures of entanglement

- Replace for pure states von-Neumann entropy by **Renyi entropies**, $\alpha > 0$

$$S_\alpha(\rho_A) = \frac{1}{1-\alpha} \log_2 \mathrm{tr}(\rho_A^\alpha)$$

- For mixed states such as thermal states, use **mutual information** or **negativity**
- **Entanglement spectra** heavily studied (but not here :))

Hilbert space is a fiction!



- **Tiny** subset occupied by natural states of local Hamiltonian models

- Not even a **quantum computer** could prepare a large set of states

- Hilbert space is a fiction: We only need to capture natural states: **Tensor network states**

- Hilbert space dimension of spin models: $\dim(\mathcal{H}) = O(d^n)$

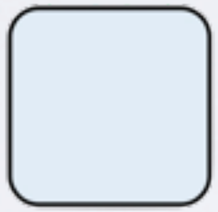
Tensors and graphical notation

Tensors and graphical notation

- **Tensor:** Multi-dimensional array of complex numbers
- Dimensionality of array **is order of tensor**
- Extensive use of **graphical notation:** Tensors are boxes, order: number of edges

Tensors and graphical notation

- This is how a **scalar** looks like



Tensors and graphical notation

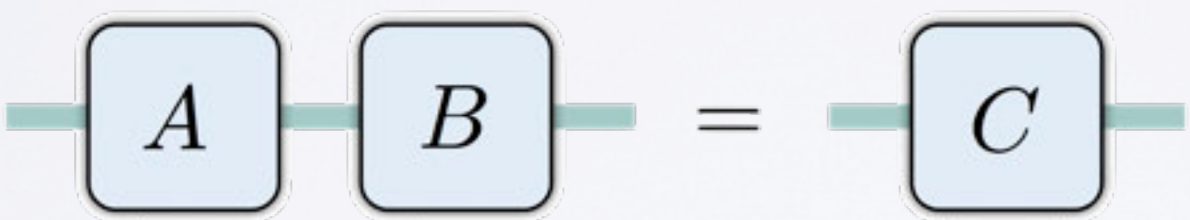
- **Vectors** and **dual vectors**

Tensors and graphical notation

- **Matrices**

- **Contraction of edge:** Summation

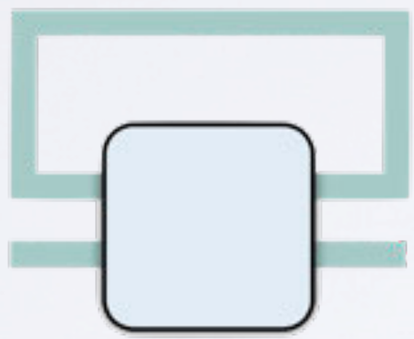
- E.g. matrix product $C_{\alpha,\beta} = \sum_{\gamma=1}^{N} A_{\alpha,\gamma} B_{\gamma,\beta}$



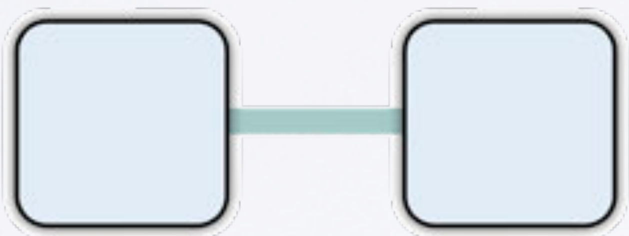
Tensors and graphical notation

- **Trace**

- **Partial trace**



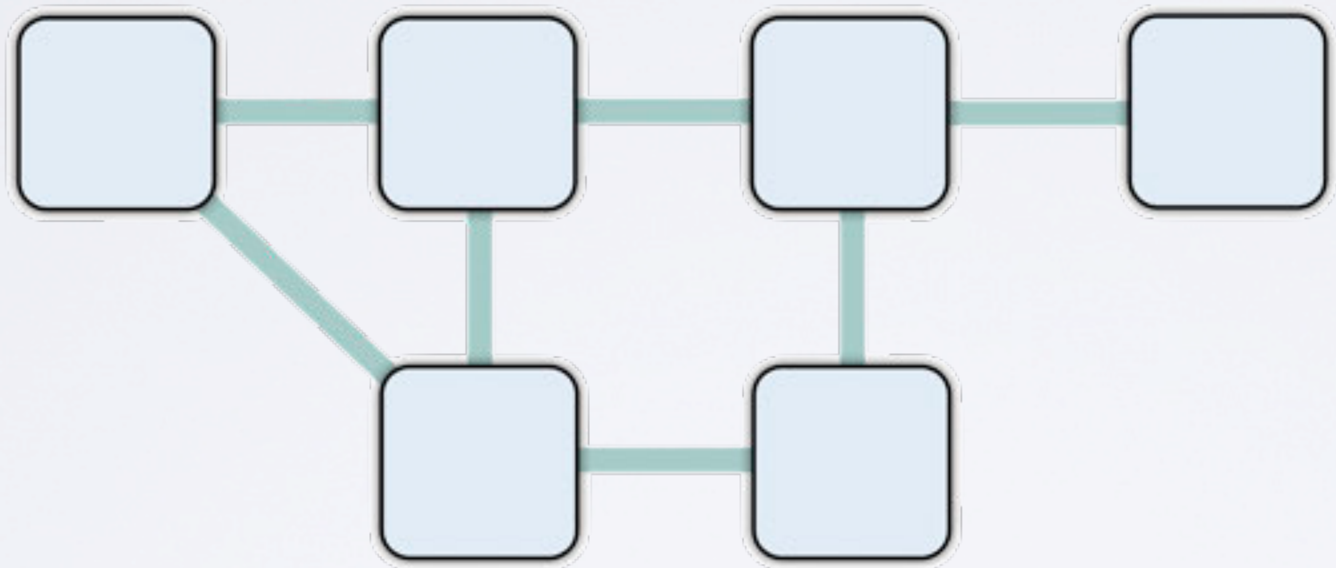
- **Scalar product**



- An uncontracted index is **open index**

Tensors and graphical notation

- **Contraction of a tensor network:** Contraction of all edges not open



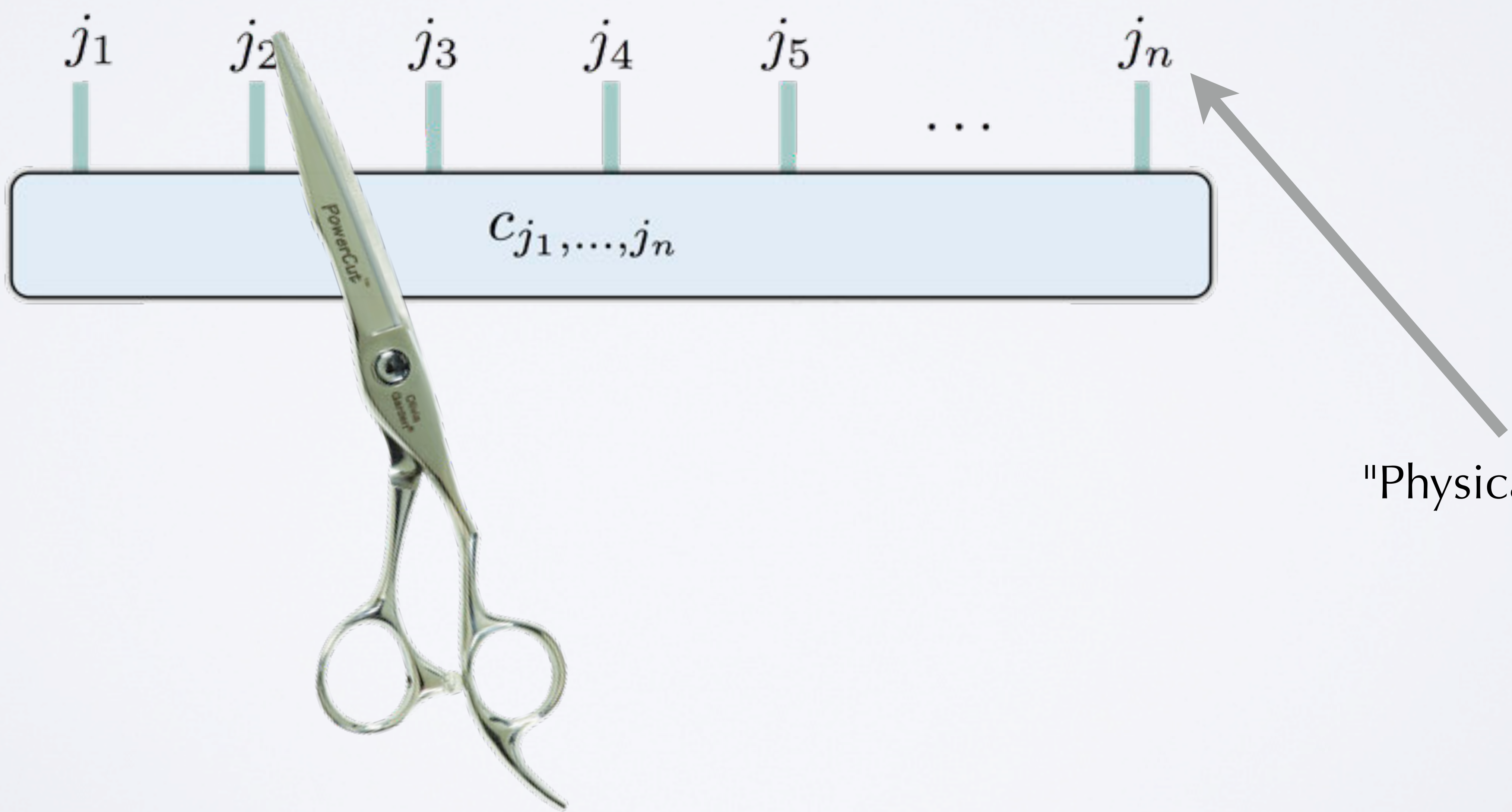
Matrix-product states

Arbitrary state vectors

- **Arbitrary state vector** $|\psi\rangle \in (\mathbb{C}^d)^{\otimes n}$

$$|\psi\rangle = \sum_{j_1,\ldots,j_n=1}^{d} c_{j_1,\ldots,j_n} |j_1,\ldots,j_n\rangle$$

graphically



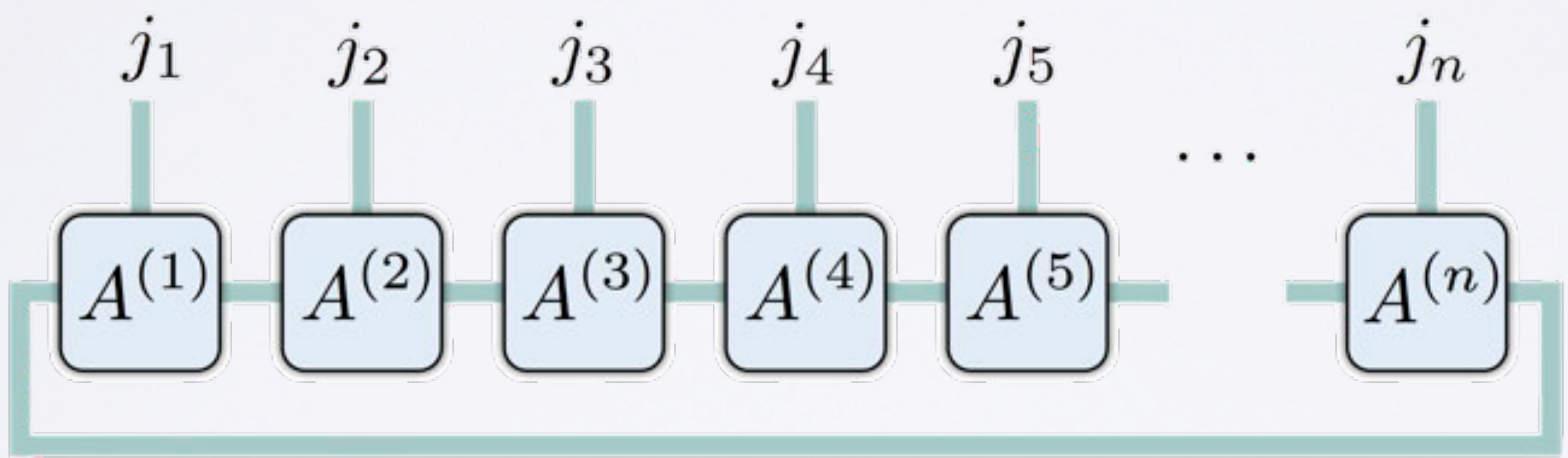
"Physical edges"

Matrix-product states

- **Matrix-product state (MPS)** vector of "bond dimension" D

$$|\psi\rangle = \sum_{j_1,\ldots,j_n=1}^{d} c_{j_1,\ldots,j_n} |j_1,\ldots,j_n\rangle$$

graphically



where

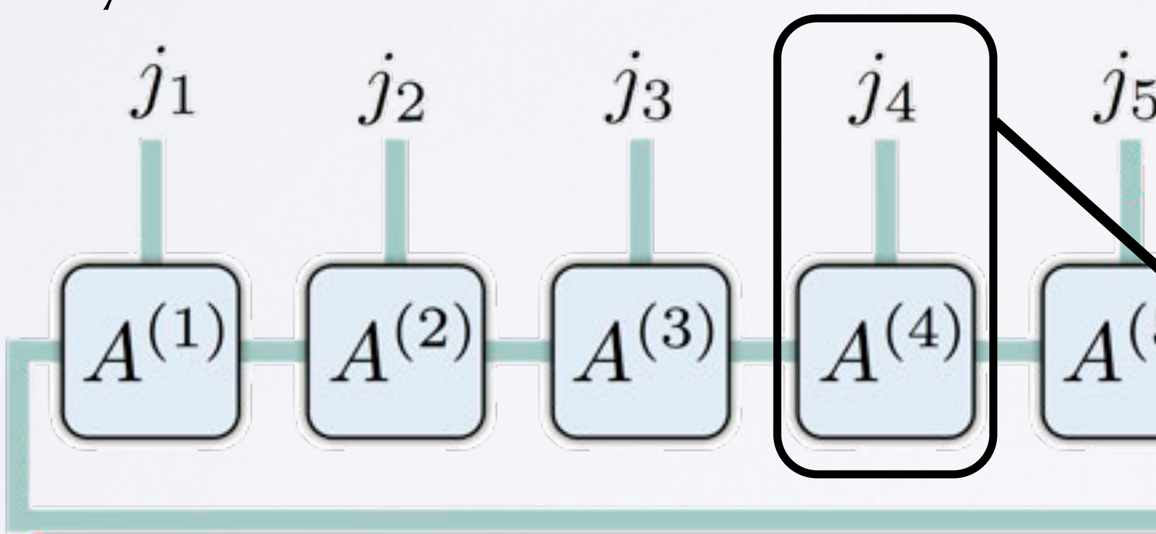
$$c_{j_1,\ldots,j_n} = \sum_{\alpha,\beta,\ldots,\omega=1}^{D} A^{(1)}_{\alpha,\beta;j_1} A^{(2)}_{\beta,\gamma;i_2} \ldots A^{(n)}_{\omega,\alpha;j_n} = \mathrm{tr}(A^{(1)}_{j_1} A^{(2)}_{j_2} \ldots A^{(n)}_{j_n})$$

Matrix-product states

- **Matrix-product state (MPS)** vector of "bond dimension" D

$$|\psi\rangle = \sum_{j_1,\ldots,j_n=1}^{d} c_{j_1,\ldots,j_n} |j_1,\ldots,j_n\rangle$$

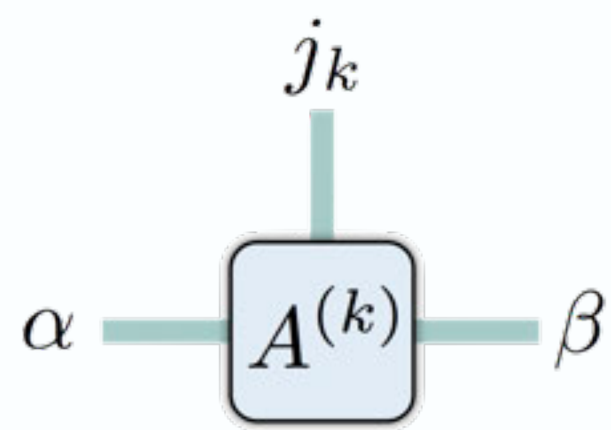
graphically



where

$$c_{j_1,\ldots,j_n} = \sum_{\alpha,\beta,\ldots,\omega=1}^{D} A^{(1)}_{\alpha,\beta;j_1} A^{(2)}_{\beta,\gamma;i_2} \cdots \quad \ldots A^{(n)}_{j_n})$$

- Each tensor



Bond dimensions

- What is D ? A **refinement parameter**
  - How many parameters for arbitrary pure state?

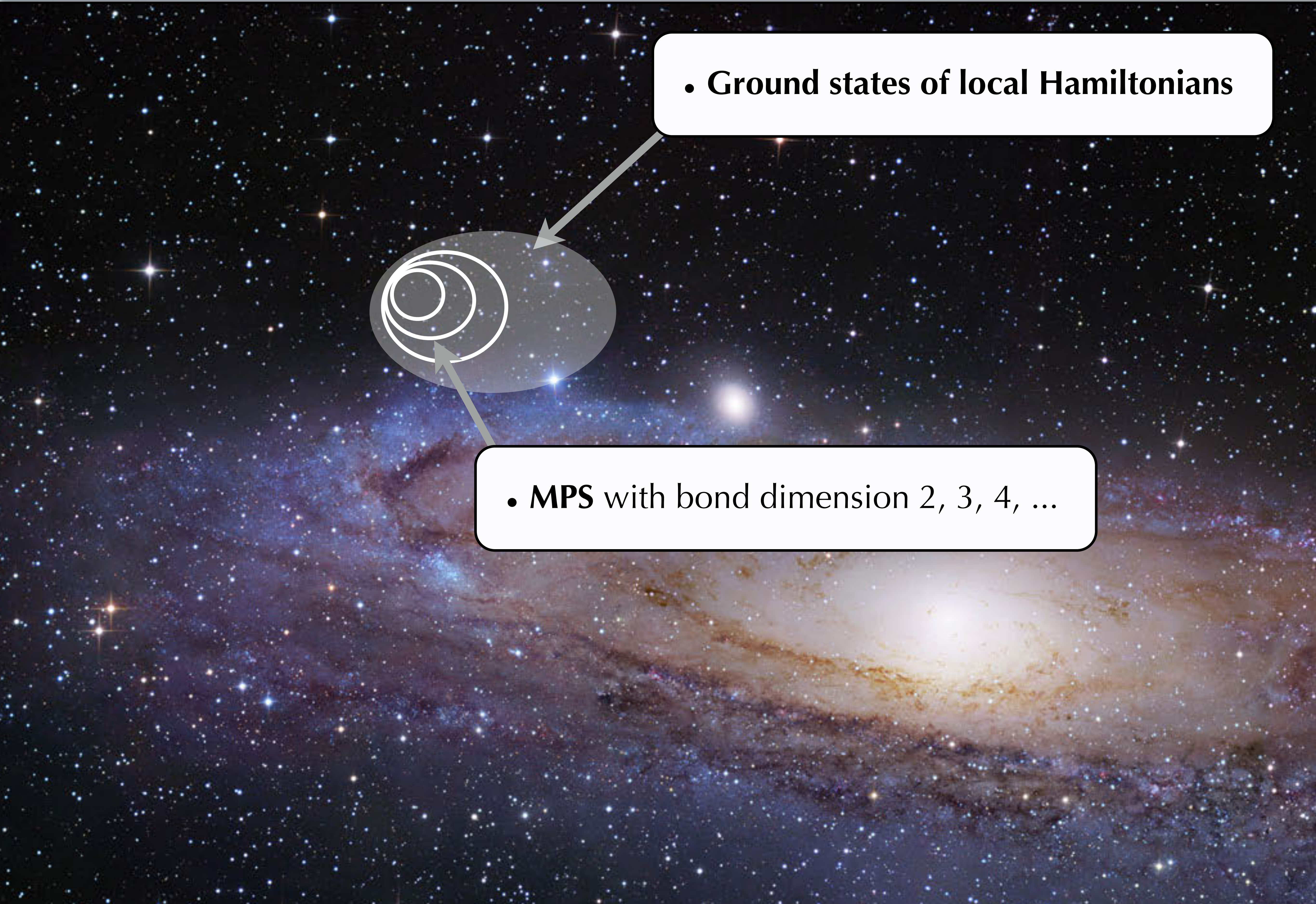
    $$O(d^n)$$

  - How many parameters for MPS?

    $$O(ndD^2)$$

- Linear in n, not exponential!
- The larger D , the larger the set of states that can be represented
- Gutzwiller mean field $D = 1$, all states can be represented for exponentially large D

Area laws and approximations with area laws



Area laws and approximations with area laws

- Easy to see: For each subset A of consecutive sites,

$$S(\rho_A) = O(\log(D))$$

- **MPS satisfy area laws**

- But the converse is also true!

- **1d states satisfying area laws can be well approximated by MPS**

- **Fine print:** If for a family of state vectors $|\psi_n\rangle$ there exist constants $c, C > 0$ such that for all $0 < \alpha < 1$ the Renyi entropies of the reduced state of any subsystem A of the one-dimensional system satisfy

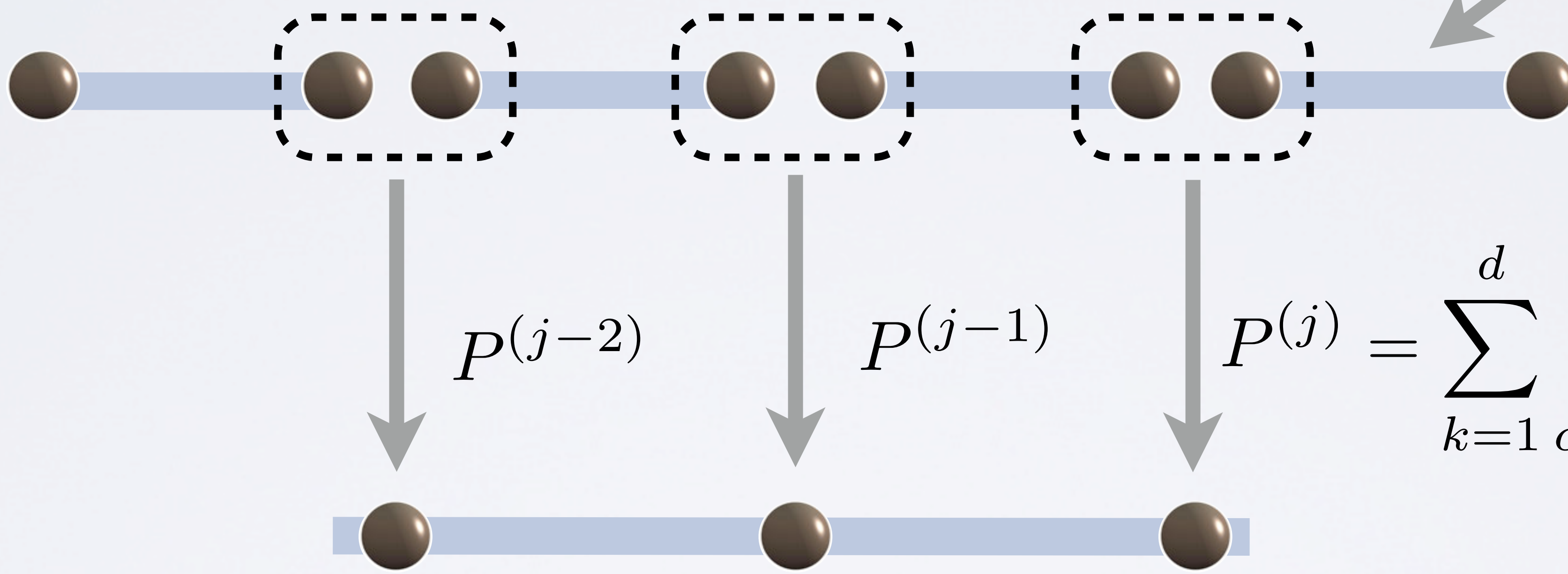
$$S_\alpha(\rho_A) \leq c \log(n) + C$$

then it can be efficiently approximated by an MPS (the bond dimension will have to grow polynomially with n, the system size, and $1/\epsilon$, where $\epsilon > 0$ is the approximation error)

Projected entangled pair state (PEPS) picture of MPS

- Start from **maximally entangled states** in **'virtual space'**

$$|\omega\rangle = \sum_{j=1}^{D} |j, j\rangle$$



$$P^{(j)} = \sum_{k=1}^{d} \sum_{\alpha,\beta=1}^{D} A^{(j)}_{\alpha,\beta;k} |k\rangle\langle\alpha,\beta|$$

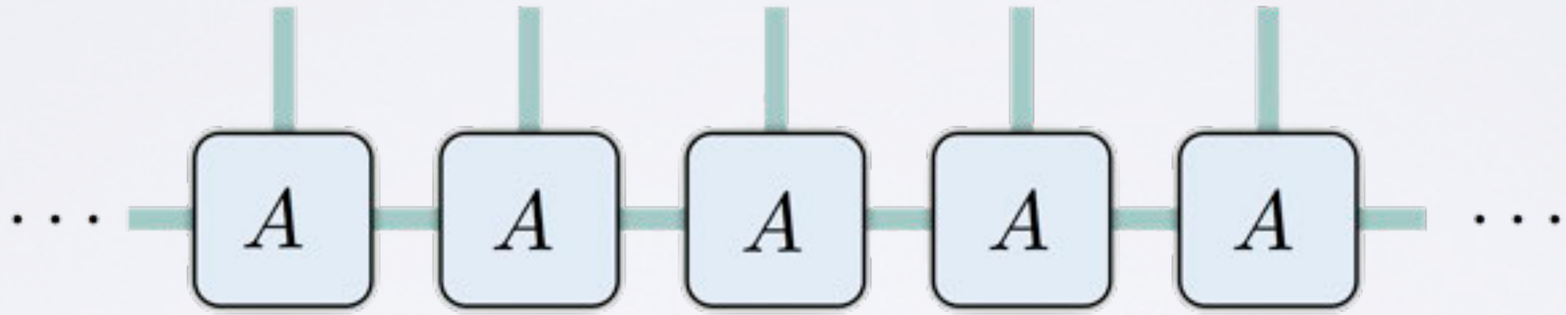
$$|\psi\rangle = (P^{(1)} \otimes \cdots \otimes P^{(n)})|\omega\rangle^{\otimes(n-1)}$$

- Generates MPS

- **Two more ways of generating MPS:** Sequential generation and successive SVD

Translationally invariant MPS

- Take for periodic boundary conditions $A^{(j)}_{\alpha,\beta;k} = A_{\alpha,\beta;k}$



- Make a lot of sense in analytical considerations, specifically in thermodynamic limit
- Numerically, advisable to break symmetry, see Uli's lecture

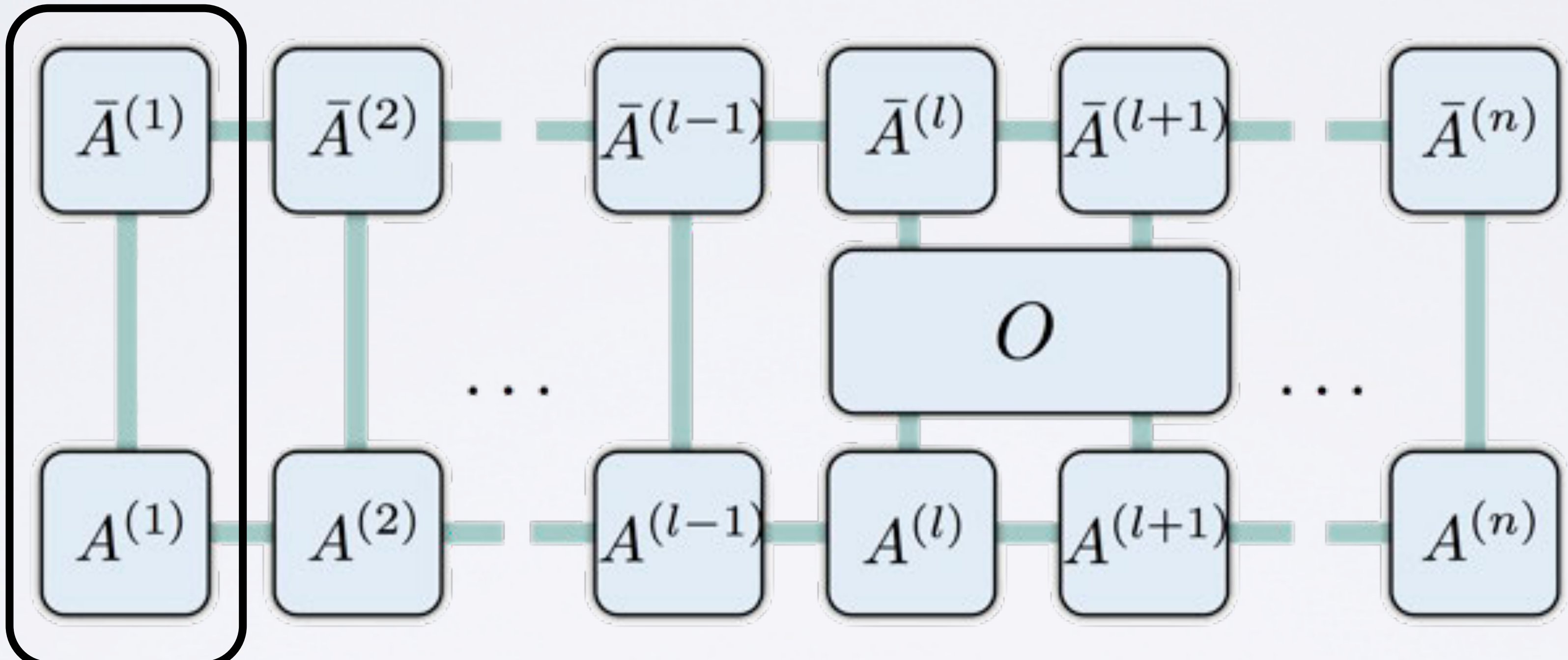
Computation of expectation values

Computation of expectation values

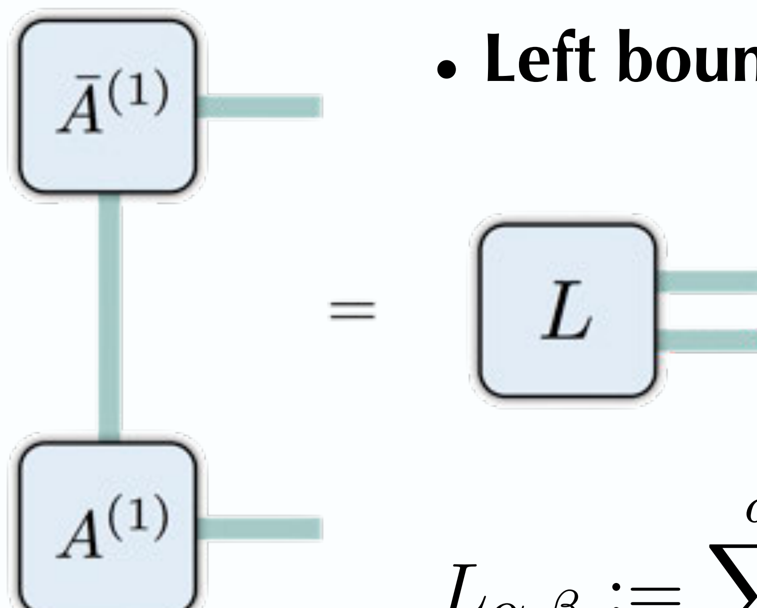
- We want to compute $\langle\psi|O|\psi\rangle$ for local observables O
- **Reasons to get worried:** Fact that MPS is described by poly many parameters alone does not mean that we can efficiently compute it (permanents in #P)
- **In fact:** In a naive way, we need exponentially many steps
- **But we can do better!**

Computation of expectation values

- Assume O is only supported on sites l and $l+1$
- Graphically



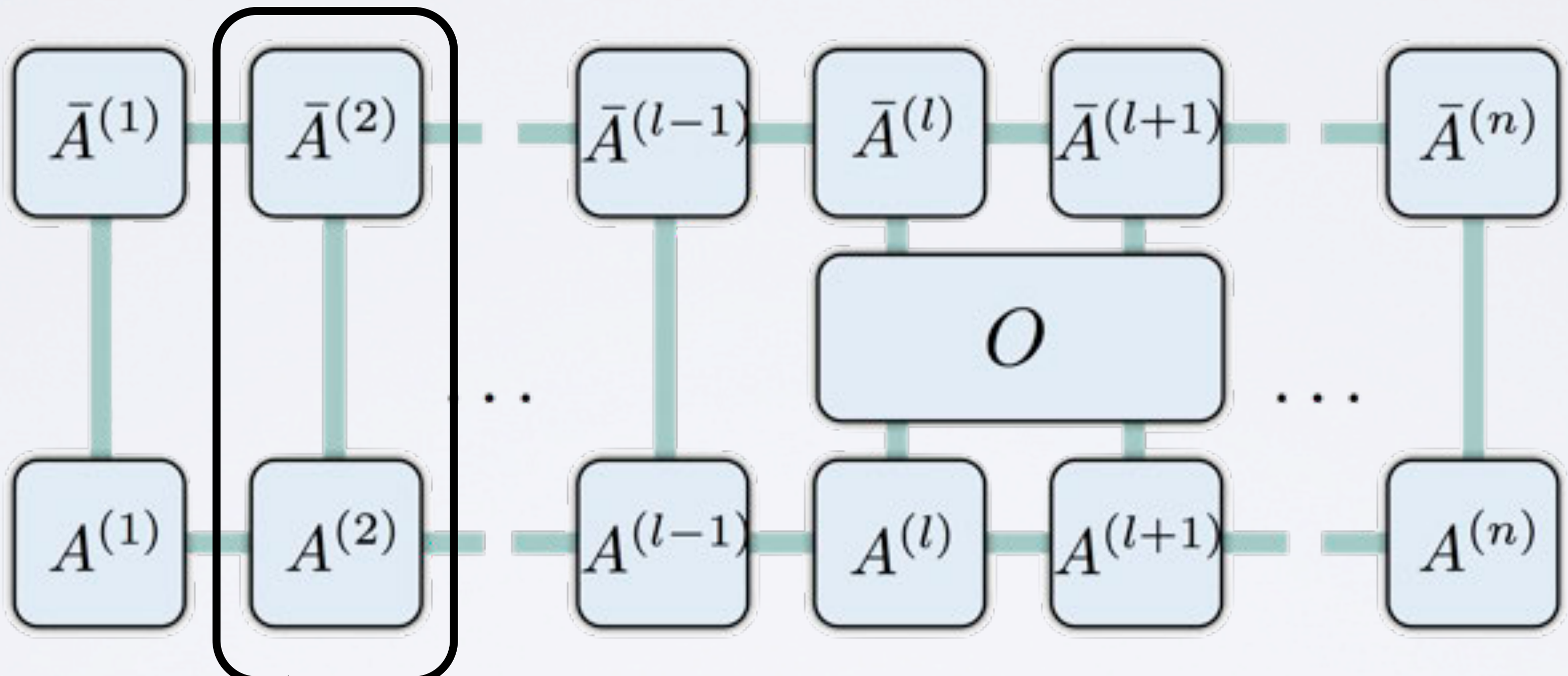
- **Left boundary**

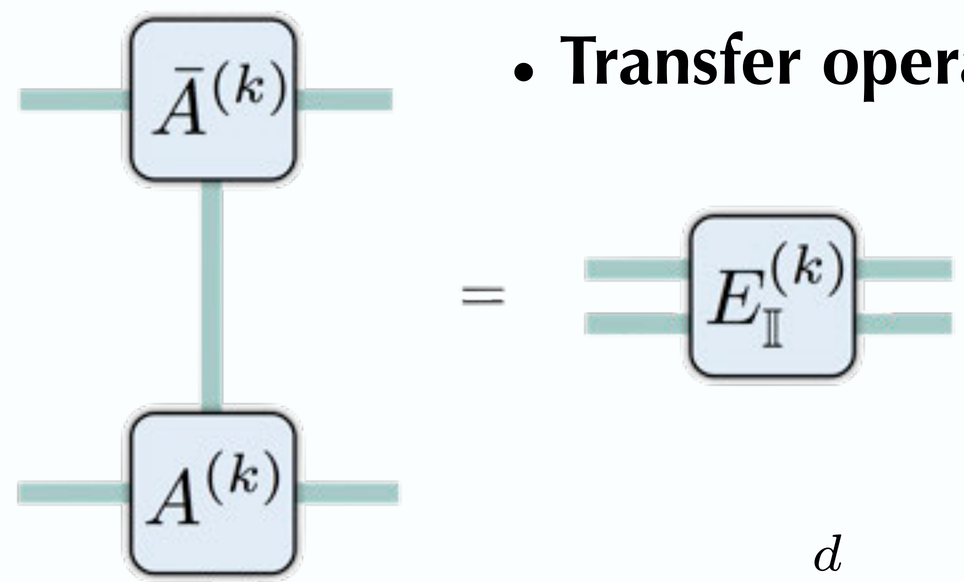


$$L_{\alpha,\beta} := \sum_{j=1}^{d} A^{(1)}_{\alpha;j} \bar{A}^{(1)}_{\beta;j}$$

Computation of expectation values

- Assume O is only supported on sites l and $l+1$
- Graphically



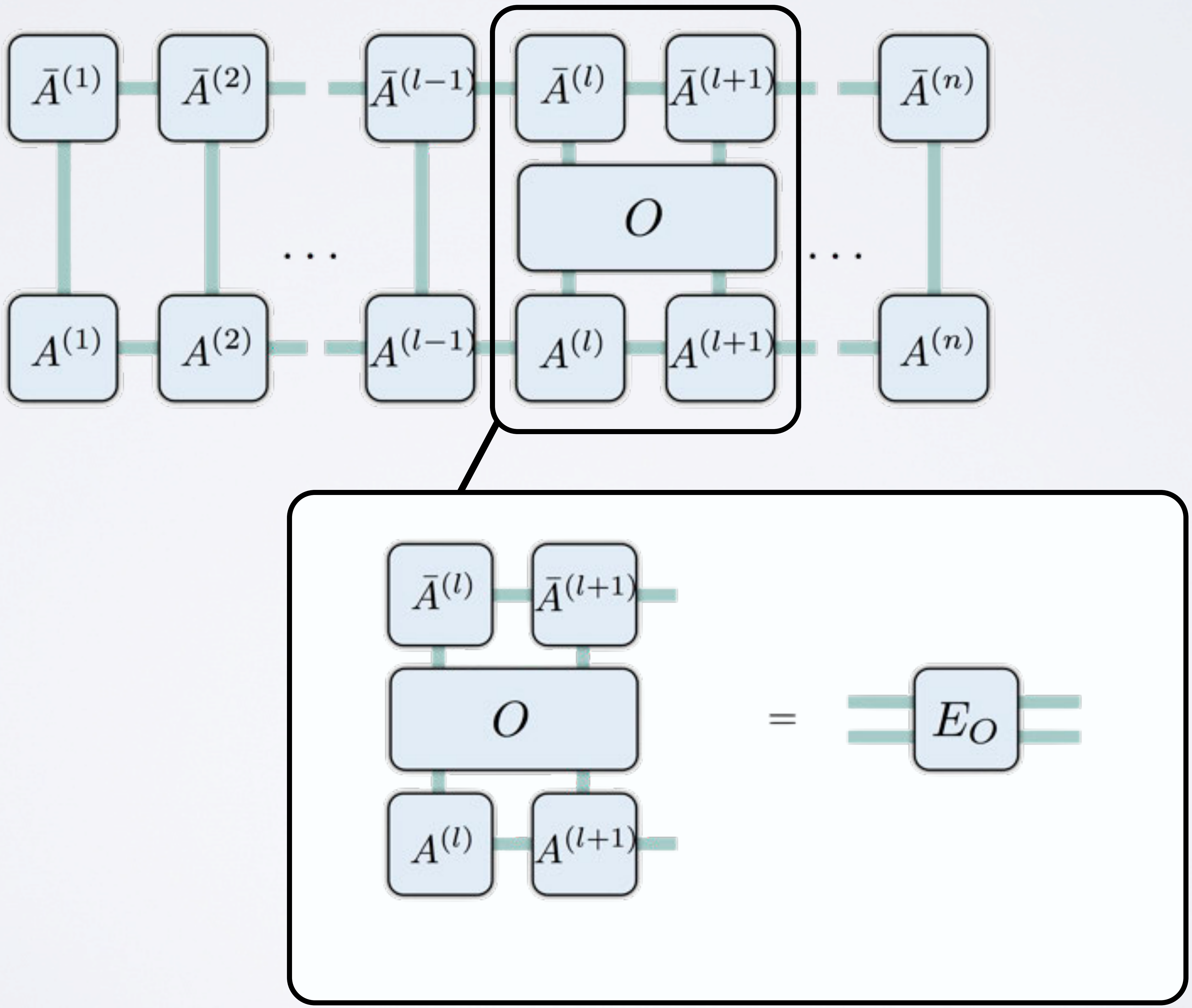


- **Transfer operator**

$$(E_{\mathbb{I}}^{(k)})_{\alpha,\beta;\gamma,\delta} = \sum_{j=1}^{d} A^{(k)}_{\alpha,\beta;j} \bar{A}^{(k)}_{\gamma,\delta;j}$$

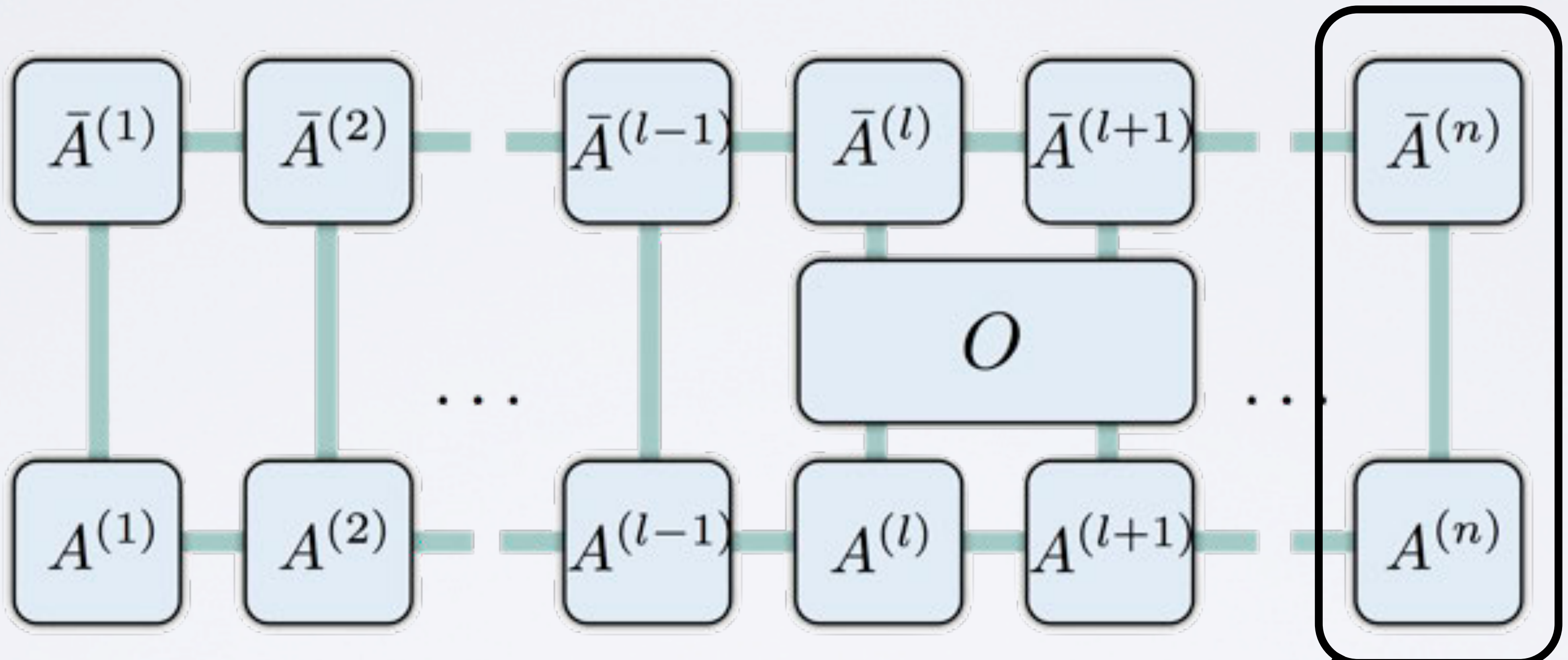
Computation of expectation values

- Assume O is only supported on sites l and $l+1$
- Graphically

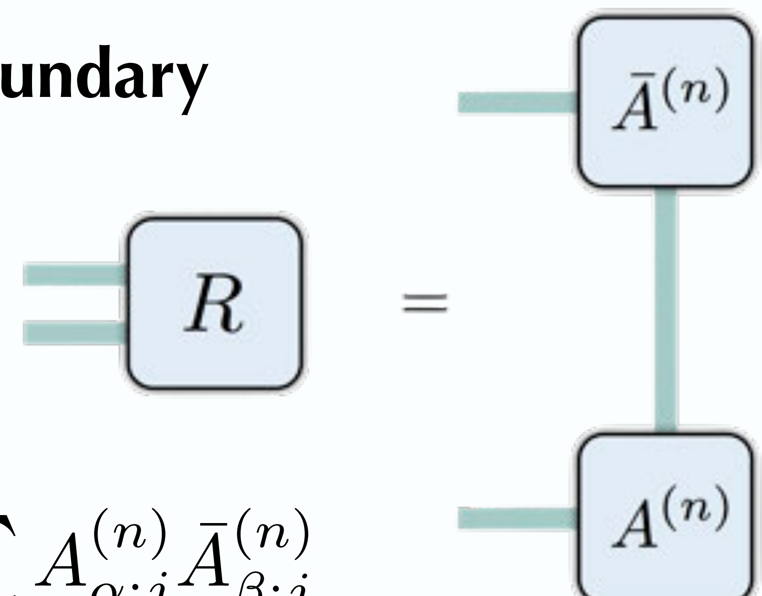


Computation of expectation values

- Assume O is only supported on sites l and $l+1$
- Graphically



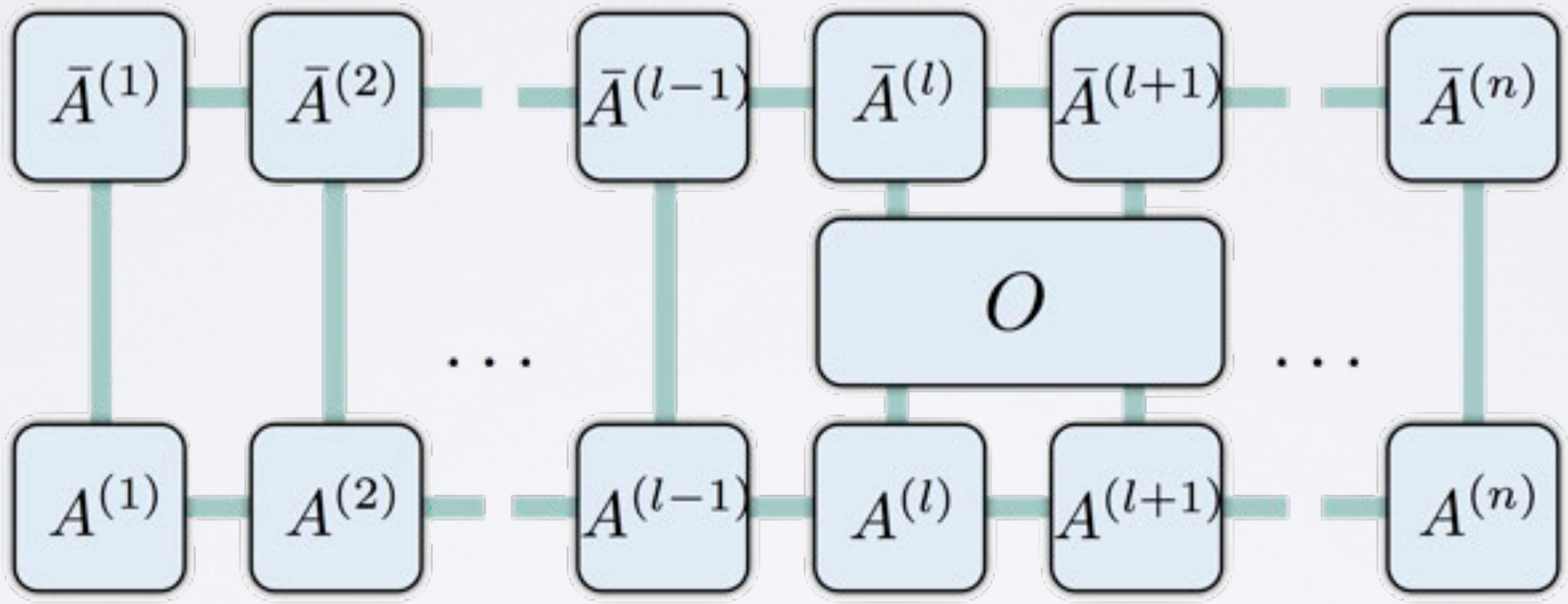
- **Right boundary**



$$R_{\alpha,\beta} = \sum_{j=1}^{d} A^{(n)}_{\alpha;j} \bar{A}^{(n)}_{\beta;j}$$

Computation of expectation values

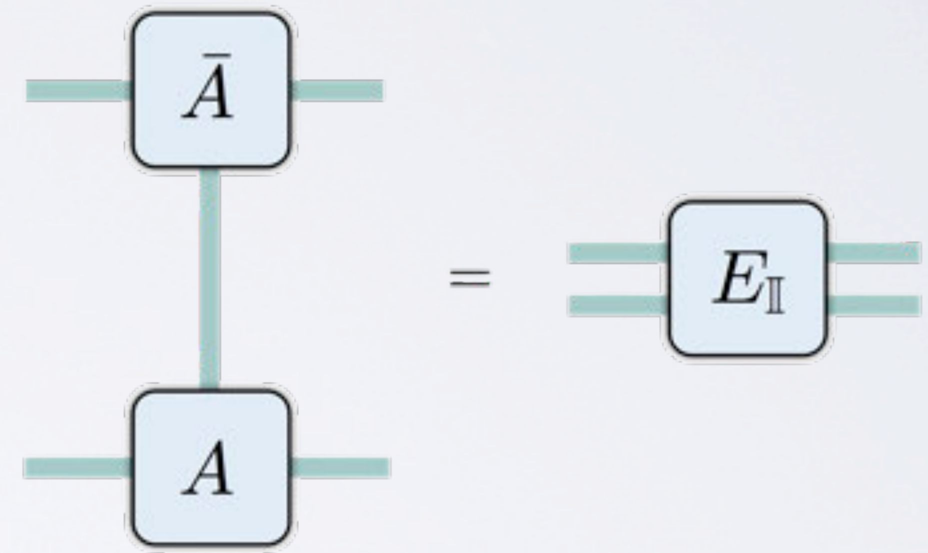
- Assume O is only supported on sites l and $l+1$
- Graphically



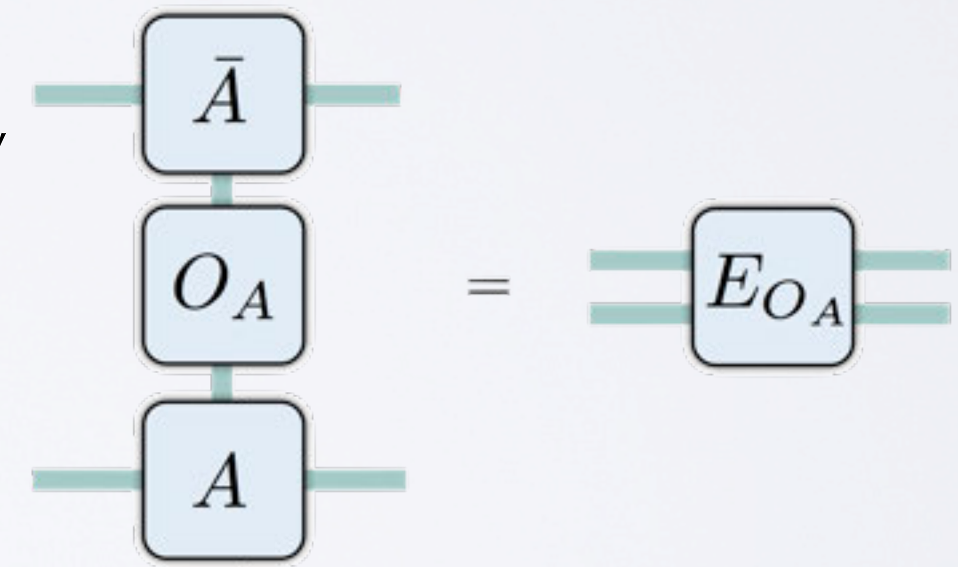
- **Can be efficiently computed!**
- There are yet smarter ways, see **Uli's lecture**

Decay of correlations

- Stick for simplicity to infinite translationally invariant MPS
- Transfer operator $E_{\mathbb{I}} = \sum_{j=1}^{d} (A_j \otimes \bar{A}_j)$, graphically



and $E_{O_A} = \sum_{j,k=1}^{d} \langle k|O_A|j\rangle (A_j \otimes \bar{A}_k)$, graphically



- Correlation function

$$\langle O_A O_B \rangle = \frac{\mathrm{tr}(E_{O_A} E_{\mathbb{I}}^{\mathrm{dist}(A,B)-1} E_{\mathbb{I}}^{n-\mathrm{dist}(A,B)-1})}{\mathrm{tr}(E_{\mathbb{I}}^{n})}$$

Decay of correlations

- Interested in $n \to \infty$
- Find $E_{\mathbb{I}}^k = |r_1\rangle\langle l_1| + \sum_{j=2}^{D^2} \lambda_j^k |r_j\rangle\langle l_j|$, so $\langle O_A O_B \rangle = \langle l_1 | E_{O_A} E_{\mathbb{I}}^{\mathrm{dist}(A,B)-1} E_{O_B} | r_1 \rangle$

becomes

$$\langle O_A O_B \rangle = \underbrace{\langle l_1 | E_{O_A} | r_1 \rangle \langle l_1 | E_{O_B} | l_1 \rangle}_{= \ \langle O_A \rangle \langle O_B \rangle} + \sum_{j=2}^{D^2} \lambda_j^{\mathrm{dist}(A,B)-1} \langle l_1 | E_{O_A} | r_j \rangle \langle l_j | E_{O_B} | l_1 \rangle$$

- So $|\langle O_A O_B \rangle - \langle O_A \rangle \langle O_B \rangle|$ decays exponentially in the distance and correlation length is given by ratio of the second largest λ_2 to the largest $\lambda_1 = 1$ (taken to be unity) eigenvalue of $E_{\mathbb{I}}$,

$$\xi^{-1} = -\log |\lambda_2|$$

Placeholder

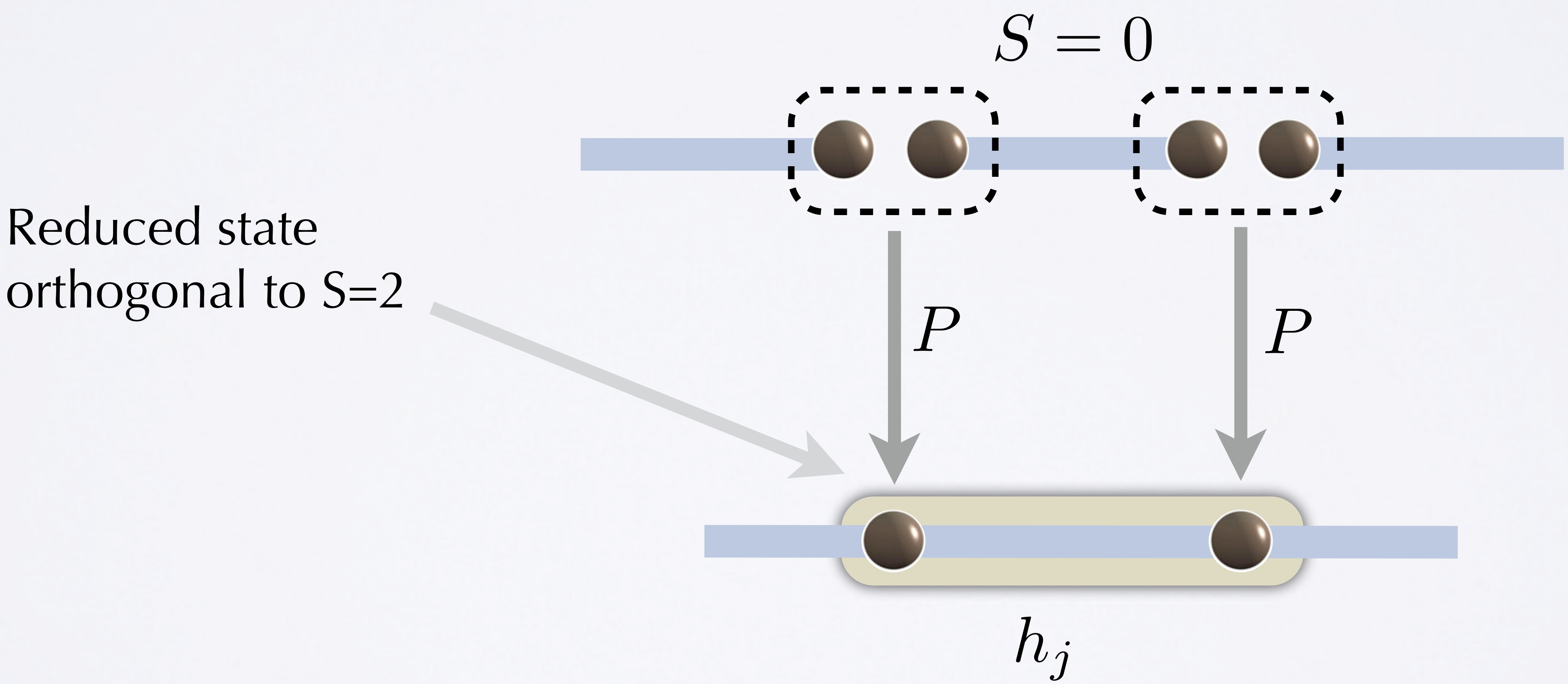
- Powerful numerical techniques, matrix-product operators, time-evolution:

  See next lecture

Matrix-product states as ground states

Exact MPS ground states

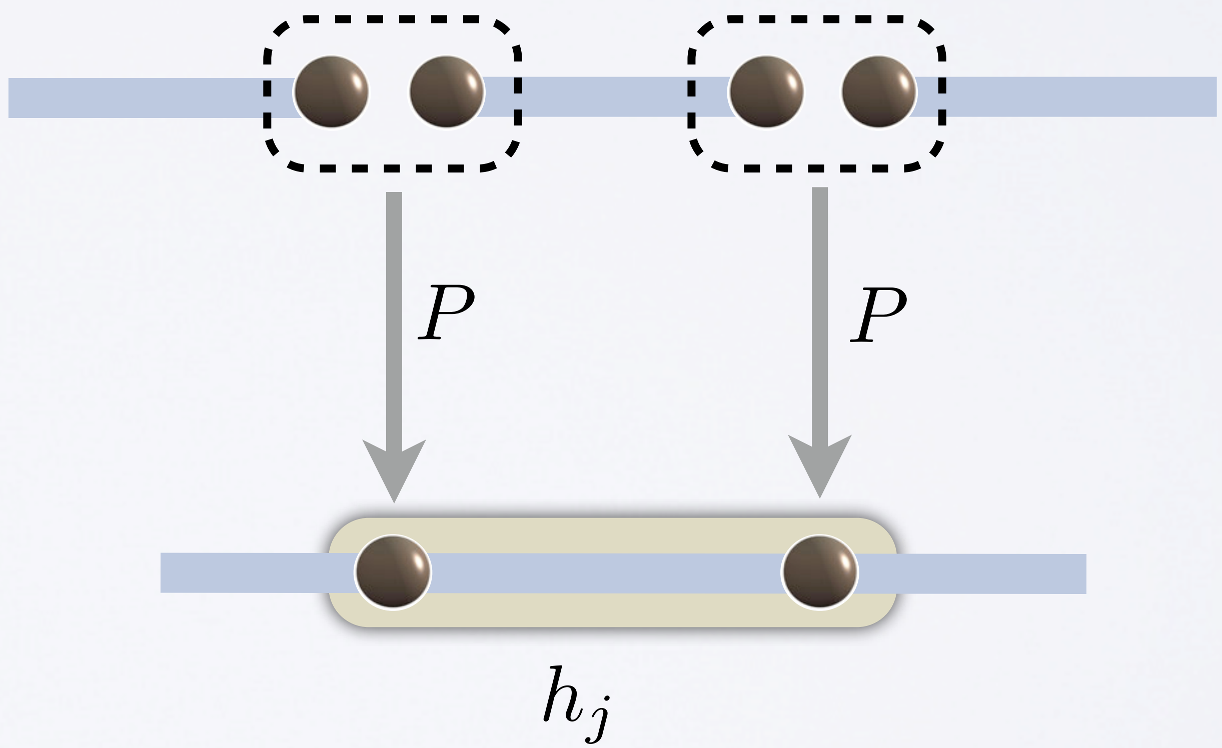
- Are there any **Hamiltonians** models that have **exact MPS ground states?**
- Take physical dimension $d = 3$, a **spin-1 model**, and bond dimension $D = 2$
- In the PEPS picture take $P = \Pi_{S=1}(\mathbb{I} \otimes iY)$, where $\Pi_{S=1}$ is projection onto the spin-1 subspace of two sites
- Surely gives rise to valid MPS $|\psi\rangle$



- Now $h_j = \Pi_{S=2}$, then $h_j|\psi\rangle = 0$

Exact MPS ground states

- But all h_j are positive, so $\langle\psi|H|\psi\rangle = \langle\psi|\sum_j h_j|\psi\rangle \geq 0$
- That is, $|\psi\rangle$ must be a **ground state vector**!



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Exact MPS ground states

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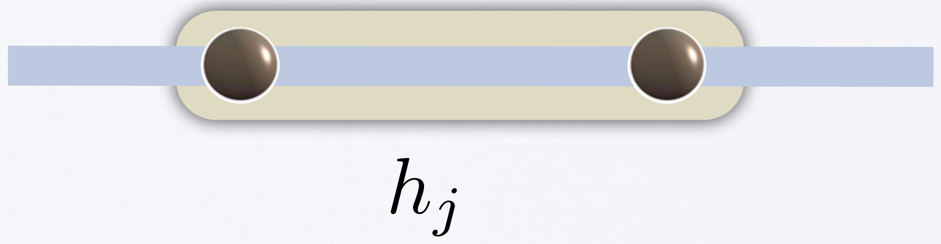
- That is, $|\psi\rangle$ must be a **ground state vector**!
- Famous **AKLT-model** (Affleck, Kennedy, Lieb, Tasaki)

$$h_j = \frac{1}{2}S^{(j)} \cdot S^{(j+1)} + \frac{1}{6}(S^{(j)} \cdot S^{(j+1)})^2 + \frac{1}{3}$$

- Resembles Spin-1 Heisenberg model

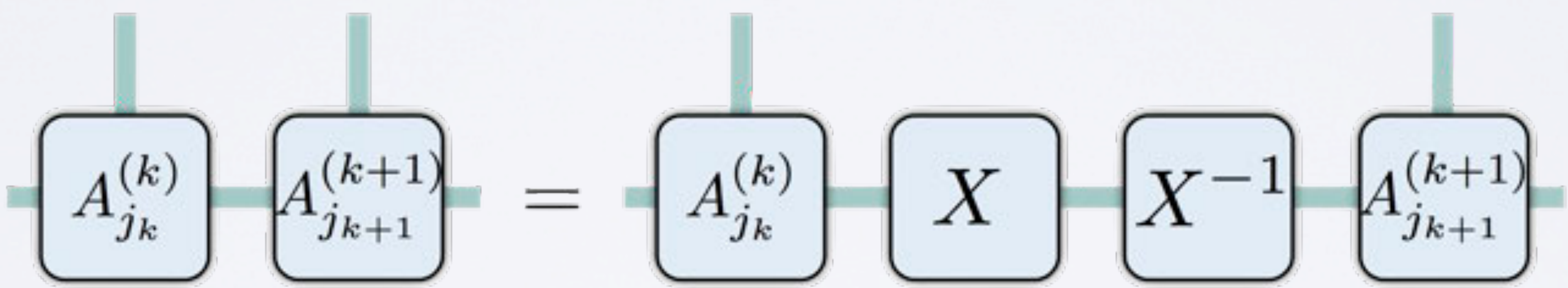


Gauge freedom in MPS

- An MPS is uniquely defined by the matrices defining it, but the converse is not true

$$A_{j_k}^{(k)} A_{j_{k+1}}^{(k+1)} = A_{j_k}^{(k)} X X^{-1} A_{j_{k+1}}^{(k+1)}$$

for every $X \in Gl(D, \mathbb{C})$



- Hence, can pick a suitable **gauge** in which matrices take simple form

$$\sum A_j^{(k)} (A_j^{(k)})^\dagger = \mathbb{I}$$

$$\sum_j (A_j^{(k)})^\dagger \Lambda^{(k-1)} A_j^{(k)} = \Lambda^{(k)}$$

$$\Lambda^{(0)} = \Lambda^{(n)} = 1$$

where each $\Lambda^{(k)} \in \mathbb{C}^{D \times D}$ for $k = 1, \ldots, n-1$ is diagonal, positive, has full rank and unit trace

Applications in quantum information theory and quantum state tomography

Matrix-product states in metrology

- Matrix-product states can be used in metrology, say, the **GHZ-state**

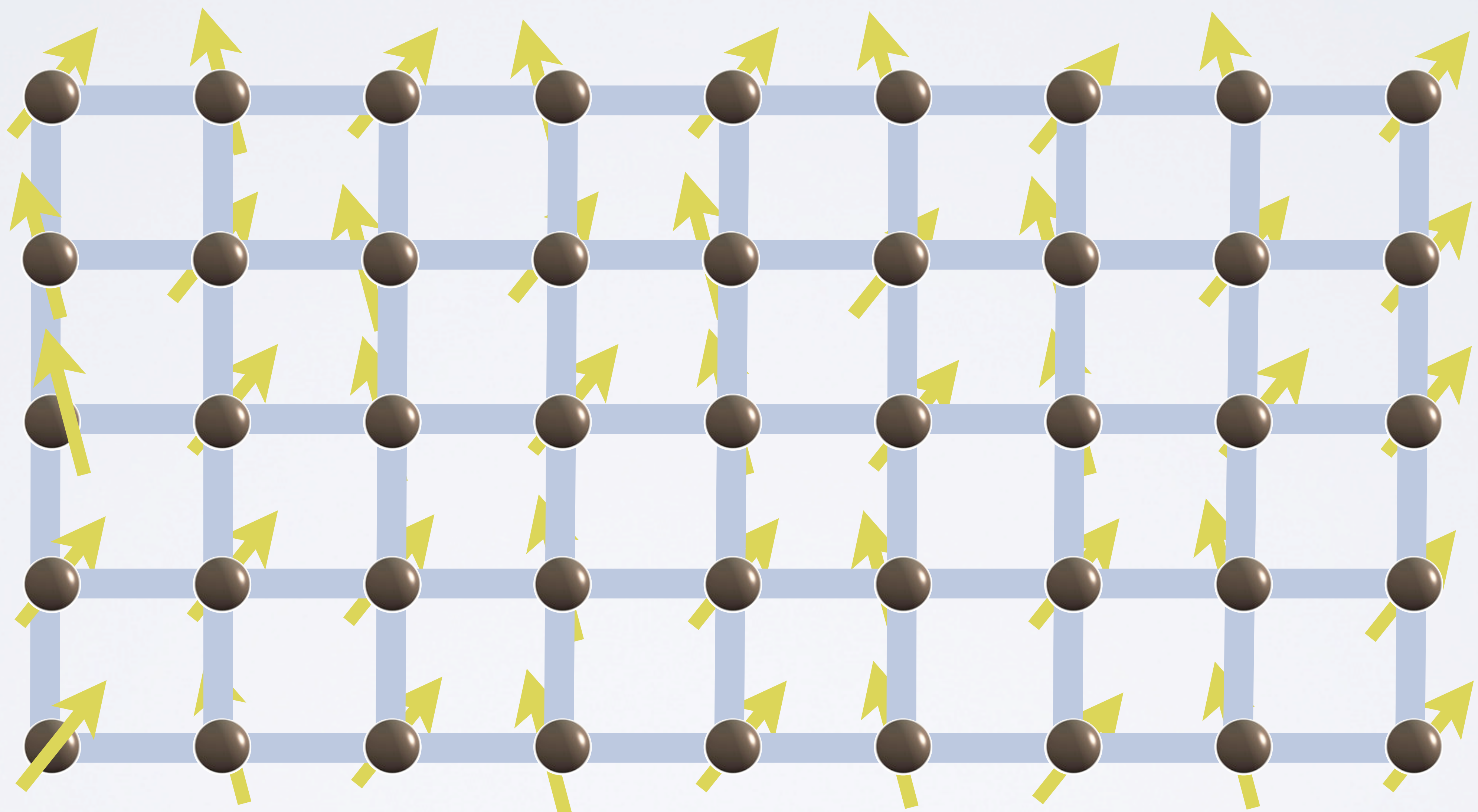
$$|\psi\rangle = (|0,\ldots,0\rangle + |1,\ldots,1\rangle)/\sqrt{2}$$

is MPS with $D = 2$ and $A_1 = |0\rangle\langle 0|$ and $A_2 = |1\rangle\langle 1|$

- **Other MPS** are better suited under noise

MPS in measurement-based quantum computing

- **Quantum computing based on measurements only**



MPS in measurement-based quantum computing

- **One-dimensional cluster states**

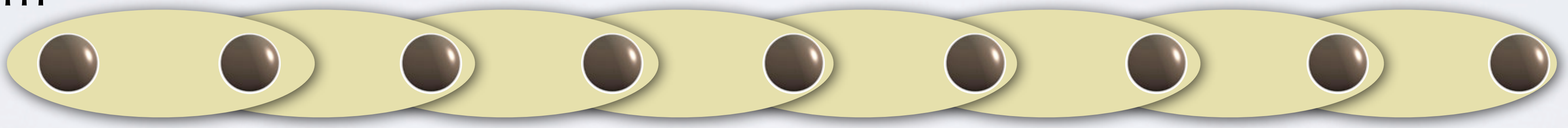
- Start from

$$|+\rangle \quad |+\rangle \quad |+\rangle \quad |+\rangle \quad |+\rangle \quad |+\rangle \quad |+\rangle \quad |+\rangle \quad |+\rangle$$

$$|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$$

MPS in measurement-based quantum computing

- **One-dimensional cluster states**
- Start from

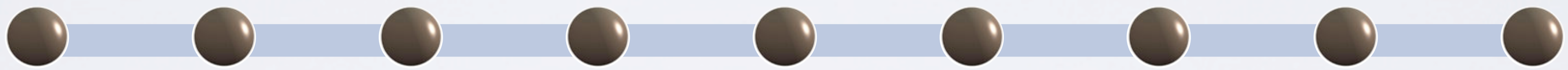


- Apply phase gates to neighbors

$$|j,k\rangle \mapsto |j,k\rangle(-1)^{\delta_{j,1}\delta_{k,1}}$$

MPS in measurement-based quantum computing

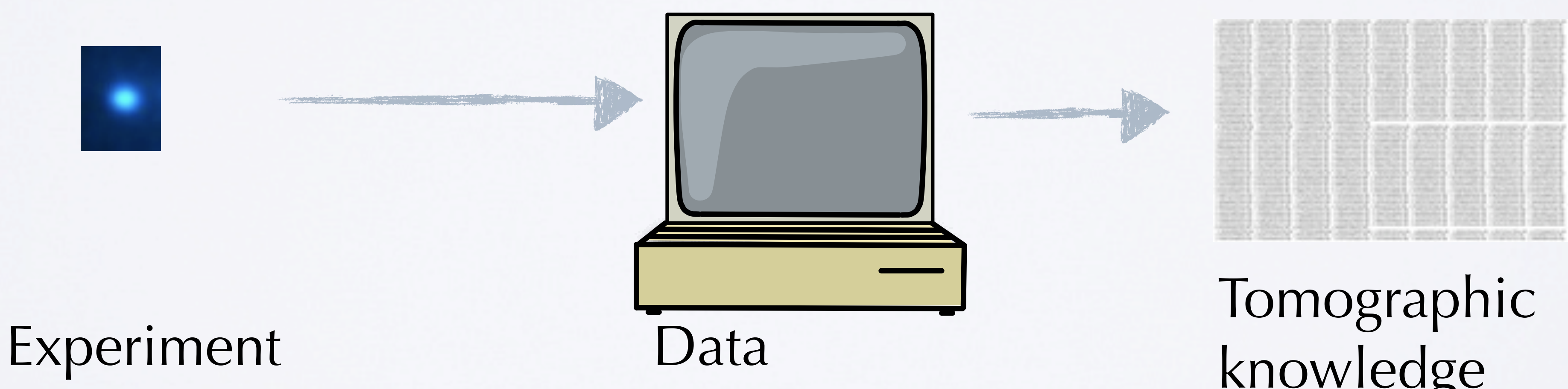
- **One-dimensional cluster states**



- Is MPS - and this picture explains how the principle works!

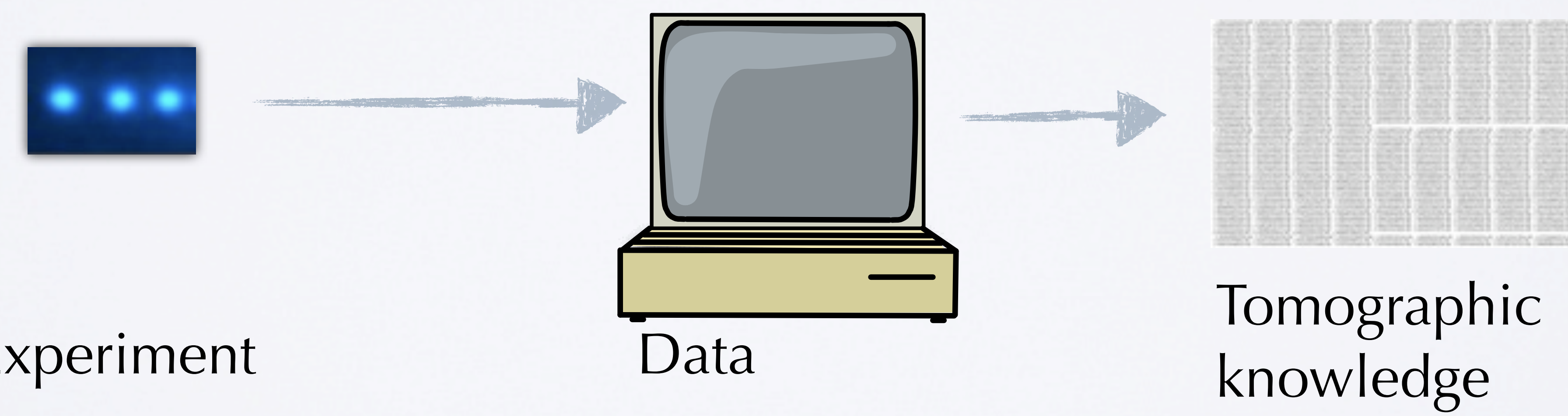
MPS in quantum state tomography

- Measure unknown quantum state of single spin
- Requires 3 measurement settings



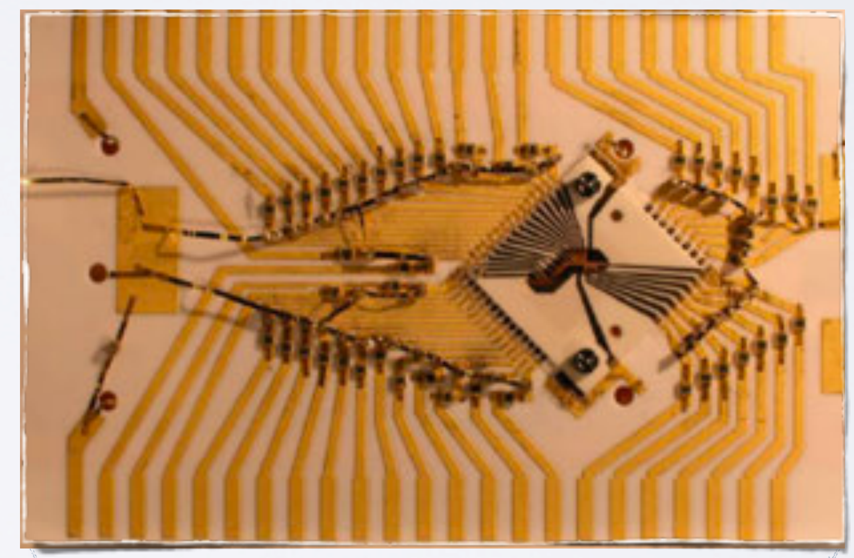
MPS in quantum state tomography

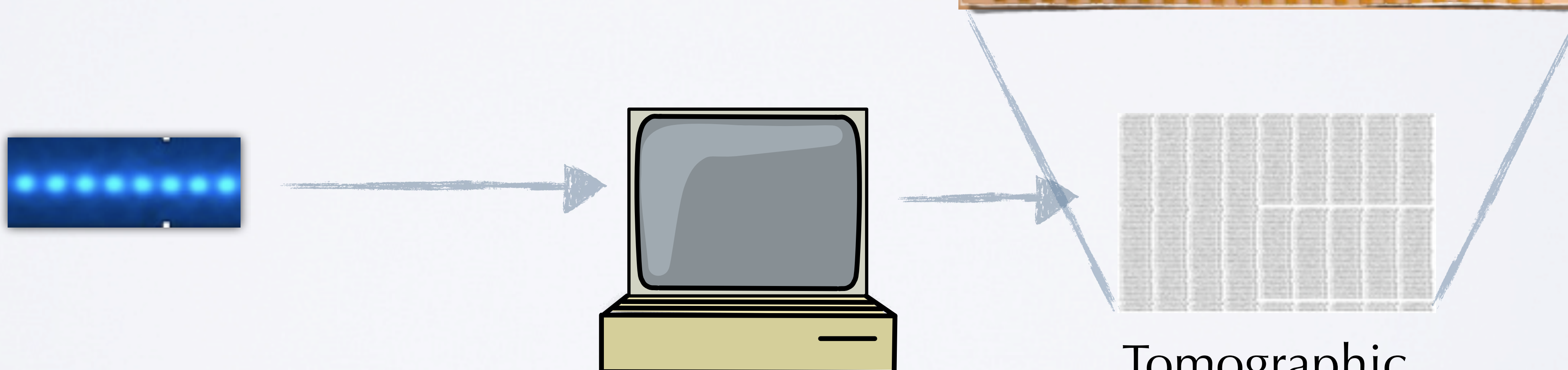
- Measure unknown quantum state of 3 spins
- Requires 63 measurement settings



MPS in quantum state tomography

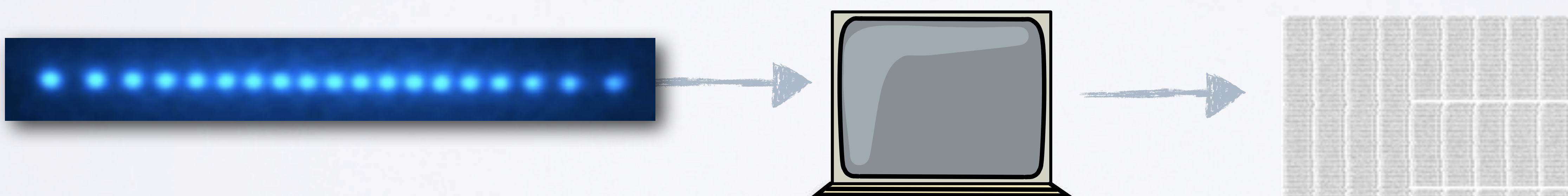
- Measure unknown quantum state of 8 spins
- Requires 65535 measurement settings





MPS in quantum state tomography

- Measure unknown quantum state of 20 spins
- Requires 1099511627775 measurement settings
- Use matrix-product states (or compressed sensing)

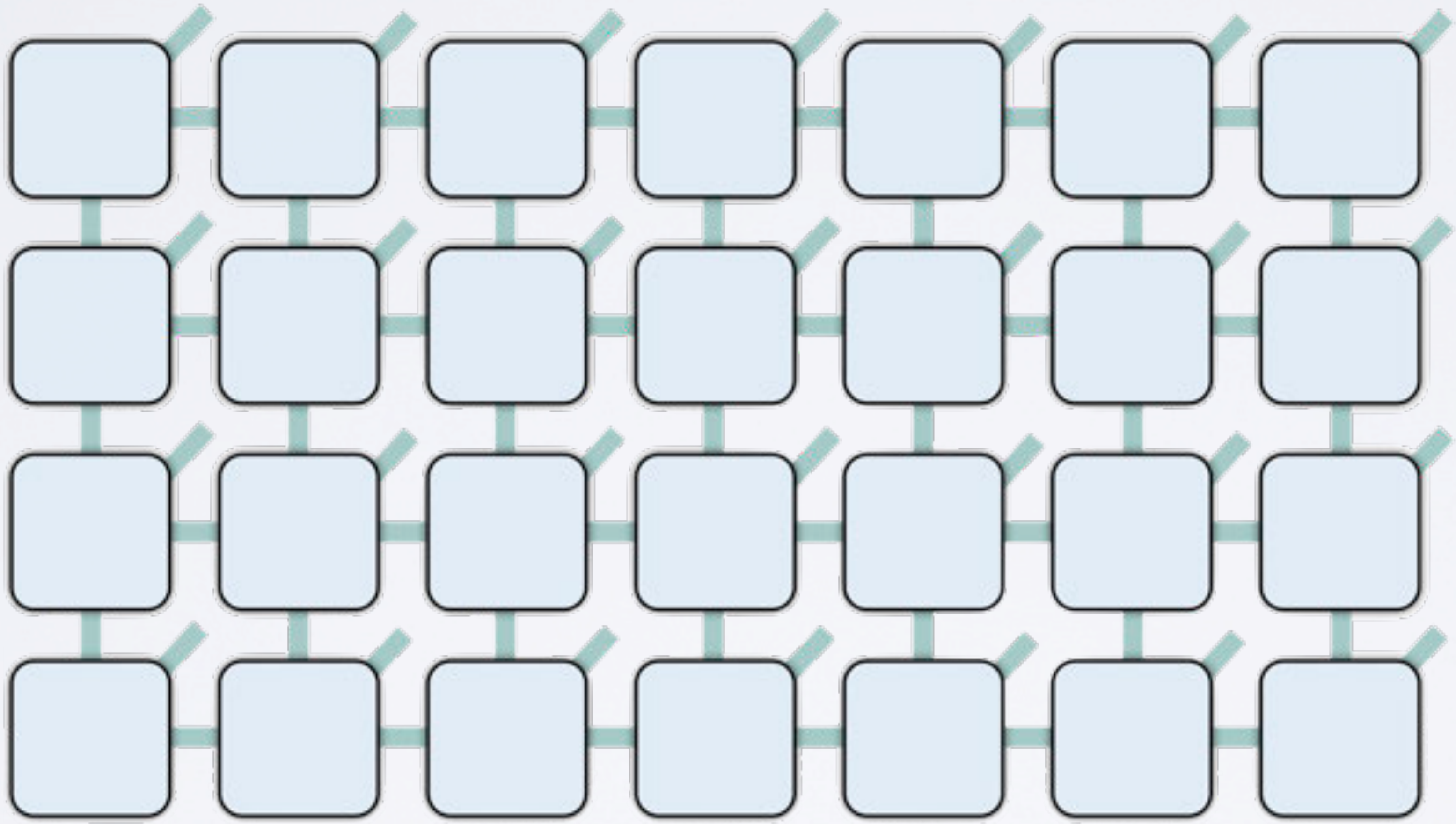


Experiment Data Tomographic knowledge

Higher-dimensional tensor network states

PEPS in higher dimensions

- For a cubic lattice $V = L^{\mathcal{D}}$ for $\mathcal{D} = 2$

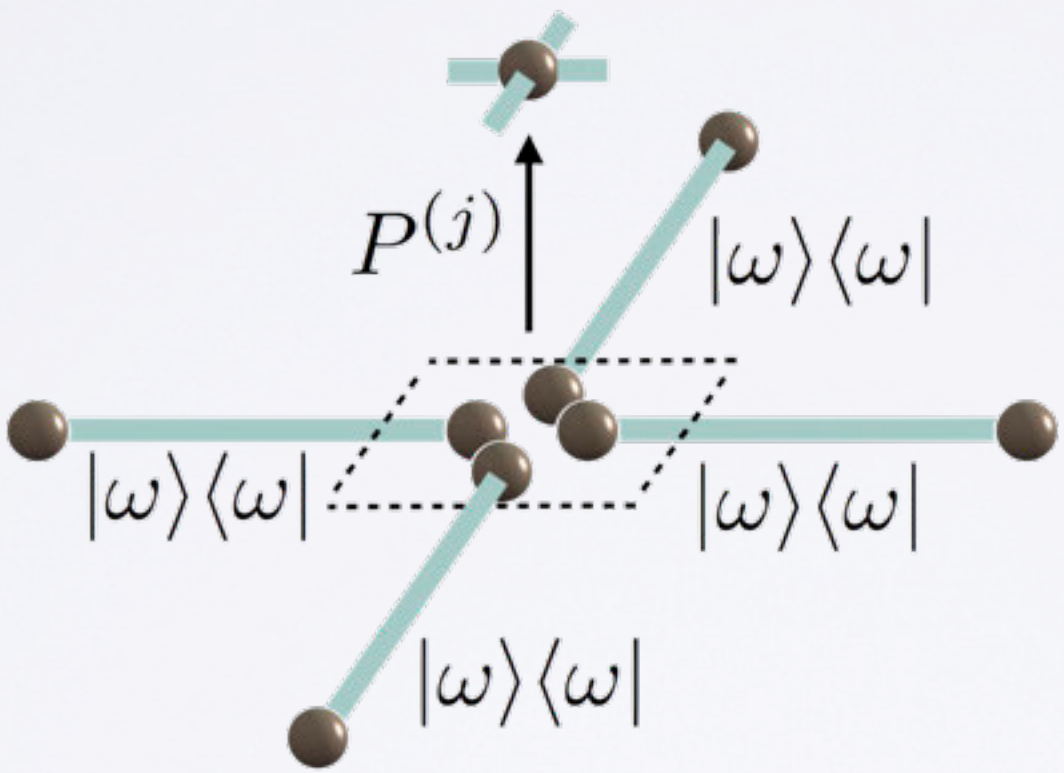


- All tensors $A^{(k)}_{\alpha,\beta,\gamma,\delta;j}$ can be taken differently per site $k \in V, j = 1, \ldots, d$ and $\alpha, \beta, \gamma, \delta = 1, \ldots, D$

PEPS in higher dimensions

- **PEPS construction**

$$P^{(k)} = \sum_{\alpha,\beta,\gamma,\delta=1}^{D} \sum_{j=1}^{d} A^{(k)}_{\alpha,\beta,\gamma,\delta;j} |j\rangle\langle\alpha,\beta,\gamma,\delta|$$

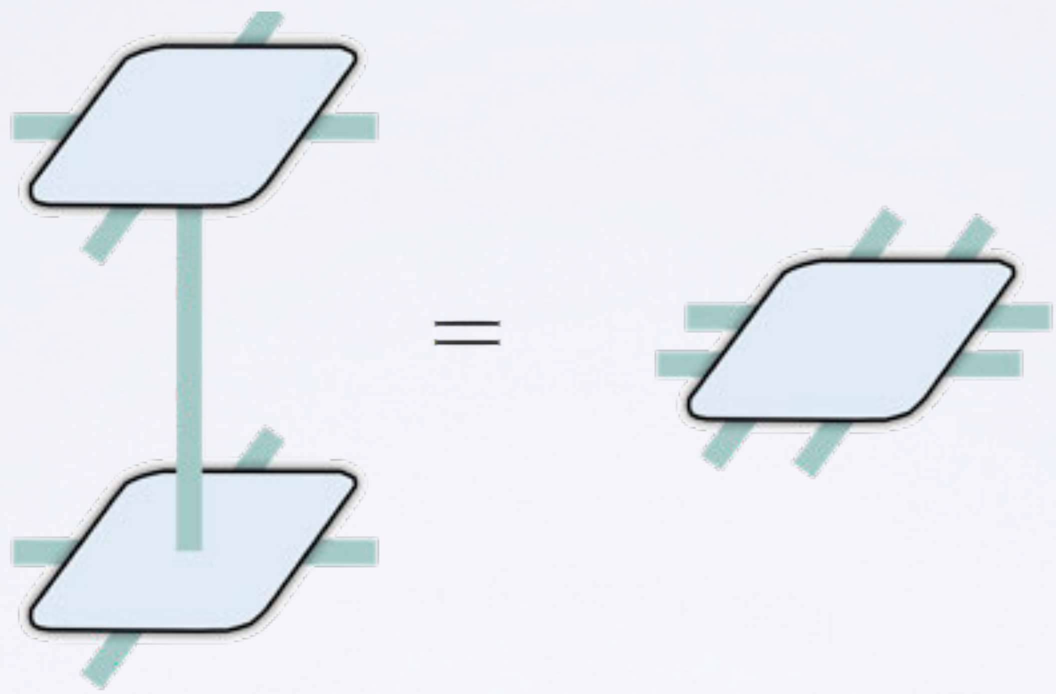


Properties of PEPS

- PEPS satisfy an **area law**: The entanglement entropy is bounded from above by $O(L\log D)$ for $\mathcal{D}=2$
- Again, if the bond dimension is large enough one can write **every state** as a PEPS
- Again, one can again have **exponentially clustering correlations**
- Interestingly, as a difference to MPS, one can construct PEPS that have **algebraically** decaying correlations in $\mathrm{dist}(A,B)$

PEPS contraction

- **Transfer operator**



- **Tricky:** Can only **approximately** contract, not **exactly!**
- Exact contraction is in #P

Exact PEPS

- **Cluster states in measurement-based computing**

- **Toric code Hamiltonian** defined on edges (!) of a cubic lattice

$$H = -J_a \sum_s A_s - J_b \sum_p B_p$$

where $\{A_s\}$ and $\{B_p\}$ are the star and plaquette operators, defined as

$$A_s = \prod_{j \in s} X^{(j)}$$

$$B_p = \prod_{j \in p} Z^{(j)}$$

More general tensor networks

- **Checklist**

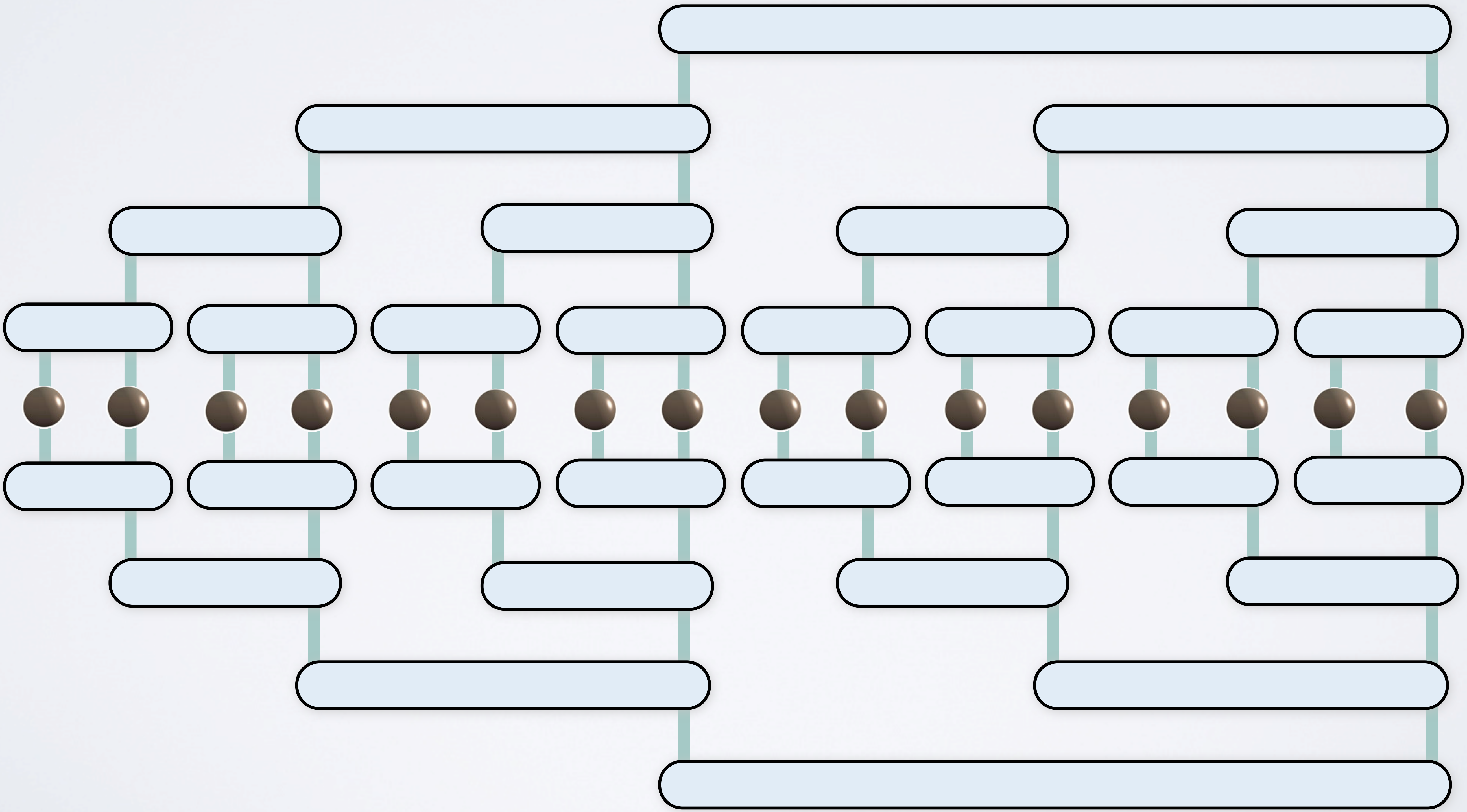
☑ the tensor network should be described by polynomially many parameters,

☑ it should be efficiently contractible, either exactly or approximately, and

☑ the corresponding class of quantum states should be able to grasp the natural entanglement or correlation structure

Trees

- Take $n = 2^T$, and think of "temporal" layers $t = 1, \ldots, T$



Trees

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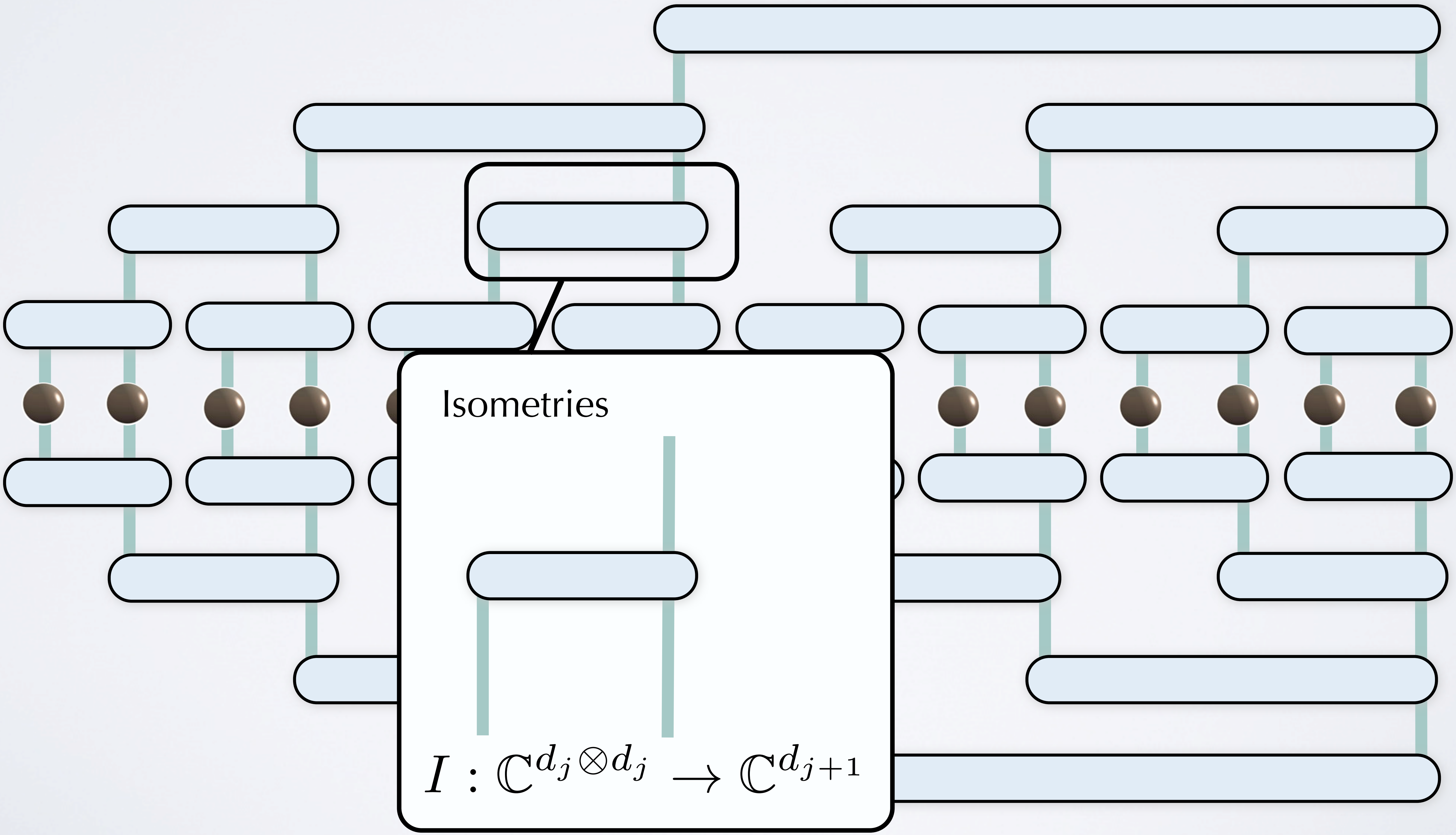

Multi-scale entanglement renormalisation

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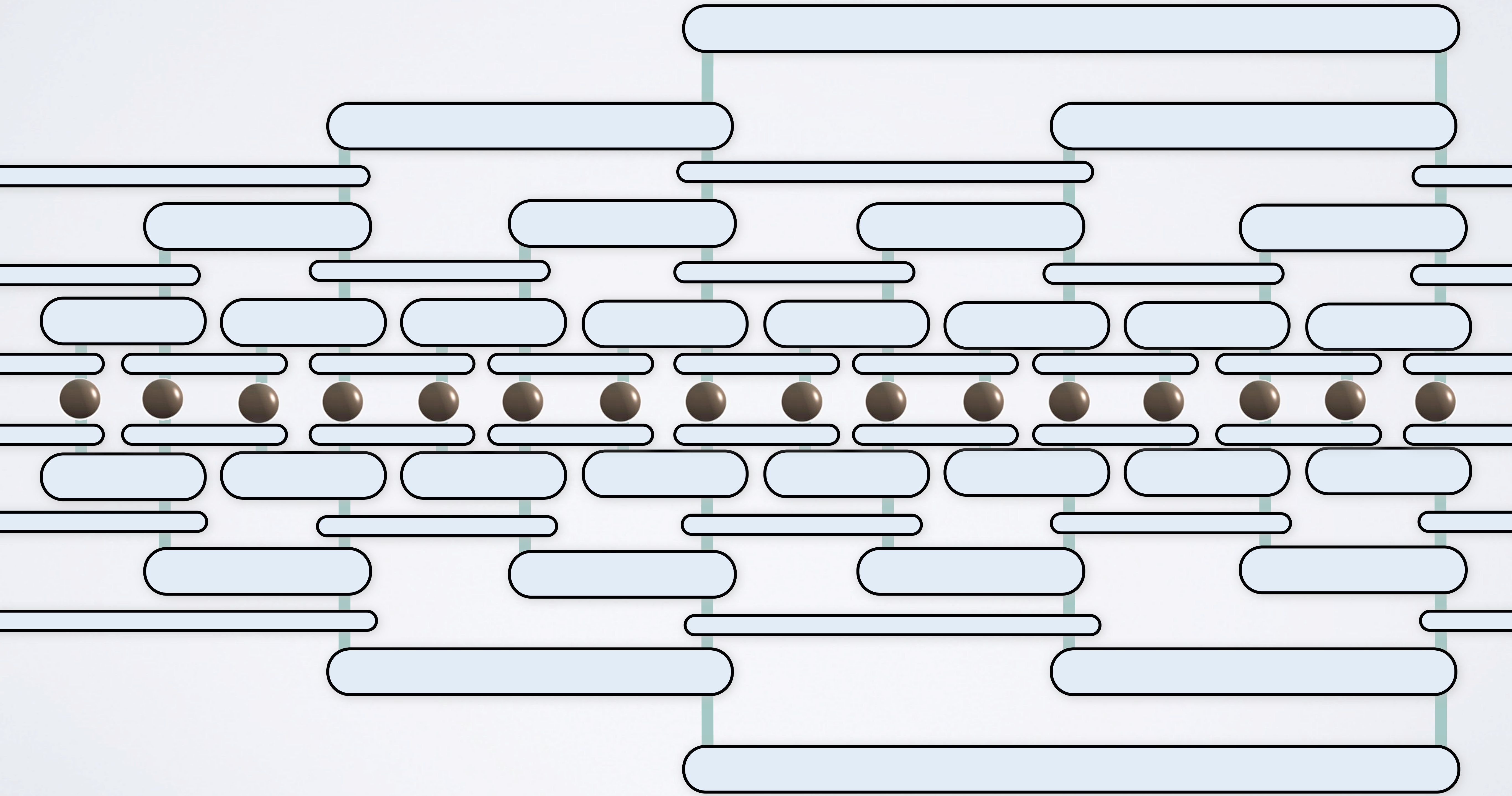

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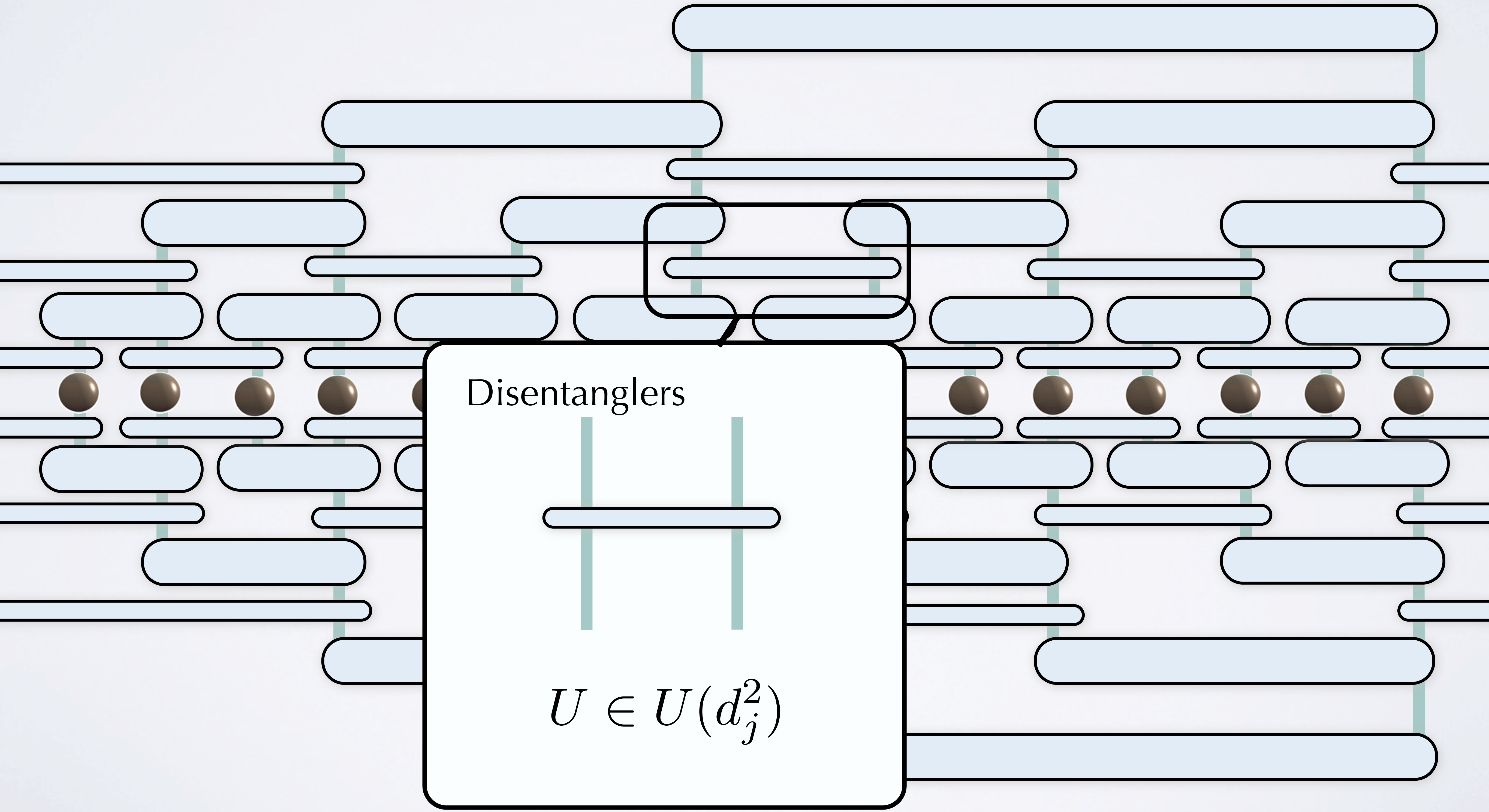
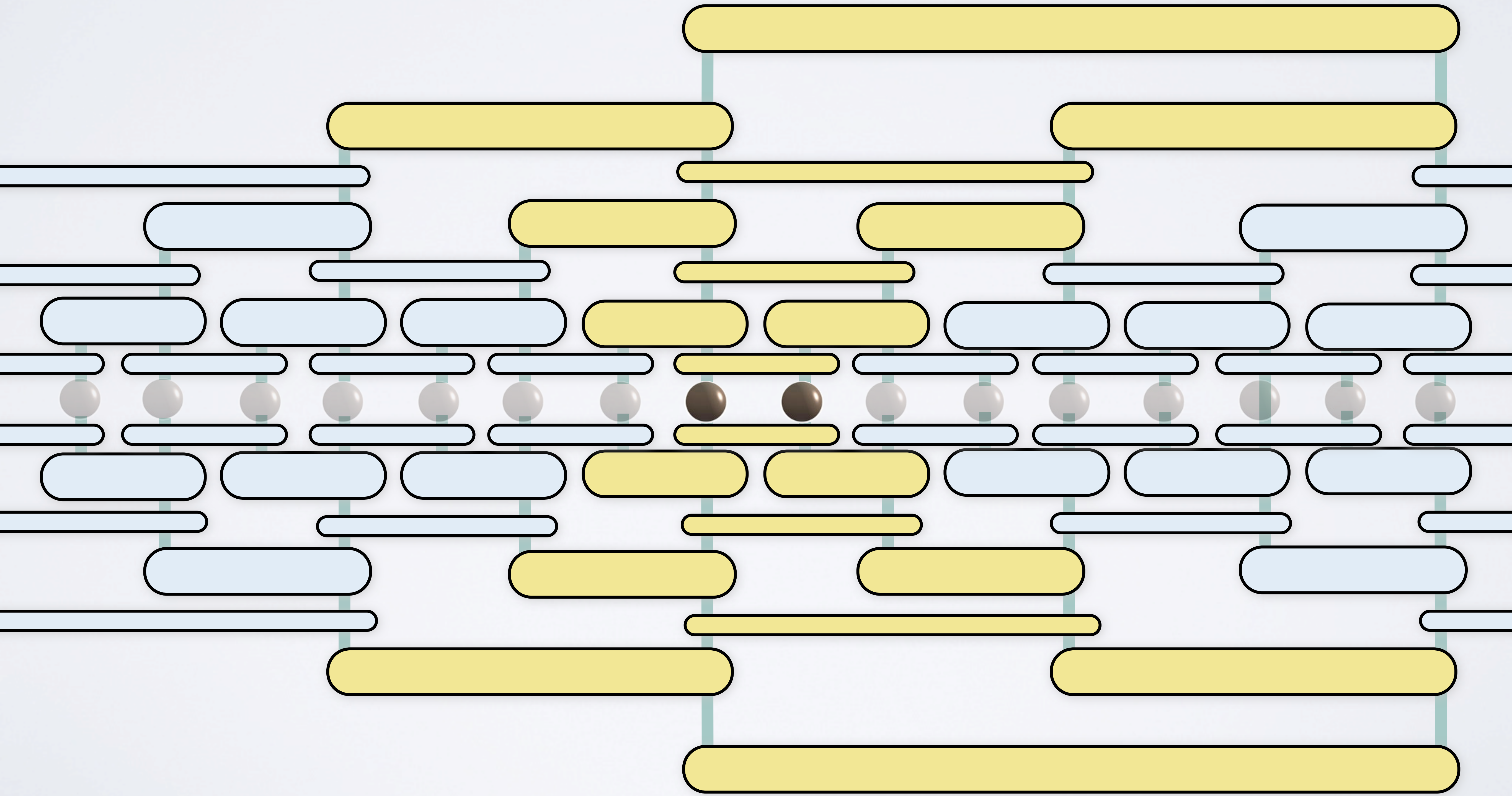


Multi-scale entanglement renormalisation

- Causal cone leads to efficient contraction



Multi-scale entanglement renormalisation

- This idea works in **any dimension**
- It also works for **fermions**
- Nice connection to **AdS-cft**
- Can be proven to be efficiently contractible PEPS

Lessons

Lessons

- **Exciting field of research!**
- Good for **numerical** and **analytical studies**
- For two dimensions, full potential is yet to be explored
- Again :)

Many natural quantum lattice models have ground states that are little, in fact very little, entangled in a precise sense. This shows that `nature is lurking in some small corner of Hilbert space', one that can be essentially efficiently parametrized. This basic yet fundamental insight allows for a plethora of new methods for the numerical simulation of quantum lattice models using tensor network states, as well as a novel toolbox to analytically study such systems

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