CENTRE FOR QUANTUM TECHNOLOGIES
NATIONAL UNIVERSITY OF SINGAPORE

AND

CLARENDON LABORATORY
UNIVERSITY OF OXFORD

THE QUANTUM THEORY OF INFORMATION AND COMPUTATION

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Tensor network simulations of strongly correlated quantum systems

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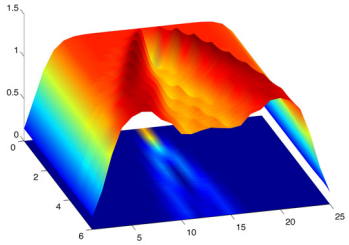
Oxford 2010 – 3rd and 8th June

Overview

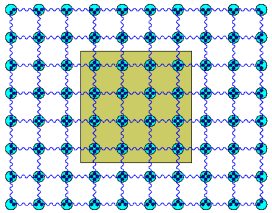
Part I – *Quantum many-body systems*

- The models and problems physicists are interested in.
- Strong correlations and quantum phase transitions.
- Difficulties in simulating many-body quantum systems.



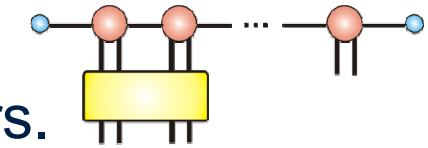
Part II – *Tensor network formalism*

- Tensors, contractions and diagrams.
- Introducing matrix product states for 1D systems.
- Approximating stationary states and time-evolution.



Part III – *Extensions and generalizations*

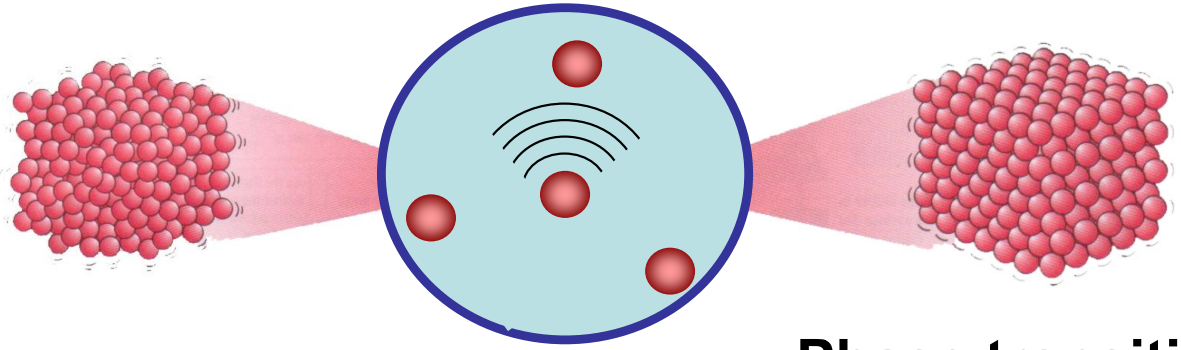
- Simulating tree and network geometries.
- Evolving with mixed states, thermal states and operators.
- Going to 2D systems and beyond.

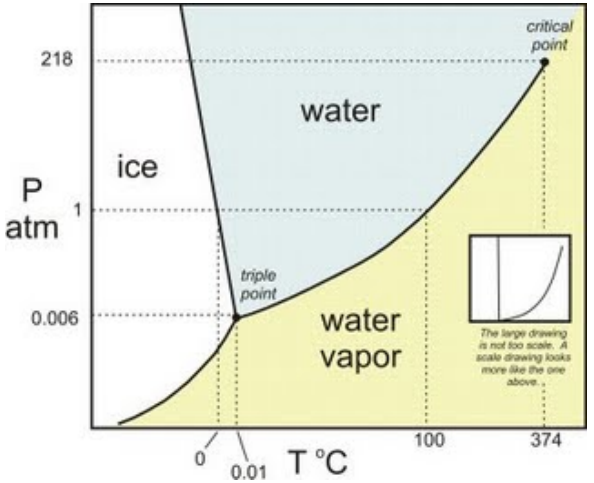


Part I – The many body problem

Consequences of strong correlations …

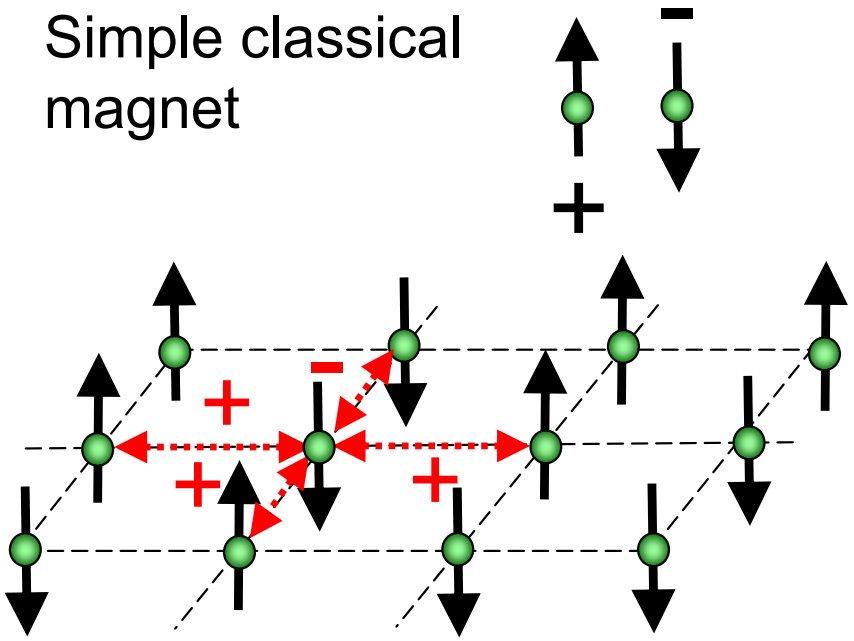
Interplay between interactions and external influences:

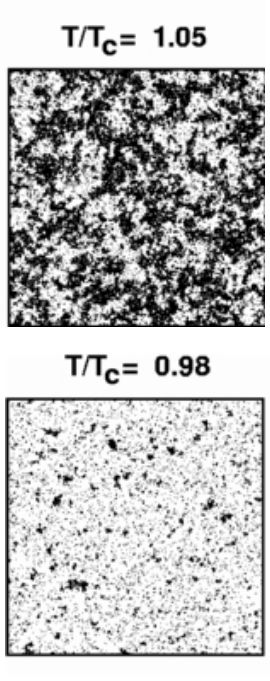


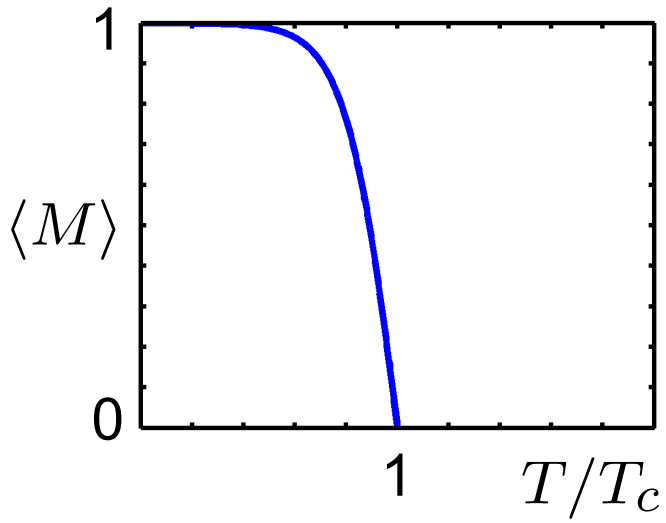


Phase transitions

Simple classical magnet







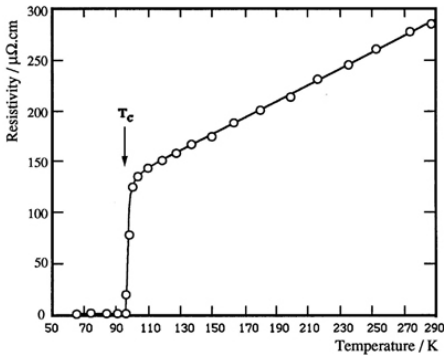
Quantum many body systems

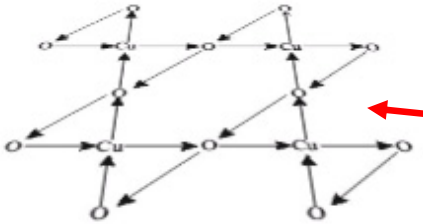
- Major interest in many-body problem focuses on lattice systems.

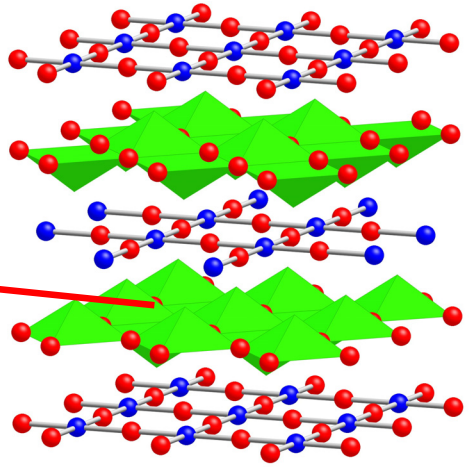
  Understanding quantum properties of electrons in materials:

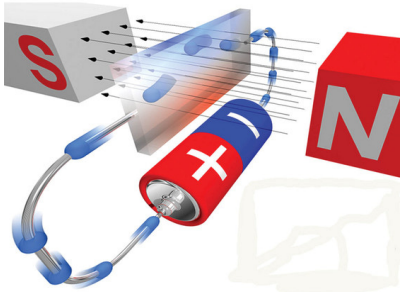
- **High-temperature superconductivity**

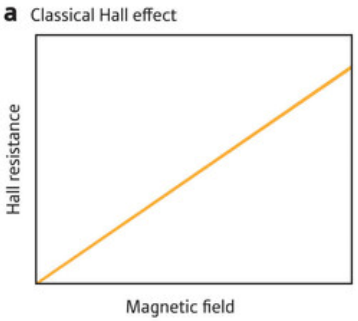
What is the physical mechanism behind it?

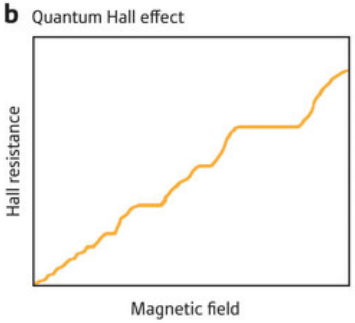










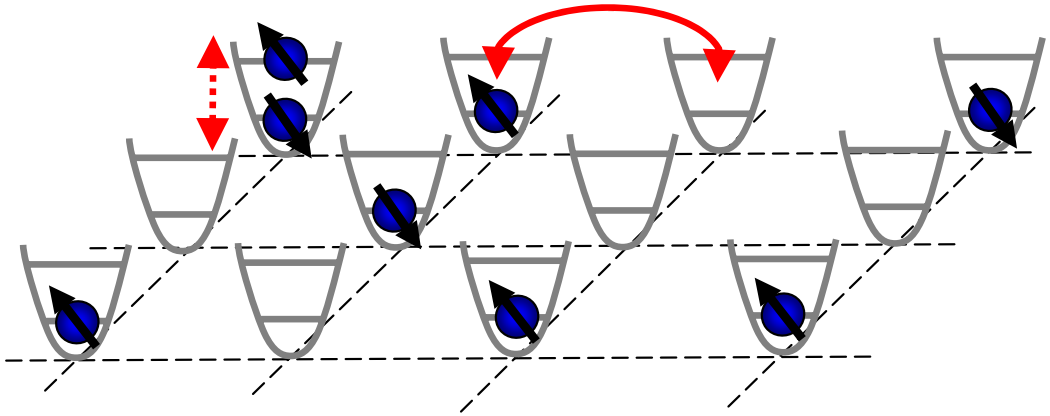


- **Quantum Hall effect**

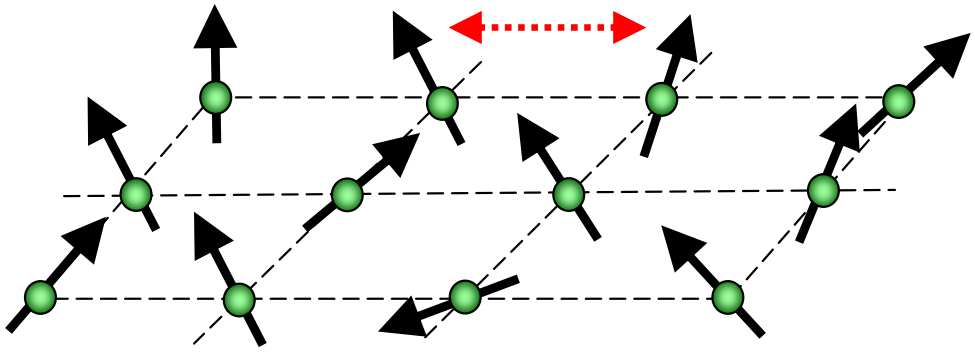
  What are the topological properties of fractional QH states?

Quantum lattice models

- Try to devise and study simpler models believed to capture the essential physics of these complex systems …



Hubbard model in 2D



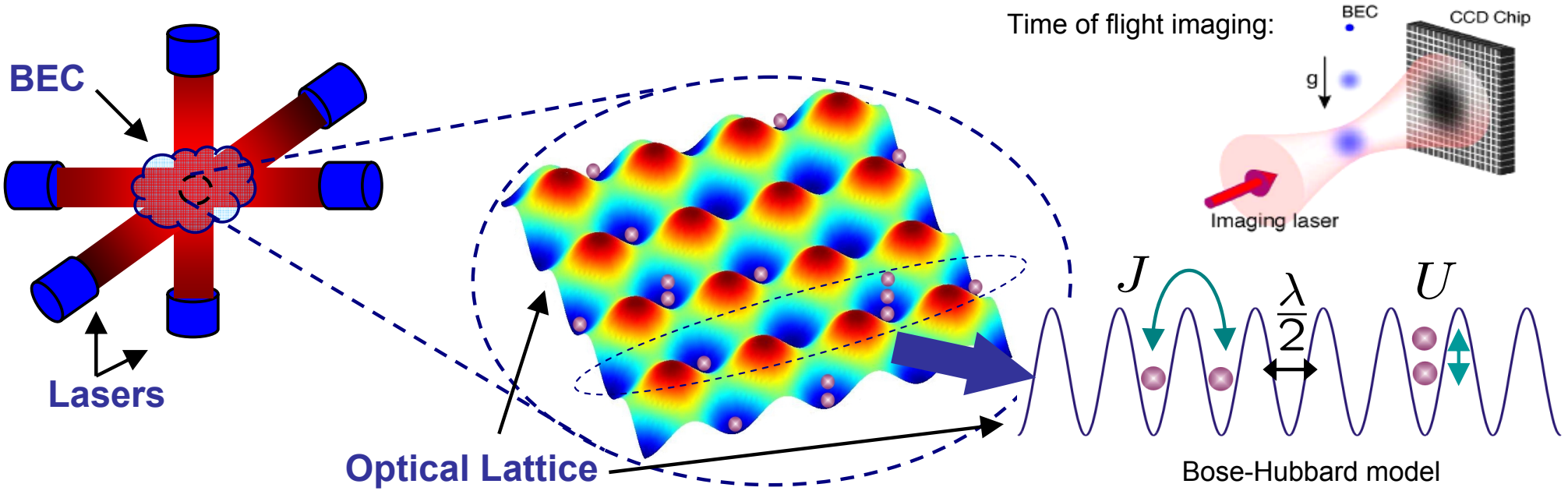
Quantum magnets $H = -\sum_{\langle jk \rangle} \sigma_j^z \sigma_k^z - B \sum_j \sigma_k^x$

- Competition between interactions – no single dominant contribution.
- Despite the simpler models much is still completely unknown.
- 1D chains

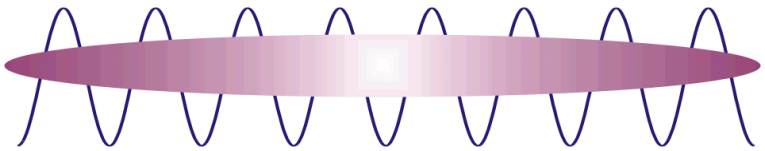
Quantum “wire”

Cold atoms in optical lattices

- Simple models now physically realizable – quantum simulators



Superfluid : $J \gg U$

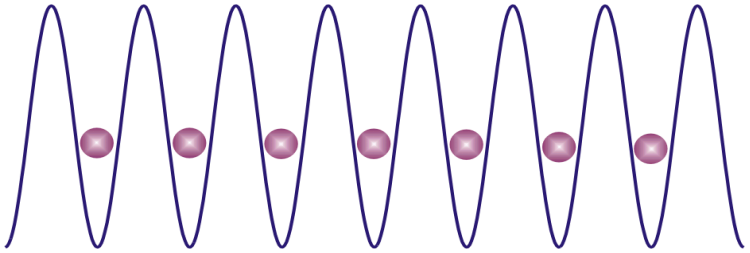


Atoms delocalised over the lattice

Laser intensity

"Quantum Phase Transition"

Mott-Insulator : $U \gg J$



Atoms pinned to a lattice site

The many body problem

- Having identified a model Hamiltonian H for our system we would now like to solve the following problems

$$H|\phi_\nu\rangle = e_\nu|\phi_\nu\rangle$$

(1) Solve the time-independent Schrodinger equation.

Hermitian matrix

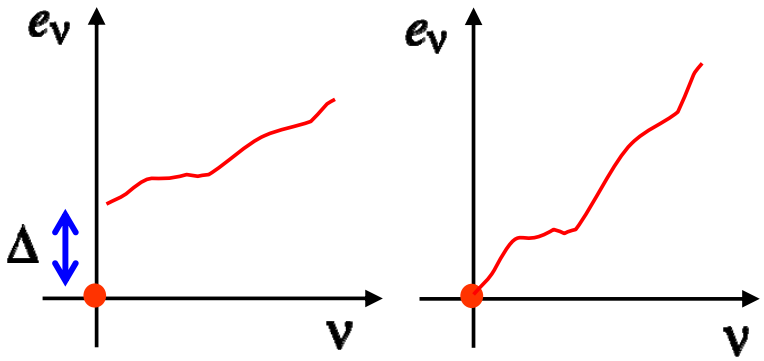
Real eigenvalue - energy

Complex vector

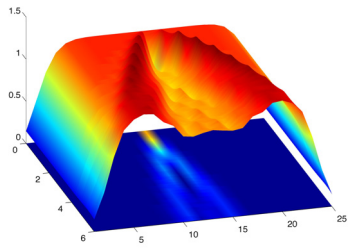
$$\begin{pmatrix} h_{00} & h_{01} & \cdots \\ h_{01}^* & h_{11} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix} = e_\nu \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix}$$

Often interested in the ground state and lowest lying excited states.

Gap vs. no gap



(2) Solve the time-dependent Schrodinger equation – simulate the real time dynamics.



$$i\frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle$$

formal solution

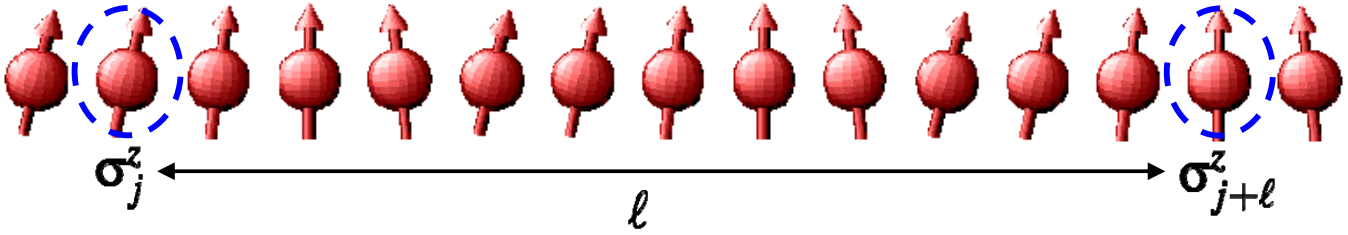
$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

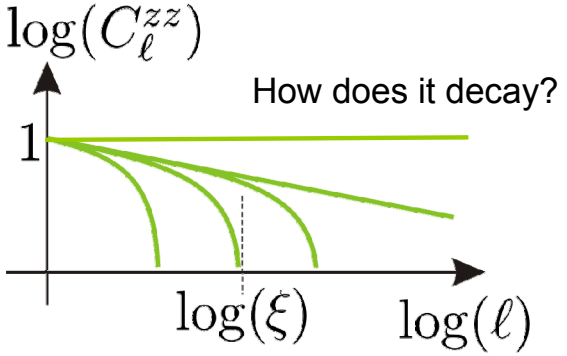
Understanding and manipulating coherent dynamics of quantum systems becoming more important.

Excitations and correlations

- Given $|\phi_0\rangle$ we want to know what correlations it contains, e.g.

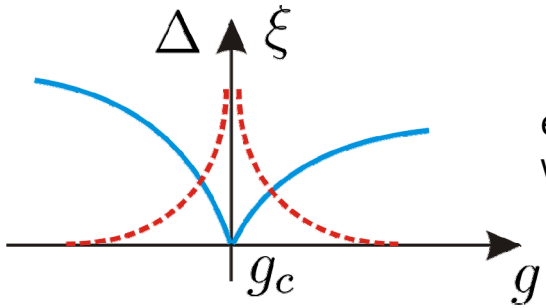
$$C^{zz}_\ell = \langle\phi_0|\sigma^z_j\sigma^z_{j+\ell}|\phi_0\rangle - \langle\phi_0|\sigma^z_j|\phi_0\rangle\langle\phi_0|\sigma^z_{j+\ell}|\phi_0\rangle$$





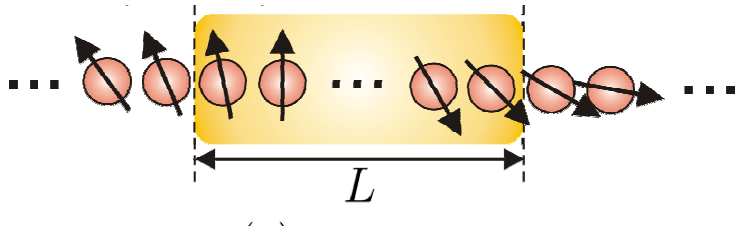
- How does the gap and correlation length depend on an external parameter, like a magnetic field?

Critical points usually coincide with a vanishing gap and a diverging correlation length – scale invariance.

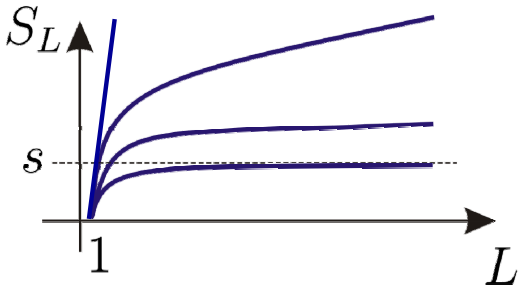


e.g. the Ising model with a transverse field

- Entanglement properties of $|\phi_0\rangle$



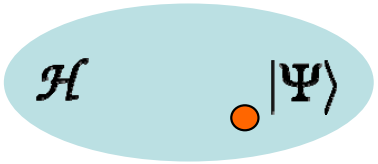
How entangled is a block of **L** spins to the rest of the system?



Does it saturate or diverge with **L**?

The “curse of dimensionality”

Classically simulating many-body quantum systems *seems* to be hard :

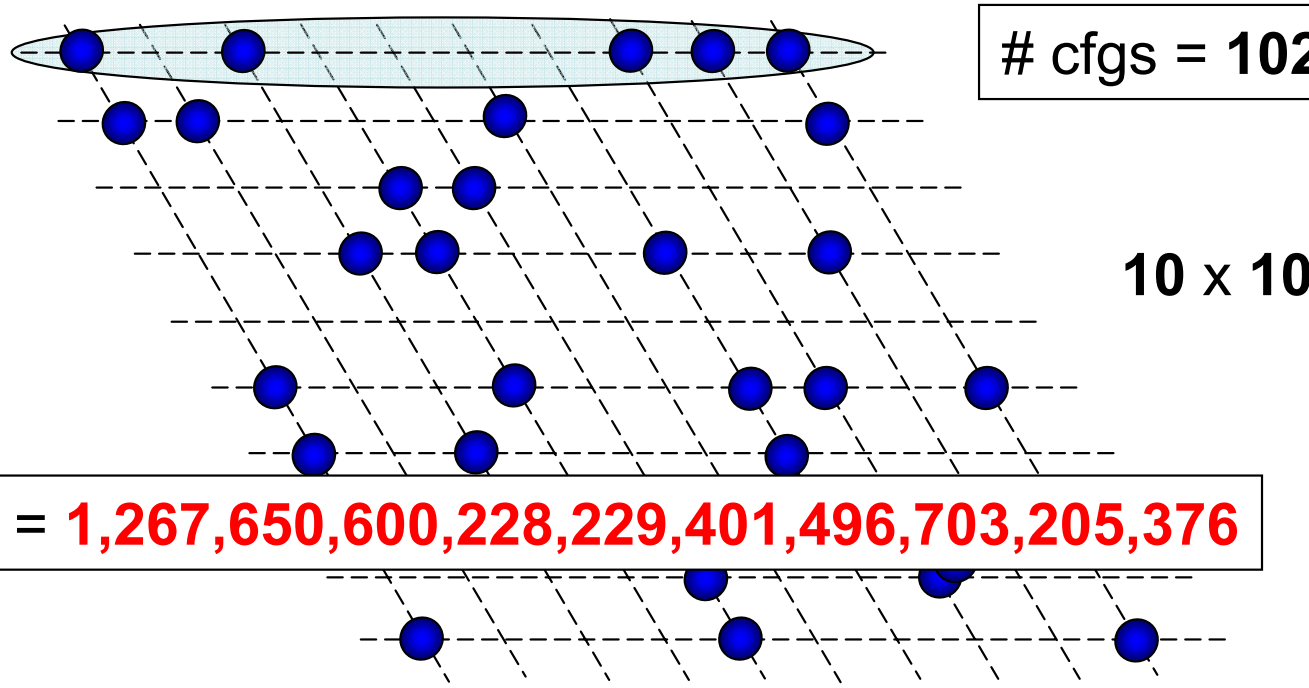


Description
Computational effort

} Scale ***exponentially*** with size

Could solve **1** x **10**

But can we solve a more useful ***“small”*** system?



cfgs = **1024**

10 x **10**

NO !

cfgs = **1,267,650,600,228,229,401,496,703,205,376**

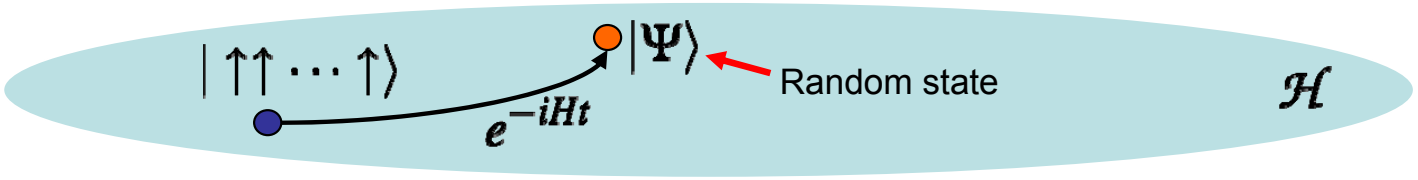
Direct approach extremely limited. New methods are needed …

Physical states – interactions

- The kinds of models which appear in nature have special structure and it is not clear a priori that the full Hilbert space is accessible. Specifically interactions are:
  - local, i.e. decay sufficiently quickly,
  - involve only a few bodies, typically just two.

$$H = -\sum_{\langle jk \rangle} \sigma_j^z \sigma_k^z - B \sum_j \sigma_k^x$$

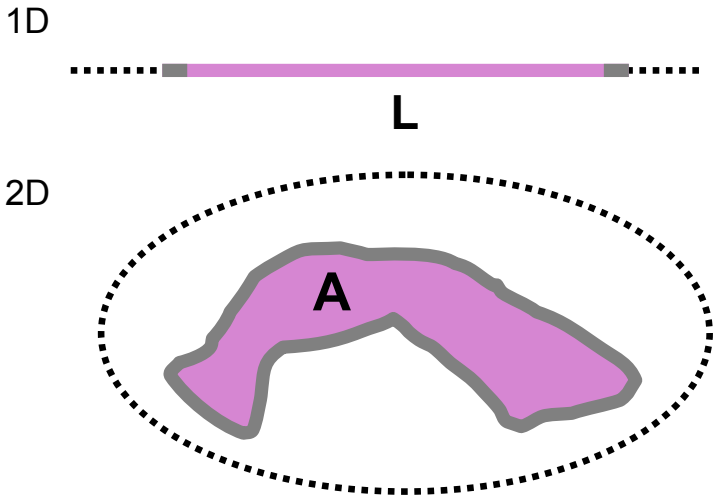
These properties put serious constraints on the states which are accessible and in fact shows that almost all states in are non-physical



Lower bound on the time required for a local Hamiltonian to evolve $|\uparrow\uparrow\cdots\uparrow\rangle$ to $|\Psi\rangle$ is found to be exponential in **N**. For **N** = 20 this is already longer than the age of the universe.

Physical states – “area laws”

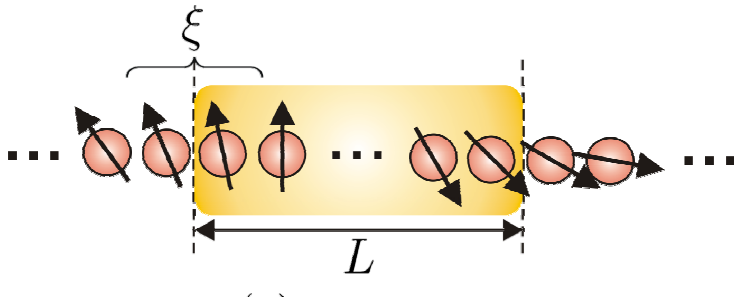
- Conclusion: the fraction of states in this exponentially large Hilbert space that are physical is in fact exponentially small.

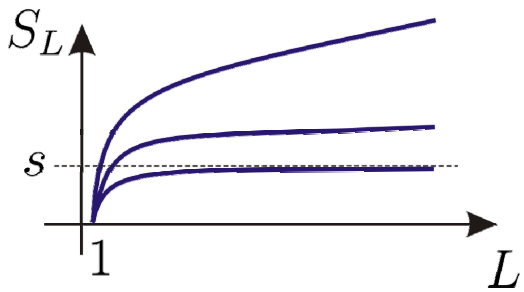


- Ground state and low-lying excitations have very little entanglement …

“Area laws”

- Entanglement is concentrated around the boundary:





Results: $S_L \approx A \ln(\xi)$ **(off-critical)** $S_L \approx B \ln(L)$ **(critical)**

Summary for Part I

- Interested in quantum lattice problems – numerous applications.
- Simulation of quantum many-body system appears to be exponentially difficult …
- but, nature prefers local few-body interactions,
- so physical states occupy only a small part of the Hilbert space,
- and such systems display an “area law” for entanglement.

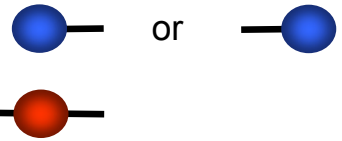
Take home message

- To simulate quantum many-body system we need to parameterize physical states in such a way as to exploit these properties.

Part II – Tensor network formalism

Tensors, contractions and diagrams

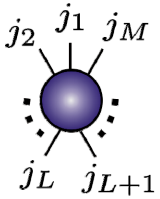
- For our purposes *"tensor"* is a fancy name for a multi-dimensional array of complex numbers.
  - A rank 1 tensor is simply a vector:
  - A rank 2 tensor is simply a matrix:



- Two basic operations – **reshape** and **contraction**:

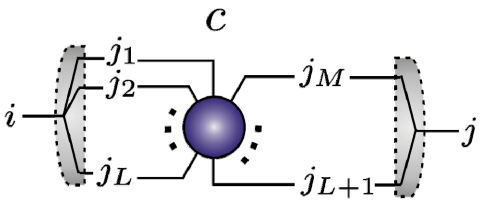
(a)

$$c_{j_1 j_2 \cdots j_L j_{L+1} \cdots j_M} =$$



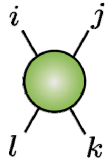
(b)

$$C_{ij} =$$

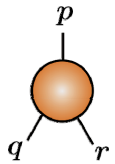


(c)

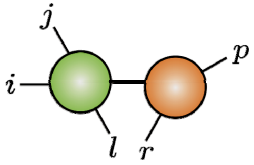
$$A_{ijkl} =$$



$$B_{pqr} =$$



$$C_{ijlpr} = \sum_\alpha A_{ij\alpha l} B_{p\alpha r} =$$

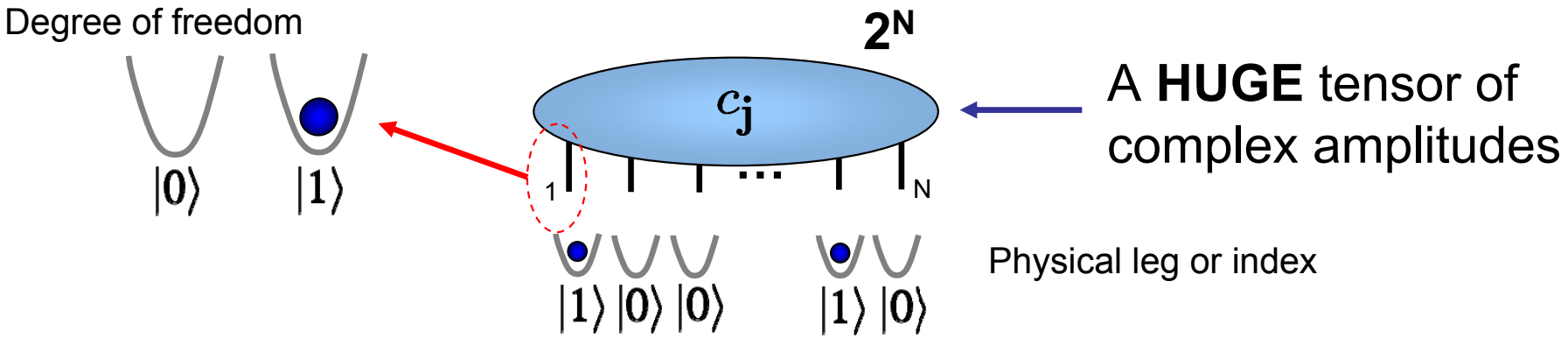


- The essential mathematical content of tensor methods actually boils down to using standard methods from linear algebra of matrices.

Aim of tensor methods in a nutshell

- An arbitrary quantum state for an **N** site system can be expanded as

$$|\psi\rangle = \sum_{\mathbf{j}} c_{\mathbf{j}} |\mathbf{j}\rangle \quad \text{in terms of cfgs basis} \quad |\mathbf{j}\rangle = |j_1\rangle |j_2\rangle \ldots |j_N\rangle$$



Approximate by *factorizing* this tensor into a network of smaller tensors.

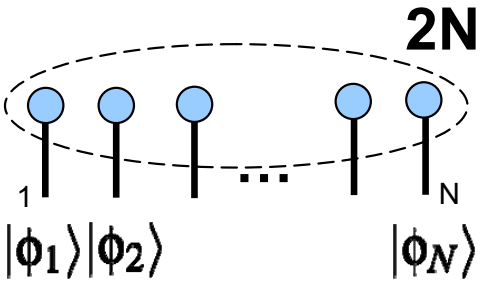
Primary aim = encode with a polynomial number of parameters.

But we also need to be able to …

(1) find and evolve this approximation efficiently.
(2) efficiently calculate physical quantities from the representation.

Aim of tensor methods in a nutshell

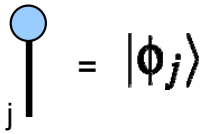
- The simplest approach possible is to describe each site (physical leg) by its own **independent** tensor



Equivalent to a product state approximation.

- Contains no entanglement.
- Cannot describe correlations $C^{zz}_{\ell} = 0$

Rank 1 tensor gives an state for each site

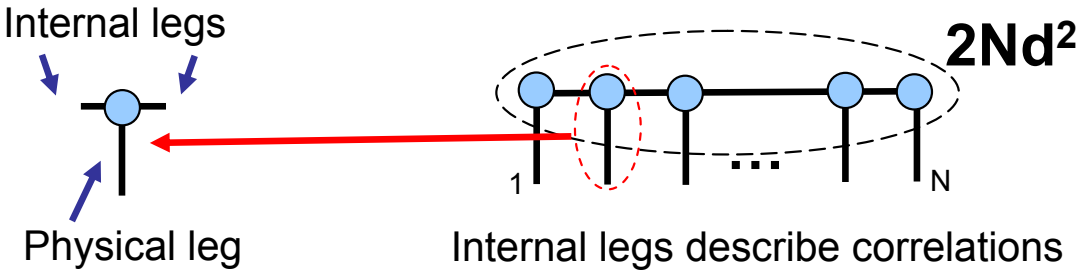


This approach is a very common technique called **mean-field theory**.

[See problem sheet for application of this in describing the SF-MI transition in the BHM]

How might we generalize this trivial tensor network?

One possible way to proceed is to elevate the site tensors to rank 3 by adding some *internal* legs of given fixed dimension **d**.

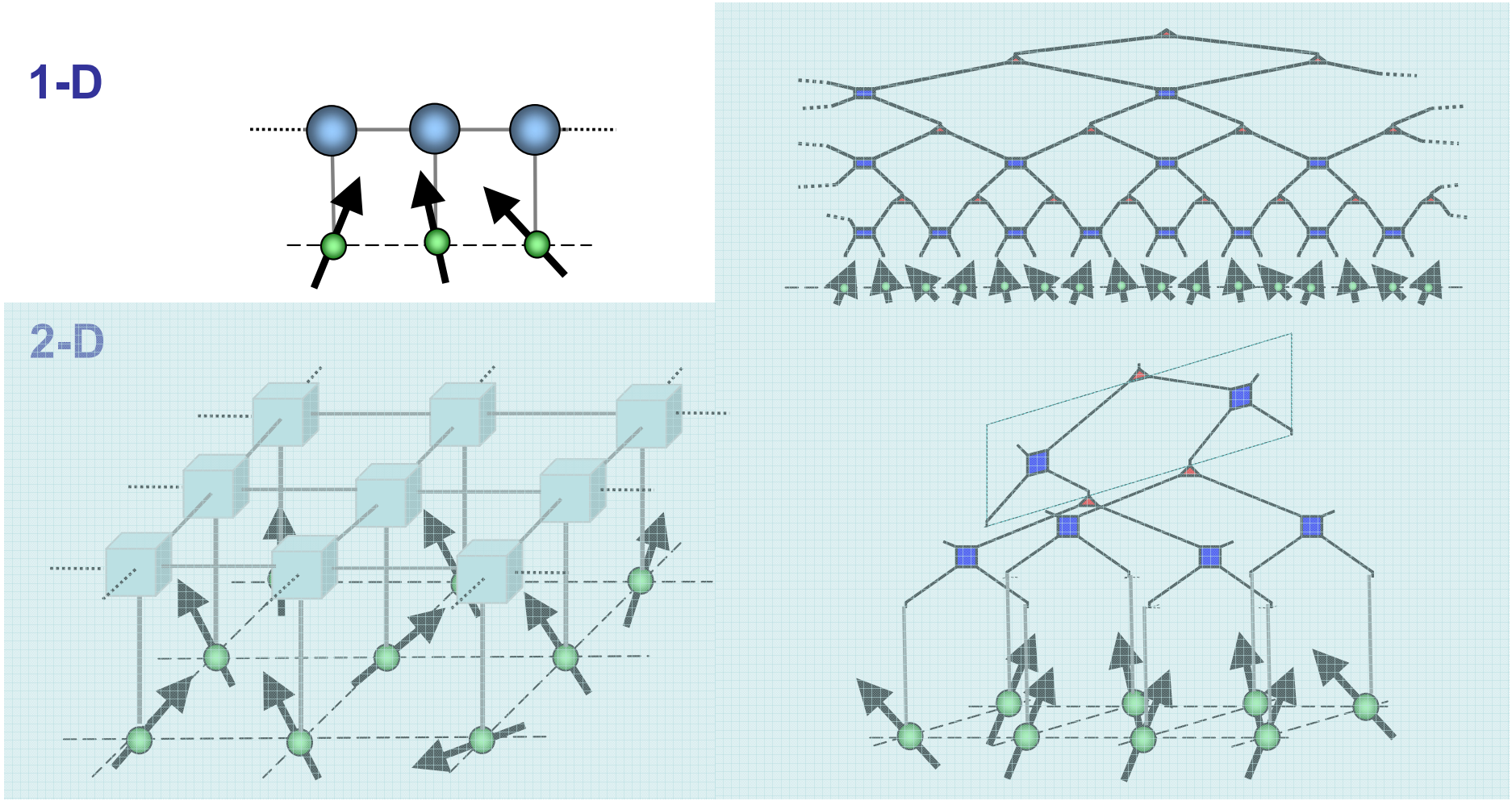


Contract all internal legs to form a comb network.

Manifestly 1D network geometry.

A zoo of tensor networks

Can physically motivate a variety of tensor networks structures:

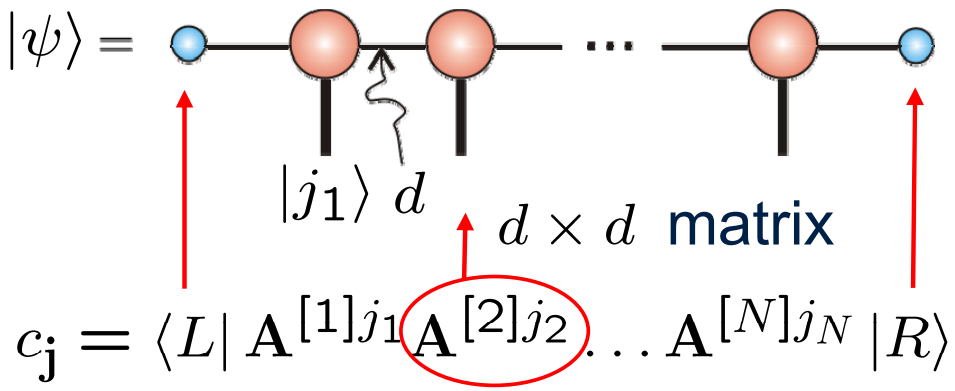


All aim to provide accurate near-lossless compression of physical states.

Matrix product states

- A state $|\psi\rangle$ described exactly by "comb"-like tensor network is called a a matrix product state since it is equivalent to an expansion:

$$|\psi\rangle = \sum_{\mathbf{j}} c_{\mathbf{j}} |\mathbf{j}\rangle = \sum_{\mathbf{j}} \langle L | \mathbf{A}^{[1]j_1} \mathbf{A}^{[2]j_2} \dots \mathbf{A}^{[N]j_N} | R \rangle |\mathbf{j}\rangle$$



Note: can absorb the vectors into the boundary tensors making them rank 2 instead.

- Parameterizes the amplitudes as sequences of **matrix products** which collapses to a scalar via the boundary vectors.

Product states (translationally invariant) $d = 1$

$$|\psi\rangle = |\phi\rangle \otimes |\phi\rangle \otimes \cdots$$

A **1 x 1** "matrix" for each local state

$$\mathbf{A}^{\uparrow} = \alpha \quad \mathbf{A}^{\downarrow} = \beta$$

$$|\phi\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$$

Some less trivial examples …

Some familiar states built from identical 2×2 matrices for all sites:

GHZ state (antiferromagnetic) $|\psi\rangle = |\uparrow\downarrow\cdots\downarrow\rangle + |\downarrow\uparrow\cdots\uparrow\rangle$

Use matrices: $\mathbf{A}^{\uparrow} = \boldsymbol{\sigma}^{+}$ $\mathbf{A}^{\downarrow} = \boldsymbol{\sigma}^{-}$ with $\langle L| = (1 \quad 1)$ $|R\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Since $(\mathbf{A}^{\uparrow})^2 = (\mathbf{A}^{\downarrow})^2 = 0$ there are only **2** non-zero amplitudes:

$$(1 \quad 1)\Big(\underbrace{\sigma^{-}\,\sigma^{+}\,\sigma^{-}\ldots\;\sigma^{-}\sigma^{+}}_{|\downarrow\uparrow\cdots\uparrow\rangle}\Big)\begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad (1 \quad 1)\Big(\underbrace{\sigma^{+}\sigma^{-}\sigma^{+}\ldots\;\sigma^{+}\sigma^{-}}_{|\uparrow\downarrow\cdots\downarrow\rangle}\Big)\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

GHZ state (ferromagnetic) $|\psi\rangle = |\uparrow\uparrow\cdots\uparrow\rangle + |\downarrow\downarrow\cdots\downarrow\rangle$

Use matrices: $\mathbf{A}^{\uparrow} = \frac{1}{2}(\mathbb{1} + \boldsymbol{\sigma}^{z})$ $\mathbf{A}^{\downarrow} = \frac{1}{2}(\mathbb{1} - \boldsymbol{\sigma}^{z})$ with $\langle L| = (1 \quad 1)$ $|R\rangle = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Again only **2** non-zero amplitudes since $\mathbf{A}^{\uparrow}\mathbf{A}^{\downarrow} = \mathbf{A}^{\downarrow}\mathbf{A}^{\uparrow} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$

Another way to expand an MPS

W state $|\psi\rangle = |\downarrow\uparrow\uparrow\cdots\uparrow\rangle + |\uparrow\downarrow\uparrow\cdots\uparrow\rangle + |\uparrow\uparrow\downarrow\cdots\uparrow\rangle + \cdots + |\uparrow\uparrow\uparrow\cdots\downarrow\rangle$

Use matrices: $\mathbf{A}^{\uparrow} = \mathbb{1}$ $\mathbf{A}^{\downarrow} = \boldsymbol{\sigma}^{-}$ with $\langle L| = (0 \quad 1)$ $|R\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

Only the **N** amplitudes associated with the translated spin-flip are non-zero since:

$\langle L|R\rangle = 0$ No flips

$\langle L|\boldsymbol{\sigma}^{-}|R\rangle = 1$ One flip

$(\mathbf{A}^{\downarrow})^2 = 0$ Multiple flips

Another helpful way of viewing this type of expansion is to absorb the physical leg inside of the **A** matrix making its elements vectors:

e.g. for the **W state** $\mathbf{A} = \begin{pmatrix} |\uparrow\rangle & 0 \\ |\downarrow\rangle & |\uparrow\rangle \end{pmatrix}$ with $|\psi\rangle = \langle L|\mathbf{A}\mathbf{A}\cdots\mathbf{A}|R\rangle$

Physical states of a lattice site

2 x 2 matrix of **N** site state vectors

Multiplication of these matrices induces tensor products of the vectors:

$$\mathbf{A}\times\mathbf{A} = \begin{pmatrix} |\uparrow\rangle\otimes|\uparrow\rangle & 0 \\ |\downarrow\rangle\otimes|\uparrow\rangle + |\uparrow\rangle\otimes|\downarrow\rangle & |\uparrow\rangle\otimes|\uparrow\rangle \end{pmatrix}$$

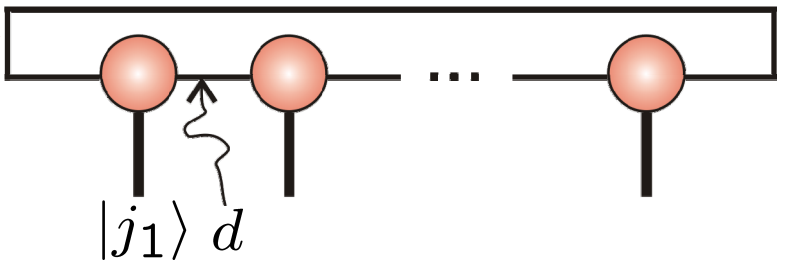
Boundary vectors select the bottom left state.

Translational invariance and PBC

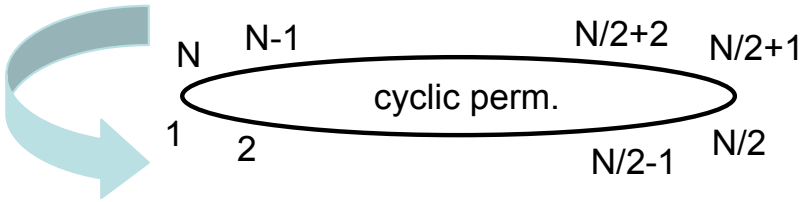
- We could have formulated our comb-like tensor network slightly differently by joining the two boundary legs together as:

$$|\psi\rangle = \sum_{\mathbf{j}} \mathrm{tr}\left(\mathbf{A}^{[1]j_1}\mathbf{A}^{[2]j_2}\ldots\mathbf{A}^{[N]j_N}\right)|\mathbf{j}\rangle$$

Trace collapses matrix product to a scalar



Results in an MPS which can share the translational symmetries of the state it describes - periodic boundary conditions (PBC).



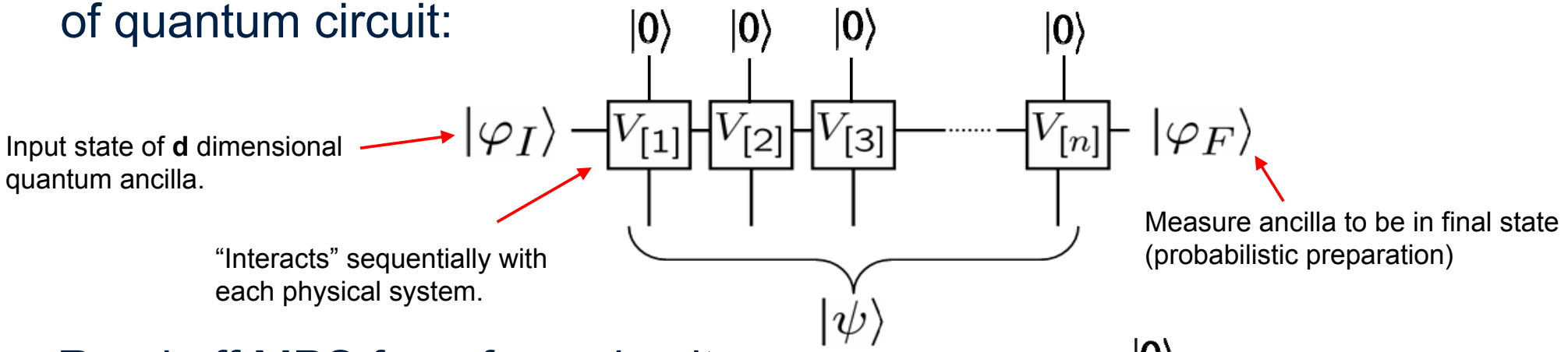
Given identical **A** matrices for all sites then the state is manifestly translationally invariant.

This formulation is often convenient theoretically (can define states with definite momentum) but comes with complications numerically.

Lets examine some physical interpretations of an MPS …

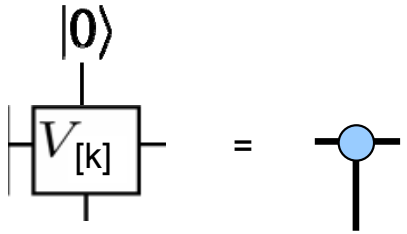
Sequential generation of an MPS

- An OBC MPS can be seen as the conditional output of a special type of quantum circuit:



- Read off MPS form from circuit:

$$V_{[k]} = \sum_{j_k,\alpha,\beta} A^{[k]j_k}_{\alpha,\beta} |\beta, j_k\rangle\langle\alpha, 0|$$

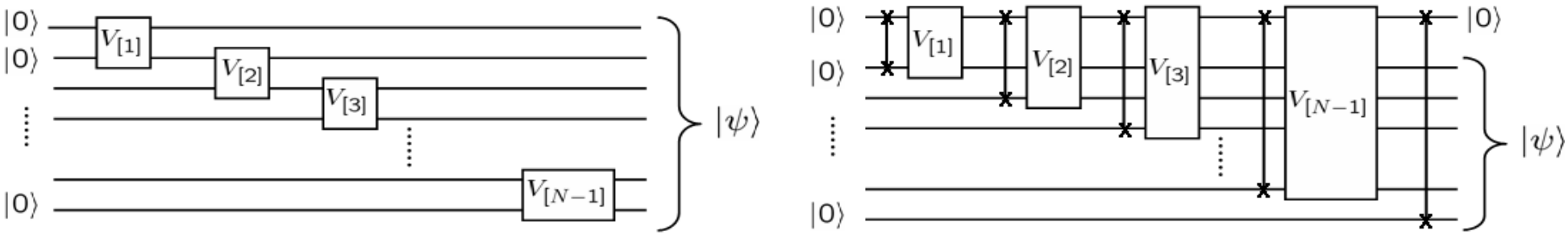


- Can enforce w.l.o.g. unitary interactions **V** and decoupling of the ancilla at the end, i.e. no measurement so deterministic preparation.

- The ancilla correlates each site with the next and its ability to do so will clearly depend heavily on its dimension **d** – more on this shortly.

Sequential generation cont …

- Consider the class of all states generated by a staircase sequence of arbitrary nearest-neighbour unitary gates:

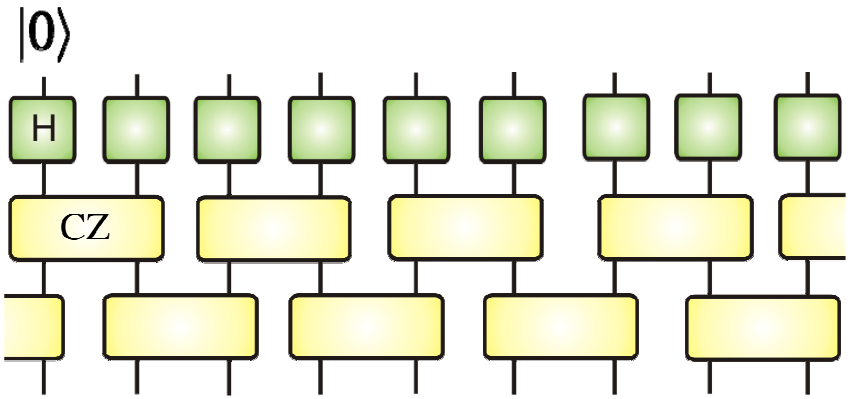


- Such states are in fact **d** = 2 MPS since the circuit is equivalent to a sequential preparation with a qubit ancilla.

Another example – **1D cluster state**

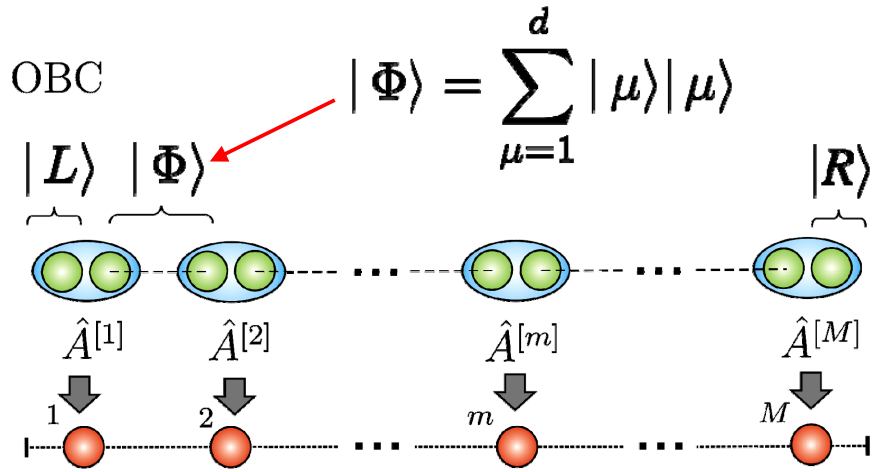
Can rearrange circuit as a staircase thus it has **d** = 2. Read-off matrices.

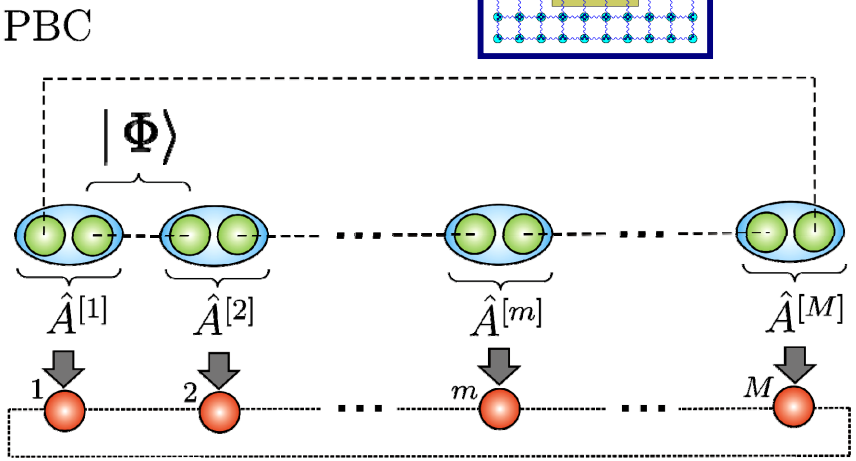
Exercise for the audience …

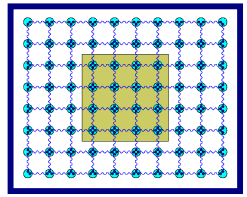


MPS from Projected Entangled Pairs

- Can view an MPS as being generated from maximally entangled qudit ancillae shared between neighbouring sites with all the ancillae on one site being "projecting" down to a physical site:







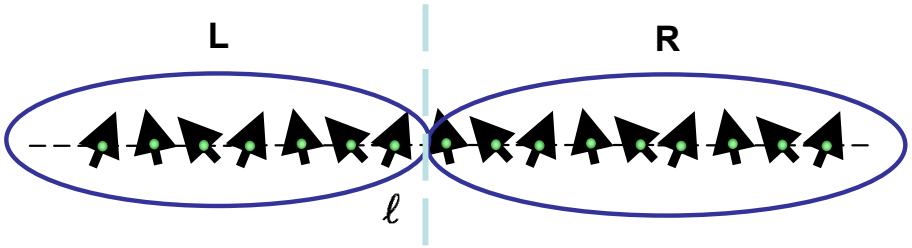
- Matrices define arbitrary linear maps $\hat{A}^{[\ell]} = \sum_{j}^{d} \sum_{\mu=1}^{d} \sum_{\nu=1}^{d} A_{\mu\nu}^{[\ell]j} |j\rangle\langle\mu|\langle\nu|$

- Shows that MPS obey an area law by construction. The entanglement of any block limited by the ancillae dimension d

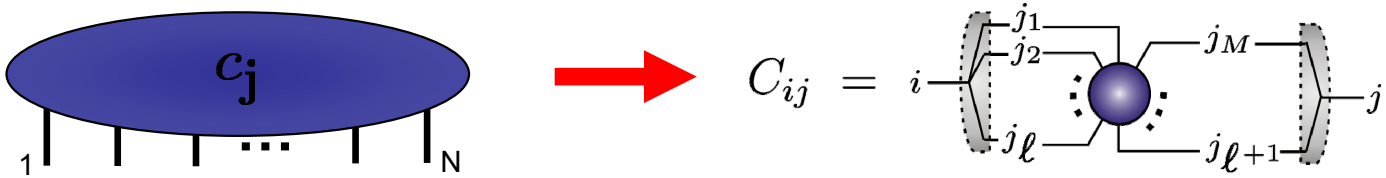
Schmidt decomposition

- We need to introduce an important tool from quantum information theory – the Schmidt decomposition:

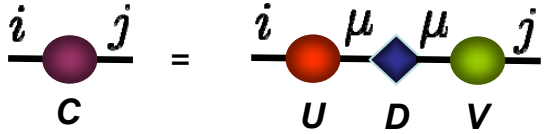
Suppose we split the system into two pieces after site ℓ :



Reshape tensor of amplitudes as a conventional matrix:



Now SVD this matrix



$$|\psi\rangle = \sum_{\mu=1}^{r} \lambda_\mu^{[\ell]} |\mathrm{L}_\mu^{[\ell]}\rangle |\mathrm{R}_\mu^{[\ell]}\rangle$$

Normalization implies $\sum_{\mu=1}^{r} (\lambda_\mu^{[\ell]})^2 = 1$ while $r = \min\left(2^\ell, 2^{N-\ell}\right)$ for qubits.

The corresponding entropy $S_{LR} = -\sum_{\mu=1}^{r} (\lambda_\mu^{[\ell]})^2 \log\left[(\lambda_\mu^{[\ell]})^2\right]$ then quantifies the entanglement.

Determining an exact OBC MPS

- Given any state we can find an exact MPS representation of it with OBC by repeatedly using the Schmidt decomposition:

$$|\mathrm{L}^{[1]}_{\mu_1}\rangle = \sum_{i_1} A^{[1]i_1}_{\mu_1} |i_1\rangle$$

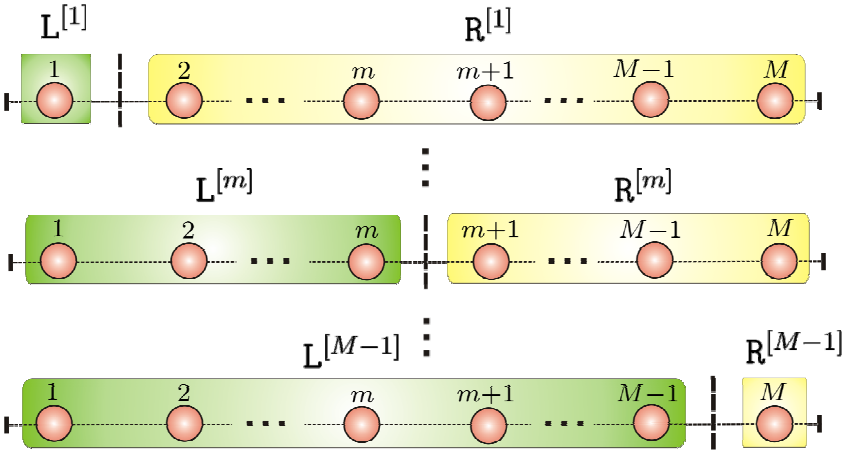
$$|\mathrm{L}^{[2]}_{\mu_2}\rangle = \sum_{i_2} \sum_{\mu_1=1}^{r_1} A^{[2]i_2}_{\mu_1\mu_2} |\mathrm{L}^{[1]}_{\mu_1}\rangle |i_2\rangle$$

$$\vdots$$

$$|\mathrm{L}^{[\ell]}_{\mu_\ell}\rangle = \sum_{i_\ell} \sum_{\mu_{\ell-1}=1}^{r_{\ell-1}} A^{[\ell]i_\ell}_{\mu_{\ell-1}\mu_\ell} |\mathrm{L}^{[\ell-1]}_{\mu_{\ell-1}}\rangle |i_\ell\rangle$$

$$|\psi\rangle = |\mathrm{L}^{[N]}_{\mu_N=1}\rangle = \sum_{i_N} A^{[N]i_N}_{\mu_{N-1}} |\mathrm{L}^{[N-1]}_{\mu_{N-1}}\rangle |i_N\rangle$$

Determine the Schmidt decomposition for each contiguous bipartition of the system:



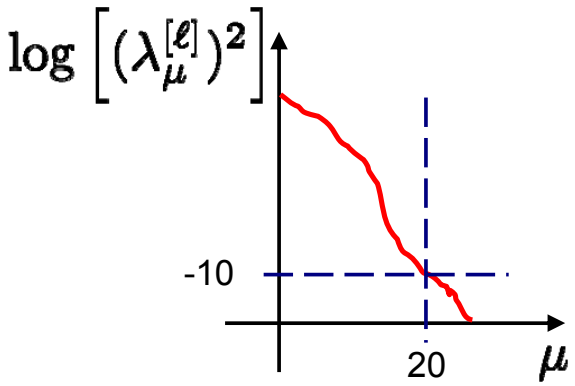
Recursively expand *left* Schmidt states.

$$|\psi\rangle = \sum_{\mathbf{i}} \left\{ \sum_{\mu_1=1}^{r_1} \sum_{\mu_2=1}^{r_2} \cdots \sum_{\mu_{N-1}=1}^{r_{N-1}} A^{[1]i_1}_{\mu_1} A^{[2]i_2}_{\mu_1\mu_2} \cdots A^{[N]i_N}_{\mu_{N-1}} \right\} |\mathbf{i}\rangle$$

Insert each expansion into the final one spanning the entire system. Obtain a MPS representation of any state.

What was the point of that?

- It seems like we have gained nothing from this because the matrices obtained can have a dimension scaling exponentially with ***N***.
- But … low-lying eigenstates of **1D** quantum systems the Schmidt spectrum $(\lambda_\mu^{[\ell]})^2$ which decays very quickly as a function of μ



A manifestation of the "area law" in 1D.

States are very weakly entangled.

Only a small number of relevant d.o.f.

Has been demonstrated numerically for many systems and proven analytically for several different models.

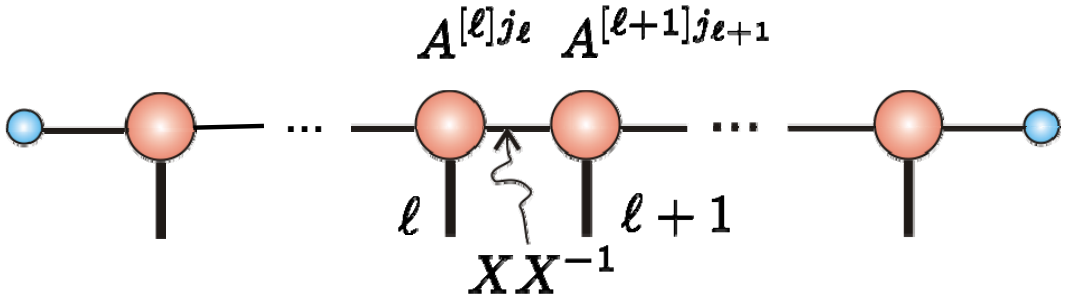
- We can truncate our matrices to some small dimension d and incur an overall 2-norm error

Can **compress** our description of the state and retain extremely high fidelity.

$$\| |\psi\rangle - |\psi_d\rangle \|^2 \leq 2 \sum_{\ell=1}^{N-1} \left[\sum_{\mu=d+1}^{r_\ell} (\lambda_\mu^{[\ell]})^2 \right]$$

Some technicalities of MPS

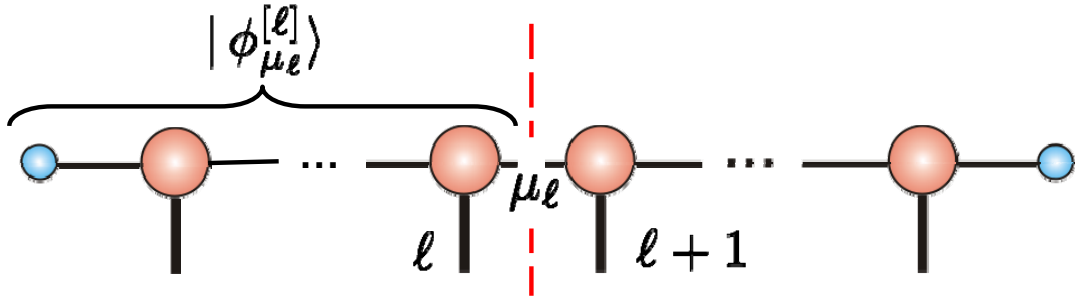
- A MPS representation of a state is not unique – it is invariant to any transformation of the internal legs via square invertible matrix X. :



$$\begin{cases} A^{[\ell]j_\ell} \rightarrow A^{[\ell]j_\ell} X \\ A^{[\ell+1]j_{\ell+1}} \rightarrow X^{-1} A^{[\ell+1]j_{\ell+1}} \end{cases}$$

- Exploiting this gauge freedom is crucial for the numerical stability of MPS algorithms. Key property is ***orthonormality*** …

- Consider splitting an MPS into two and the resulting left states:



The partial product defines a set of states indexed by μ_ℓ over the subsystem.

From our exact Schmidt expansion these left states are Schmidt states

$$|\phi^{[\ell]}_{\mu_\ell}\rangle = |\mathrm{L}^{[\ell]}_{\mu_\ell}\rangle$$

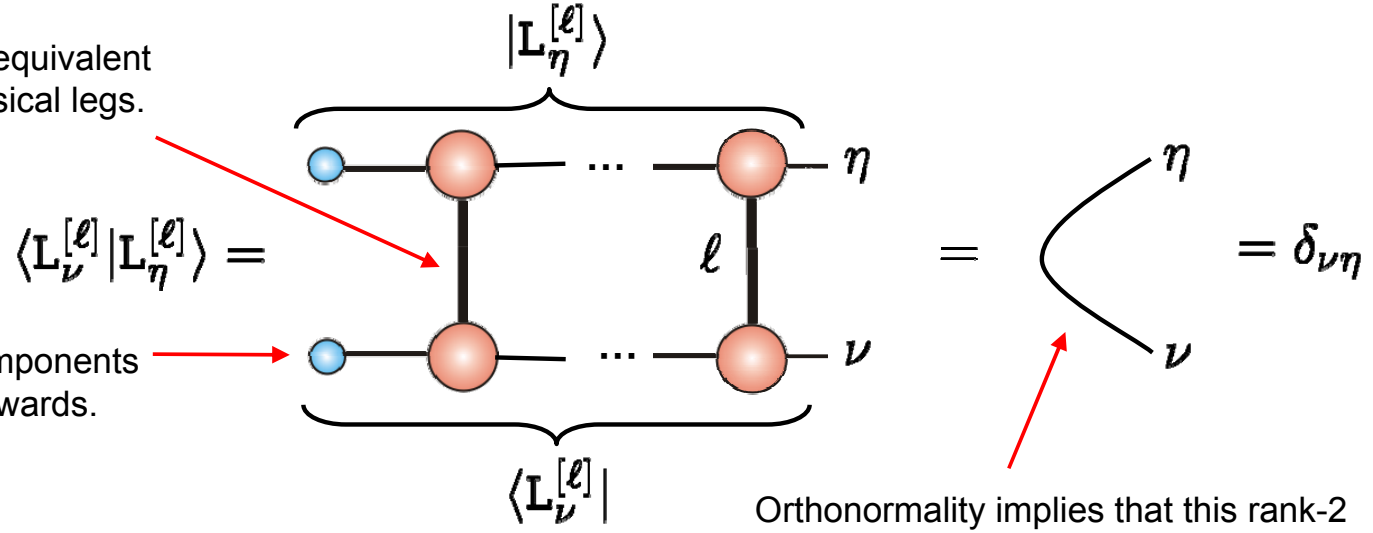
and are an orthonormal set:

$$\langle \mathrm{L}^{[\ell]}_{\nu} | \mathrm{L}^{[\ell]}_{\eta} \rangle = \delta_{\nu\eta}$$

Orthonormality and MPS

- The scalar product of the left subsystem states is given by:

Scalar product of two states is equivalent to the contraction of all the physical legs.



Complex conjugate tensor components when flipping physical legs upwards.

Orthonormality implies that this rank-2 tensor is simply the identity matrix.

- Recall that:

$$|\mathrm{L}_{\mu_\ell}^{[\ell]}\rangle = \sum_{i_\ell} \sum_{\mu_{\ell-1}=1}^{r_{\ell-1}} A_{\mu_{\ell-1}\mu_\ell}^{[\ell] i_\ell} |\mathrm{L}_{\mu_{\ell-1}}^{[\ell-1]}\rangle |i_\ell\rangle$$

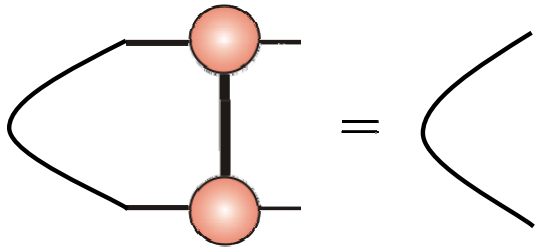
- Thus assuming that $\langle \mathrm{L}_{\nu}^{[\ell-1]} | \mathrm{L}_{\eta}^{[\ell-1]} \rangle = \delta_{\nu\eta}$ this means that:

The **A** matrices obey the constraint:

$$\sum_{j_\ell} (A^{[\ell] j_\ell})^\dagger A^{[\ell] j_\ell} = I_\ell$$

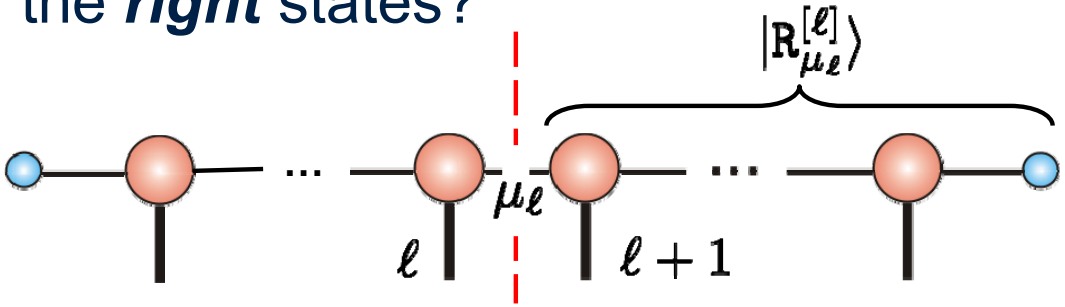
Identity matrix

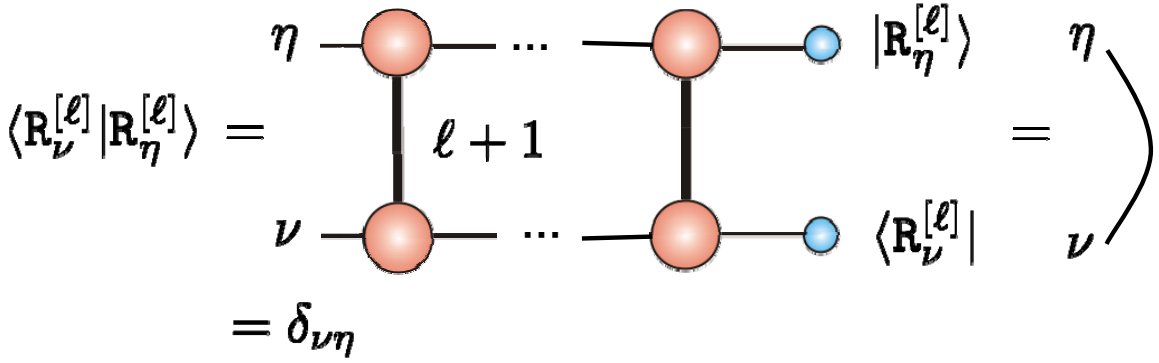
Or graphically:

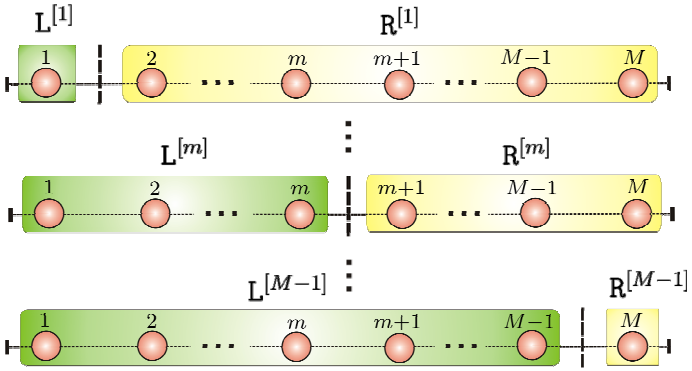


Orthonormality and MPS cont.

- Applying this recursively forces $\sum_{j_k} (A^{[k]j_k})^\dagger A^{[k]j_k} = I_k \quad \text{for} \quad 1 \le k \le \ell$
- The exact Schmidt MPS expansion using ***left*** states in fact makes all the matrices obey this constraint.
- What if we had done everything with the ***right*** states?



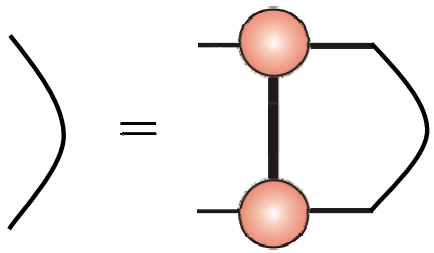




Now all the **A** matrices obey the constraint:

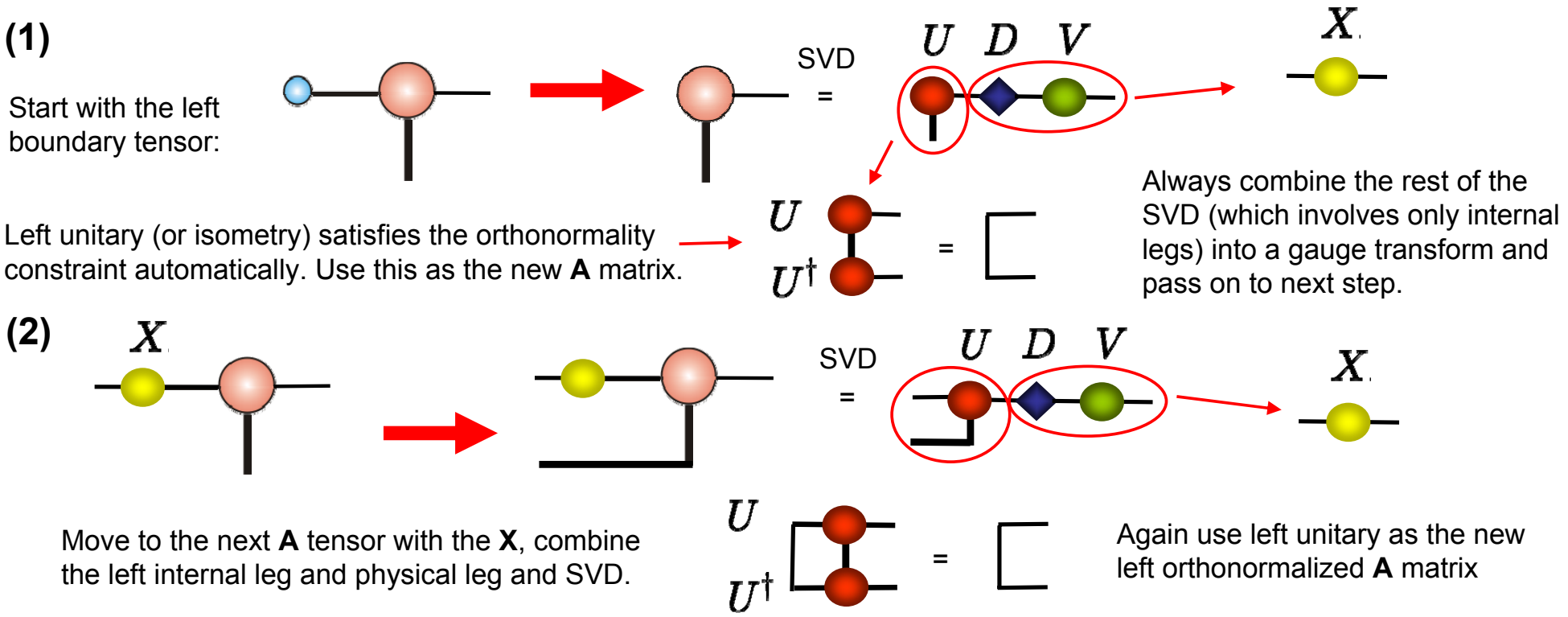
$$\sum_{j_\ell} A^{[\ell]j_\ell} (A^{[\ell]j_\ell})^\dagger = I_{\ell-1}$$

Or



Establishing an orthonormal MPS

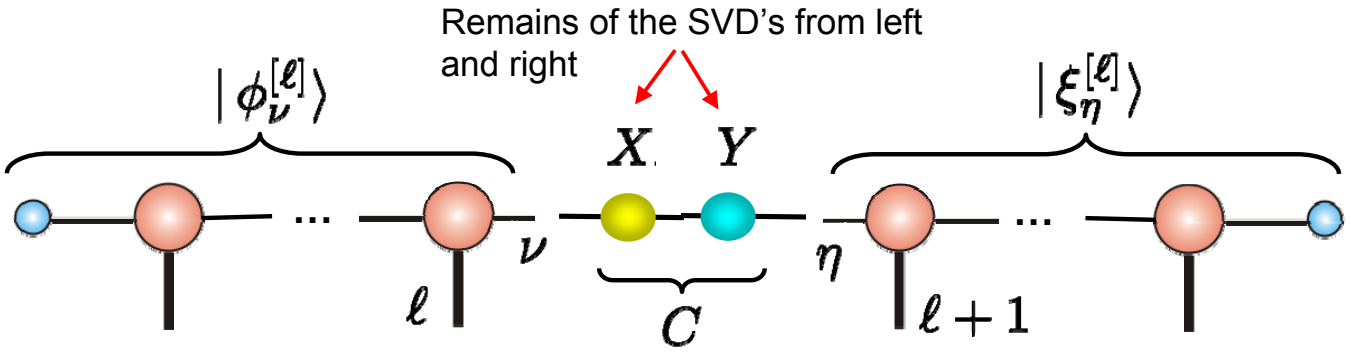
- Given an MPS, like the examples earlier that obey no constraints, how can we gauge transform it to be orthonormal?



- Continuing this process until the last site left orthonormalizes all the matrices. Could have done an analogous process from the right boundary resulting in all right orthonormalized matrices.

Orthonormal Schmidt form MPS

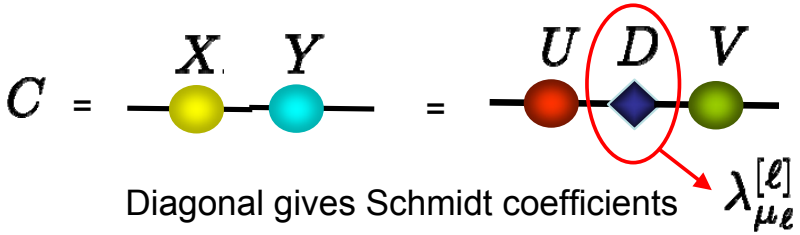
- If we work from the **left** *and* **right** up to site ℓ then we obtain orthonormal left and right states:



Equivalent to an expansion of the state in some orthonormal basis

$$|\psi\rangle = \sum_{\nu\eta} C_{\nu\eta} |\phi_\nu^{[\ell]}\rangle |\xi_\eta^{[\ell]}\rangle$$

- The MPS is said to have a twist in its handedness at ℓ.
- Put the MPS into a Schmidt form via an SVD (again!) of C:



$$|\psi\rangle = \sum_{\mu_\ell} \lambda_{\mu_\ell}^{[\ell]} |\mathrm{R}_{\mu_\ell}^{[\ell]}\rangle |\mathrm{L}_{\mu_\ell}^{[\ell]}\rangle$$

Use the unitaries to transform the left and right bases:

$$|\mathrm{L}_{\mu_\ell}^{[\ell]}\rangle = \sum_\nu U_{\nu\mu_\ell} |\phi_\nu^{[\ell]}\rangle \qquad |\mathrm{R}_{\mu_\ell}^{[\ell]}\rangle = \sum_\eta V_{\mu_\ell\eta} |\xi_\eta^{[\ell]}\rangle$$

Same as absorbing **U** and **V** into the adjacent **A** matrices.

$$A^{[\ell]j_\ell} \to A^{[\ell]j_\ell} U \qquad A^{[\ell+1]j_{\ell+1}} \to V A^{[\ell+1]j_{\ell+1}}$$

Matrix product operators - digression

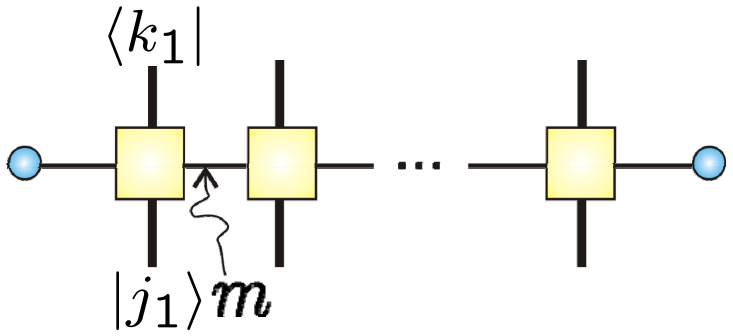
- We now make a small but important digression which will help us answer some useful questions:

  (i) What expectation values can be computed efficiently from an MPS?

- To answer this we apply the matrix product ansatz to operators:

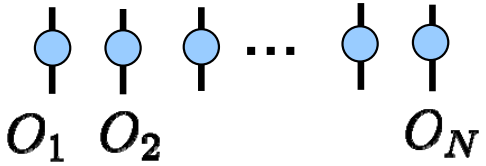
$$O = \sum_{\mathbf{j},\mathbf{k}} o_{\mathbf{j},\mathbf{k}} |\mathbf{j}\rangle \langle \mathbf{k}| \quad \text{with} \quad o_{\mathbf{j},\mathbf{k}} = \langle L| \mathbf{A}^{[1]j_1 k_1} \mathbf{A}^{[2]j_2 k_2} \dots \mathbf{A}^{[N]j_N k_N} |R\rangle$$

and $|\mathbf{j}\rangle = |j_1\rangle |j_2\rangle \dots |j_N\rangle$

$O =$ 

- Many useful operators have a very small m.

- Again the simplest example is a product operator where



Includes n-point correlations operators , e.g.

$$I \otimes \cdots \otimes I \otimes \sigma^z \otimes I \otimes \cdots \otimes I \otimes \sigma^z \otimes I \otimes \cdots \otimes I$$

Matrix product operators cont.

- Can understand MPO's "analytically" using the lower-triangular form:

$$O = \langle L| \mathbf{A}\mathbf{A}\dots\mathbf{A} |R\rangle \quad \text{where} \quad \mathbf{A} = \begin{bmatrix} p & 0 \\ q & r \end{bmatrix}$$

Single site operators

Wrap physical legs into the matrix elements

- Matrix multiplication results in the tensor product of the operators:

$$\langle L| = \begin{bmatrix} 0 & 1 \end{bmatrix} \quad \mathbf{A}\times\mathbf{A} = \begin{bmatrix} p\otimes p & 0 \\ q\otimes p + r\otimes q & r\otimes r \end{bmatrix} \quad |R\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

- For longer strings $\mathbf{A}\times\mathbf{A}\times\cdots\times\mathbf{A}$ boundary vectors select the sum of all translates of ($r\otimes\cdots\otimes r\otimes q\otimes p\otimes\cdots\otimes p$) c.f. W state earlier

- Examples: $\sum_j \sigma^z_j$ $\sum_j \sigma^x_j\sigma^x_{j+1} + B\sum_j \sigma^z_j$

Sum of Z mag. $\mathbf{A} = \begin{bmatrix} \mathbb{1} & 0 \\ \sigma^z & \mathbb{1} \end{bmatrix}$

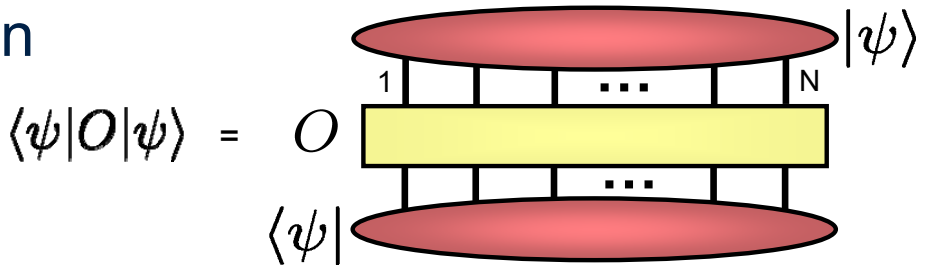
Ising Hamiltonian $\mathbf{A} = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ \sigma^x & 0 & 0 \\ B\sigma^z & \sigma^x & \mathbb{1} \end{bmatrix}$

I.P. McCulloch J. Stat. Mech. **P10014** (2007) and arxiv:0804.2509

Computing expectation values

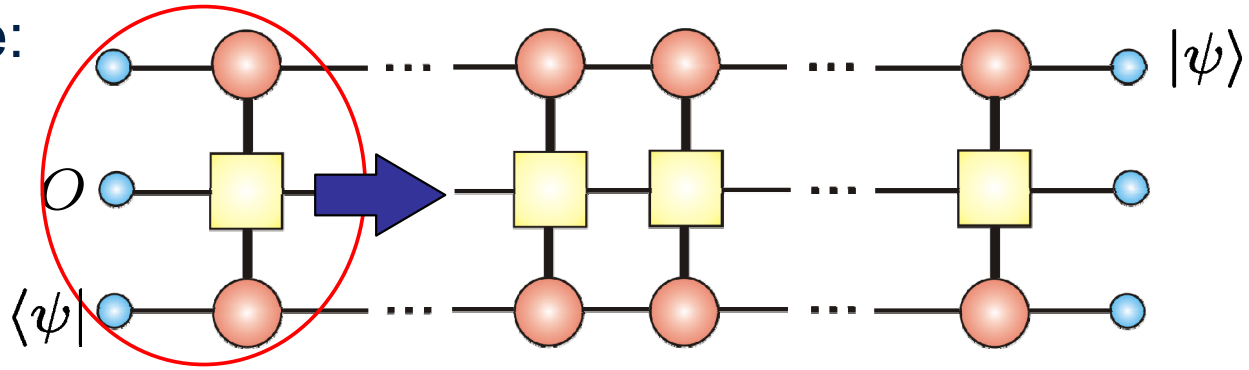
- Calculating an expectation value can be viewed as a tensor network:

Must deal with huge structureless tensors.
Have no choice but to contract vertically



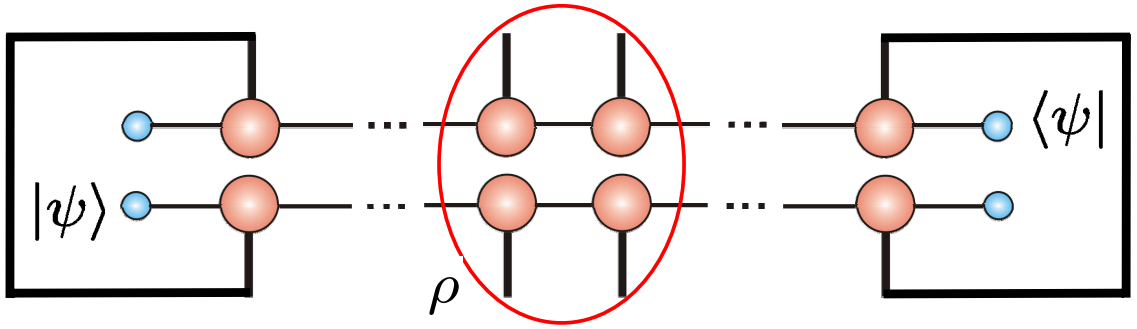
- In contrast for an MPS and an MPO this contraction is efficient due to the internal tensor structure:

Can contract vertically on local pieces and then contract horizontally across the system dealing at most with a d^2m tensor.



- Moreover any density matrices for a tractable sized subsystem are efficiently accessible:

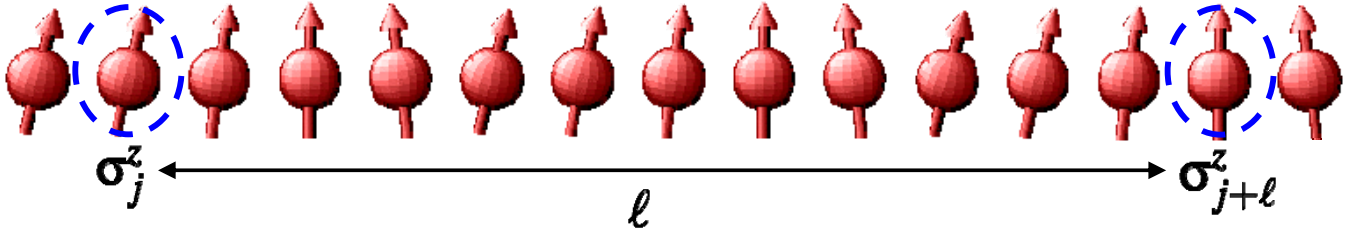
Partial tracing is equivalent to contracting physical legs together. Contract horizontally the local tensors. Physical legs of relevant sites are left uncontracted giving

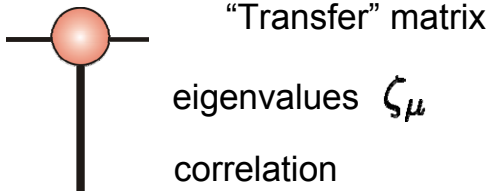


Decay of correlations in an MPS

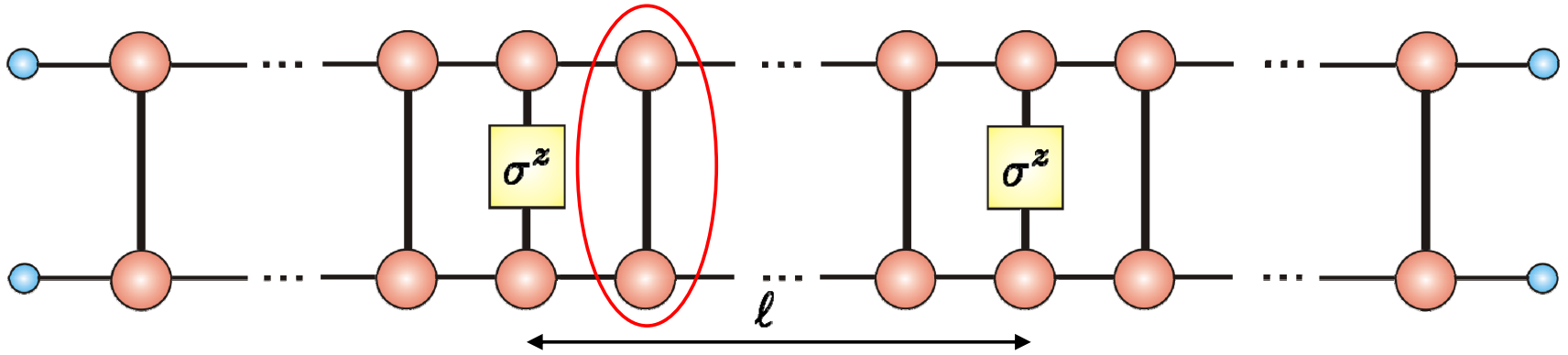
- Recall that we were interested in long-range correlations:

$$C_\ell^{zz} = \langle \phi_0 | \sigma_j^z \sigma_{j+\ell}^z | \phi_0 \rangle - \langle \phi_0 | \sigma_j^z | \phi_0 \rangle \langle \phi_0 | \sigma_{j+\ell}^z | \phi_0 \rangle$$





- For an MPS this boils down to a contraction of the form:



- MPS manifestly have exponentially decaying correlations given by:

$$C_\ell = \sum_{\mu>1}^{d^2} \kappa_\mu \left(\frac{\zeta_\mu}{|\zeta_\mu|}\right)^\ell \exp\left(-\frac{\ell}{\xi_\mu}\right) + c$$

- Can still model a power-law decay as a sum of exponential decays.

Variational minimization of an MPS

- We now come to the second question:

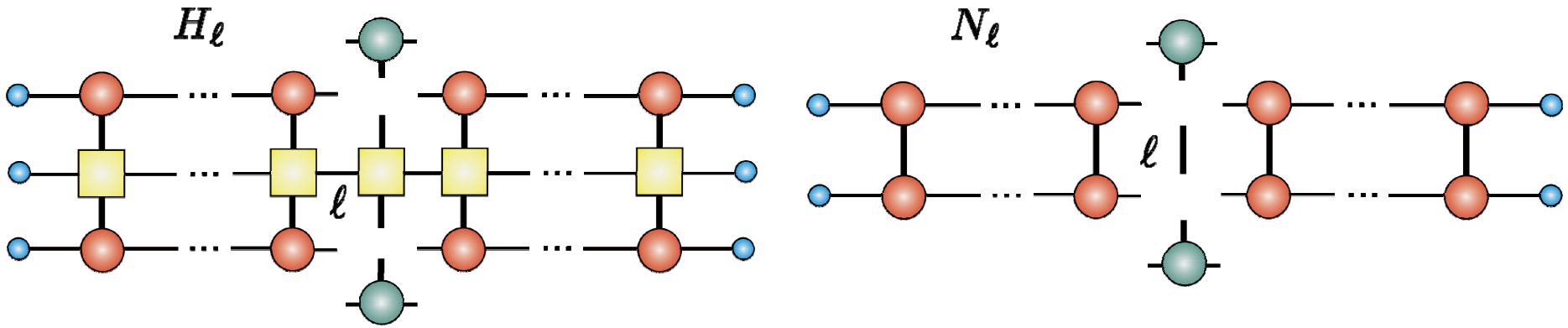
  (ii) Can we efficiently find an MPS approximation to a ground state?

- Want to *variationally* minimize over the class of MPS with a fixed dimension d:

$$\min \{\langle\psi|H|\psi\rangle,\ \text{s.t. } \langle\psi|\psi\rangle = 1,\ |\psi\rangle \in \mathrm{MPS}(d)\}$$

- One strategy is to minimize w.r.t. one **A** matrix at a time, keeping all others fixed, and then alternate over all matrices.

Start by picking one **A** matrix, say ℓ, and remove it from the tensor networks defining energy and normalization:

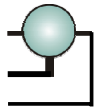


Contraction of remaining tensors defines two matrices sandwiched by **A** matrices (after reshaping them as a vector).

Variational minimization cont.

- We are then left with a quadratic minimization problem of the form:

$$\min_{x_\ell} \left\{ e = \frac{x_\ell^\dagger H_\ell x_\ell}{x_\ell^\dagger N_\ell x_\ell} \right\}$$

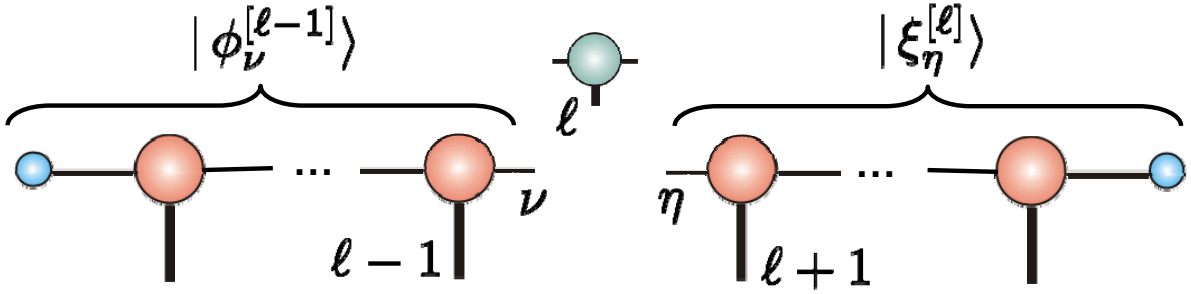
$x_\ell =$ 

The **A** matrix reshaped as a vector.

- It follows that H_ℓ is hermitian and N_ℓ is positive, thus e is real and the minimum is determined by a generalized eigenvalue equation:

$$H_\ell x_\ell = \lambda N_\ell x_\ell$$

- One issue is that N_ℓ can be ill-conditioned. This can be circumvented by ensuring that the twist in the MPS is always located at ℓ



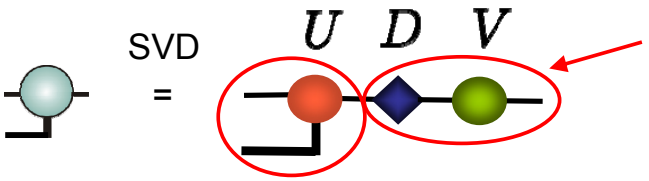
All matrices frozen to the left and right are appropriately constrained so that the left and right bases are orthonormal

- Orthonormality makes $N_\ell = \mathbb{1}$ and reduces the problem to $H_\ell x_\ell = \lambda x_\ell$

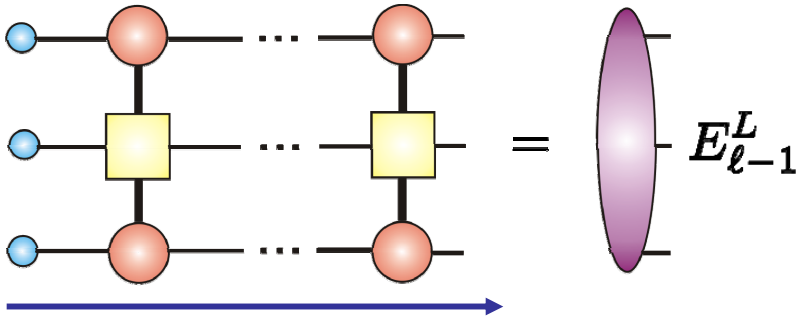
Variational minimization cont.

- Having solved the eigenvalue problem we now constrain the solution so that the updated **A** matrix is appropriately orthonormalized:

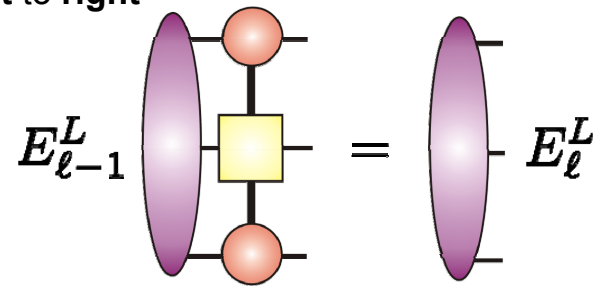
When sweeping from left to right combine physical leg to the left and use the left unitary as the new **A** matrix.



Can discard the rest since the next sites **A** matrix will be updated anyhow.



Sweep **left** to **right**

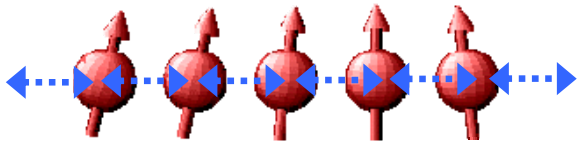


- Combine the new **A** matrix and part of Hamiltonian MPO with an accumulated left environment tensor E^L_ℓ.
- Move to site $\ell+1$ and use this updated environment to form $H_{\ell+1}$. Analogous actions for right to left sweep.
- Algorithm is essentially density matrix renormalization group.

- Common DMRG approach is to minimize two **A** matrices at a time.

Time evolution of an MPS

- Consider a 1D Hamiltonian with nearest-neighbour interactions: $H = \sum_{j=1}^{N-1} h_{j,j+1}$



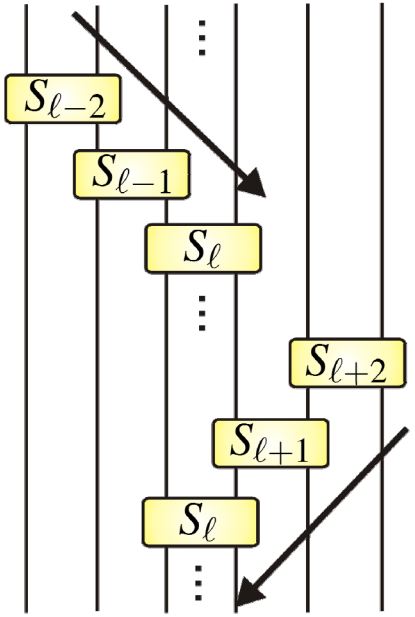
- Want discretize the time evolution $|\psi(t)\rangle = U(\delta t)U(\delta t)\cdots U(\delta t)|\psi(0)\rangle$

where $U(\delta t) = \exp\left(-i\delta t \sum_{j=1}^{N-1} h_{j,j+1}\right)$

Storing let alone computing this many-body unitary operator is infeasible.

- Better strategy "**Trotterize**" the exponential …

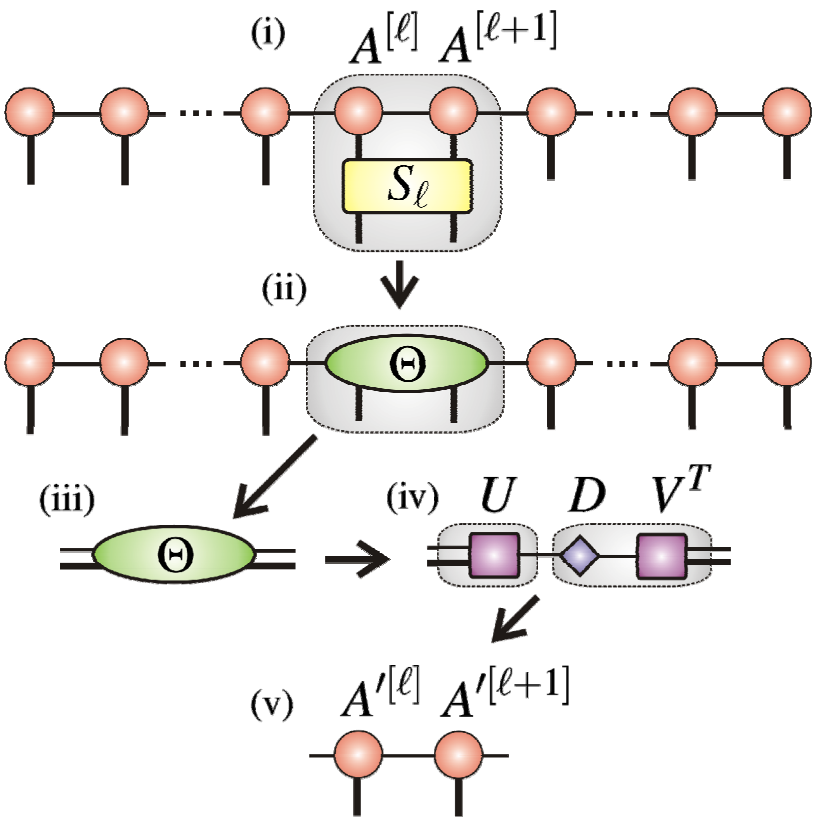
$$e^{-iH\delta t} = \underbrace{\left(\prod_{j=1}^{N-1} e^{-\frac{i}{2}h_{j,j+1}\delta t}\right)}_{S_j \text{ = two-site gate}} \left(\prod_{j=N-1}^{1} e^{-\frac{i}{2}h_{j,j+1}\delta t}\right) + O\left(\delta t^3\right)$$



- Have broken the evolution into a sequence of gates.

Applying a two-site gate to an MPS

- We now need to apply a sequence of two-site *n.n.* gates to the MPS:



(i) Apply local "gate" by contracting it with the relevant physical legs.

(ii) Resulting merged tensor now needs to be broken up.

(iii) Reshape tensor into a matrix.

(iv) Factorize the matrix via an SVD.

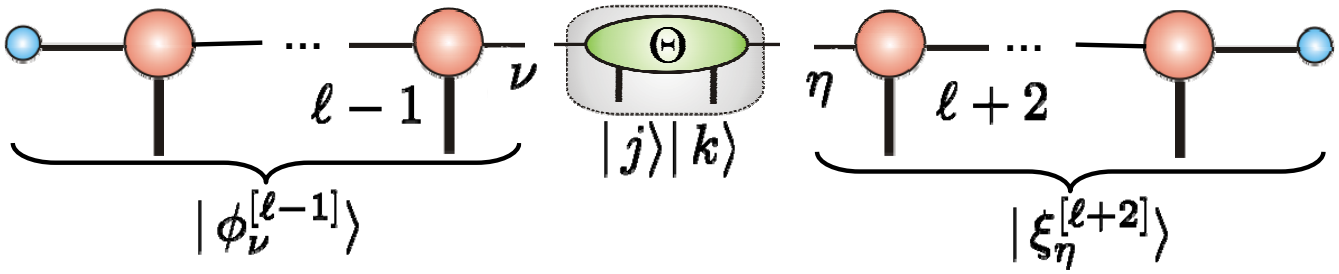
(v) Truncate the inner dimension and extract new **A** matrices.

- Most expensive step numerically is the SVD whose cost scales as $O(d^3)$ for each gate.

Optimality of MPS truncation

- What does the truncation of the local SVD mean physically?
- Resulting two-site tensor is a set of expansion coefficients for $S_\ell|\psi\rangle$

$$S_\ell|\psi\rangle = \sum_{\nu\eta jk} \Theta^{jk}_{\nu\eta} |\phi^{[\ell-1]}_\nu\rangle |j\rangle |k\rangle |\xi^{[\ell+2]}_\eta\rangle$$



Note that we do not need to assume that S_ℓ is unitary. To ensure optimality we need only that the left and right bases are orthonormal.

- Want to factorize and truncate inner dimension to d optimally by solving:

$$\min\{\||S_\ell|\psi\rangle - |\psi'\rangle\|_2, \text{ s.t. } |\psi'\rangle \in \mathrm{MPS}(d)\}$$

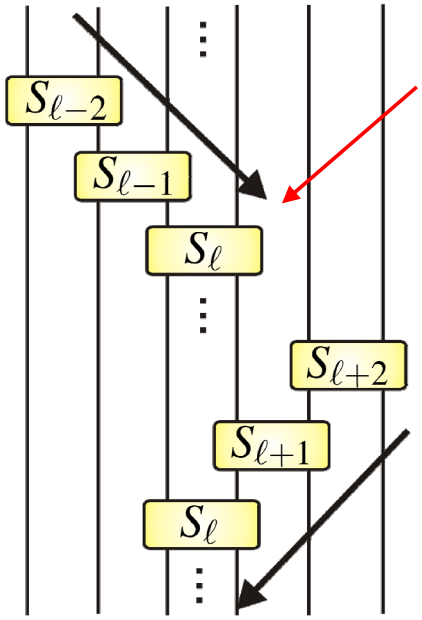
- The SVD is already the optimal solution to the problem:

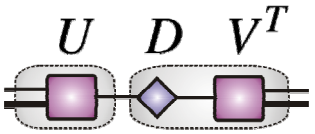
$$\min\{||\Theta - Q||_2, \text{ s.t. } Q \in \mathbb{C}^{m\times n}, \text{ rank}(Q) = d\}$$

- So long as all legs are orthonormal optimal truncation for the state is solved by the SVD of the local tensor.

Real and imaginary time evolution

- Can efficiently simulate real-time unitary dynamics of 1D quantum lattice systems with this method (time-evolving block decimation).
- Remains accurate for short time – breaks down due to dynamical entanglement production so $(\lambda_{\mu}^{[\ell]})^2$ no longer decay rapidly.
- Can determine the ground state via imaginary time-evolution:





$$|\phi_0\rangle = \lim_{t\to\infty} \frac{e^{-Ht}|\psi\rangle}{\| |\psi\rangle \|}$$

- Gates are now non-unitary (not a problem).
- Works since excitation are exponentially suppressed:

$$e^{-Ht} = \sum_{\nu} e^{-e_\nu t} |\phi_\nu\rangle\langle\phi_\nu|$$

- So long as $\langle\psi|\phi_0\rangle \neq 0$

Part III – Extensions & Generalizations

Open quantum systems

- We have so far concentrated on the ground state and the temperature **T** = 0 coherent dynamics of 1D quantum systems.
- Can also simulate dissipative, incoherent evolution of a systems density matrix by representing $\rho(t)$ as an MPO.
- For Markovian noise the evolution of the system is modelled by a master equation:

$$\dot{\rho}(t) = \overbrace{-i[H,\rho(t)]+\sum_{\gamma}\left(L_\gamma\rho(t)L_\gamma^\dagger-\frac{1}{2}L_\gamma^\dagger L_\gamma\rho(t)-\frac{1}{2}\rho(t)L_\gamma^\dagger L_\gamma\right)}^{\mathcal{L}}$$

Hamiltonian for the system.

"local" Lindblad jump operators.

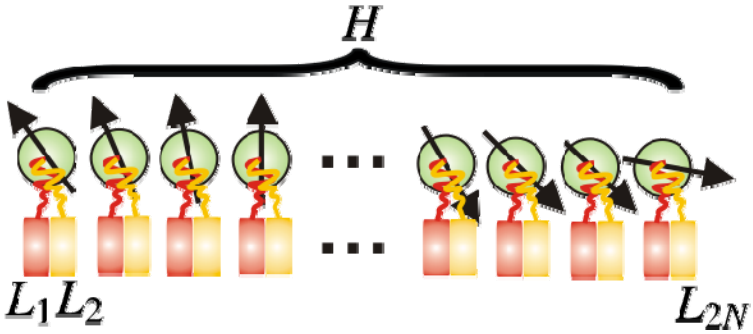
- Example: **XYZ** spin-chain subject to bulk spin damping noise:

Hamiltonian:

$$H_{xyz}=\sum_{j=1}^{N}\left(J_x\sigma_j^x\sigma_{j+1}^x+J_y\sigma_j^y\sigma_{j+1}^y+J_z\sigma_j^z\sigma_{j+1}^z\right)+B\sum_{j=1}^{N}\sigma_j^z$$

Lindblad Noise::

$$L_1=\sqrt{\Gamma_+}\sigma_1^+,\quad L_2=\sqrt{\Gamma_-}\sigma_1^-\cdots\quad L_{2N}=\sqrt{\Gamma_-}\sigma_N^-$$



Master equation evolution

- Formal solution to master equation evolution is:

Incoherent $\rho(t) = \exp(\mathcal{L}t)\{\rho\}$ where $\mathcal{L}$ is a the full superoperator.

Important special cases:

Coherent $\rho(t) = \exp(\mathcal{H}t)\{\rho\} = e^{-iHt}\rho e^{iHt}$

Form commutator superoperator: $\mathcal{H}\{o\} = -i(Ho - oH)$

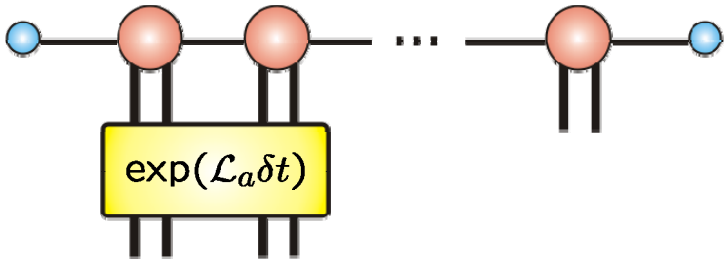
Thermal $\rho(\beta) = \exp(-\beta\mathcal{T})\{\mathbb{1}\} = e^{-\beta H/2}\mathbb{1}e^{-\beta H/2}$

Form anti-commutator superoperator: $\mathcal{T}\{o\} = \frac{1}{2}(Ho + oH)$

- "Trotterize" the exponentials as before so long as operators are local:

$$\exp(\mathcal{L}\delta t) \approx \exp(\mathcal{L}_a\delta t)\exp(\mathcal{L}_b\delta t)$$

- Can apply "gates" representing two-site superoperator evolution via TEBD:

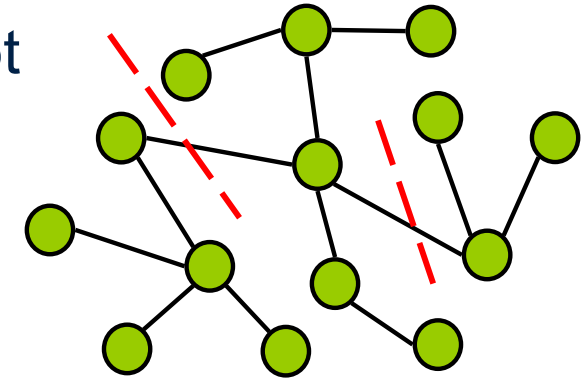


M. Zwolak and G. Vidal, PRL **93**, 207205 (2004)
F. Verstraete, J.J. Garcia-Ripoll and J.I. Cirac, PRL **93**, 207204 (2004)

A first step beyond 1D

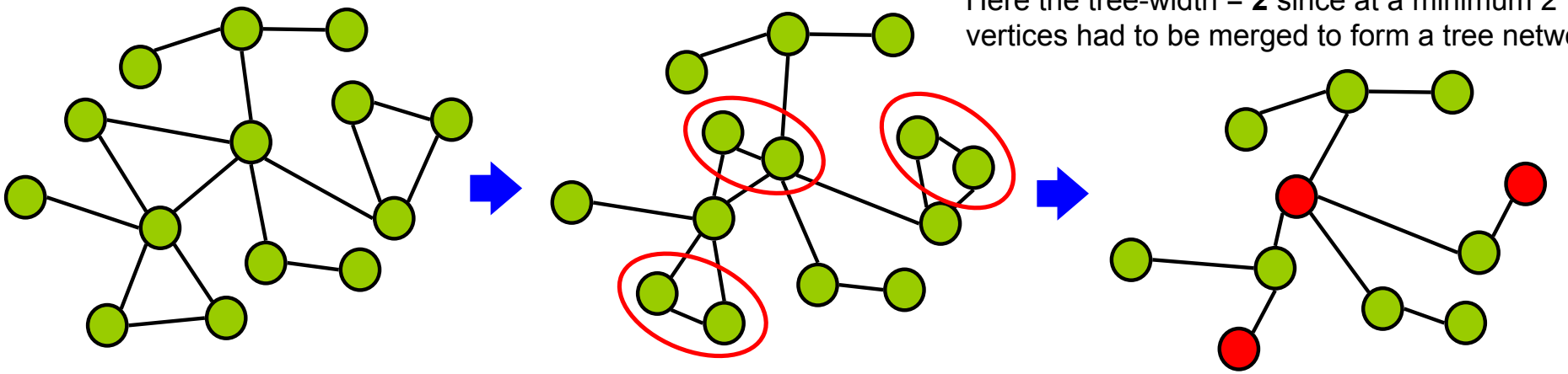
- The most general geometry in which the concept of a Schmidt decomposition remains is a *tree*:

  The network has no loops and so for any n.n. pair we can always divide the system into two halves with only that bond connecting the subsystems (i.e. governing entanglement) as in 1D.



- Can generalize slightly to networks with loops and remain efficient so long as the so-called *tree-width* is small:

Here the tree-width = **2** since at a minimum 2 vertices had to be merged to form a tree network.

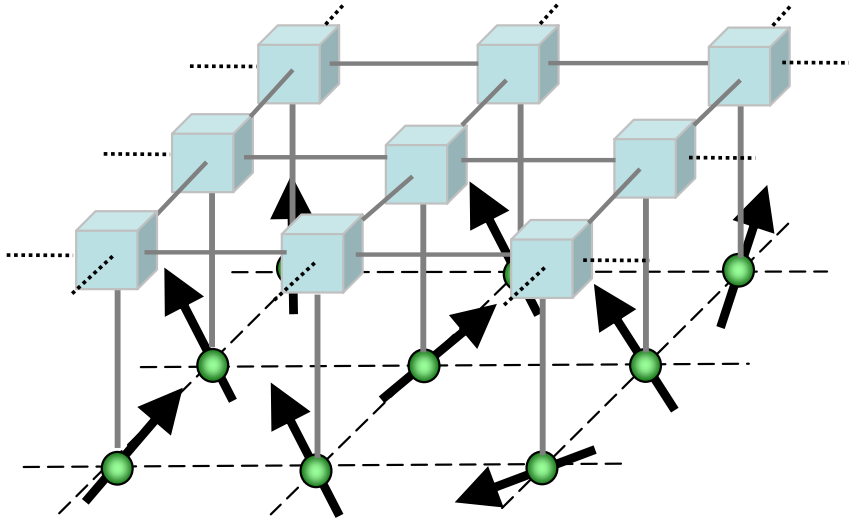


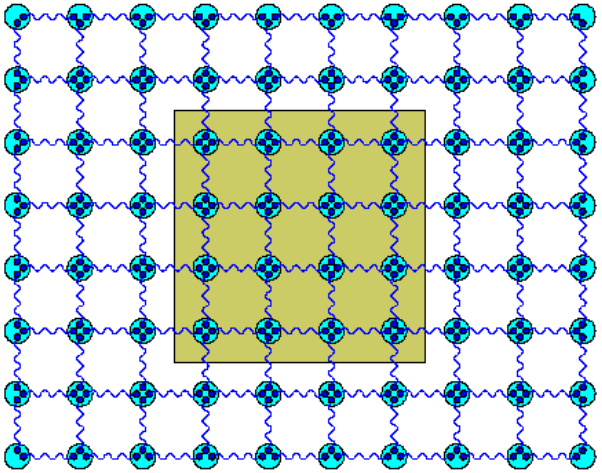
- So long as the tree-width is limited the network remains efficiently contractible and all the algorithms presented carry over.

Y. Shi, L. Duan and G. Vidal, PRA **74**, 022320 (2006)

Going to 2D with PEPS

- A direct generalization of MPS to 2D is a tensor network following a regular lattice. This picture is motivated by the PEPS construction:





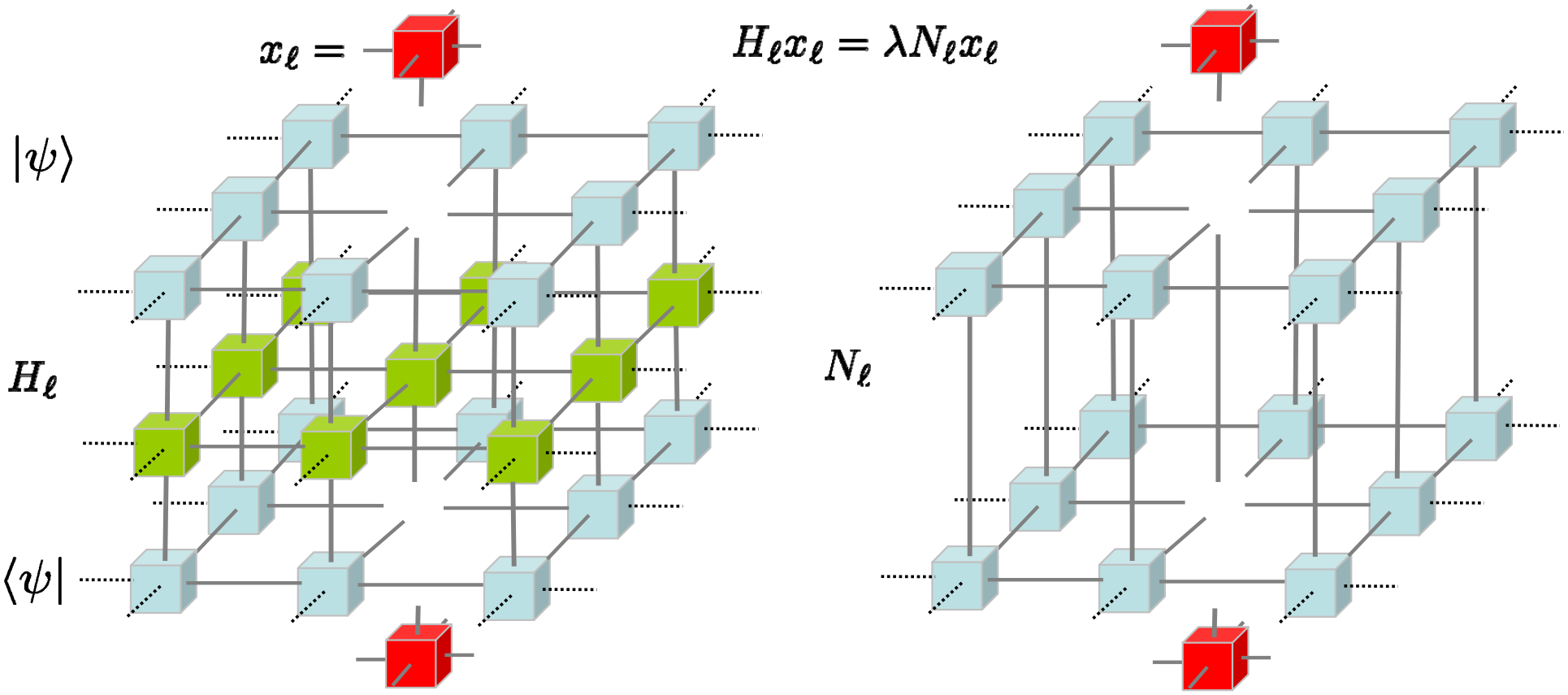
- Two problems immediately present themselves:

  (i) The 2D tensor network is not efficiently contractible (growing tree-width).

  (ii) Multiple bonds connecting regions prevents gauge transformations and concepts like orthonormality from being applicable.

Variational minimization in 2D

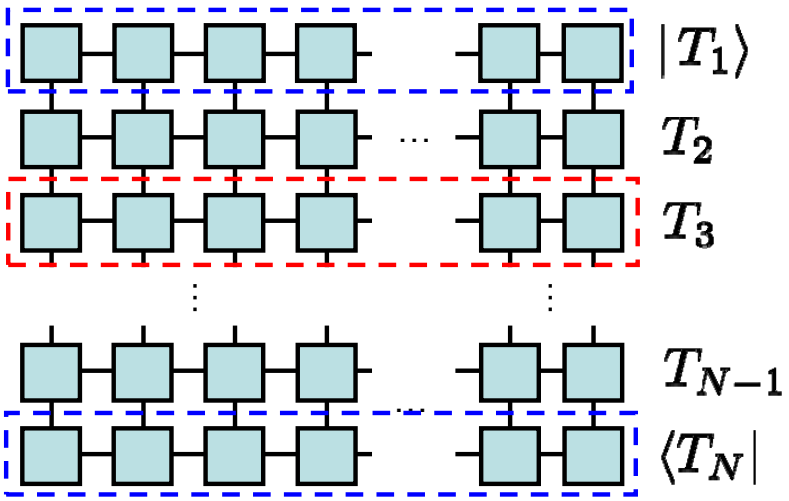
- Putting contractibility aside for the moment we can see that PEPS provide a direct generalization of DMRG to 2D quantum systems:
- Can attempt to variationally minimize one tensor at a time, as in 1D, by solving the generalized eigenvalue problem for each tensor:

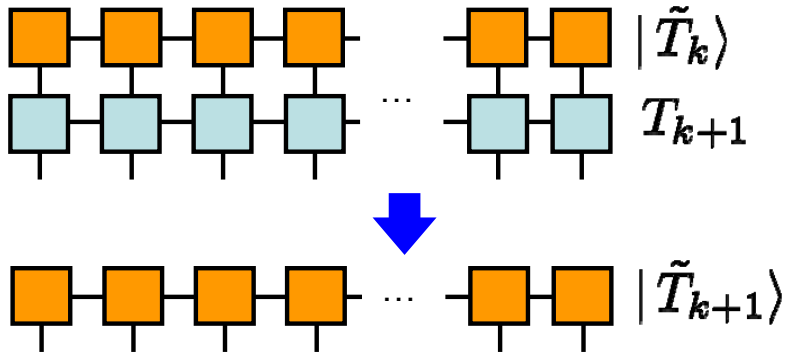


Approximate contraction via MPS

- Viewing the “double” layered network from above an approximate scheme for contracting the network can be devised using MPS:

Form MPS from the top and bottom rows. Other rows form MPO’s sandwiched between them.





Sequentially apply each MPO to the top MPS and find the best MPS approximation with some fixed dimension to the result. Finish with a contraction:

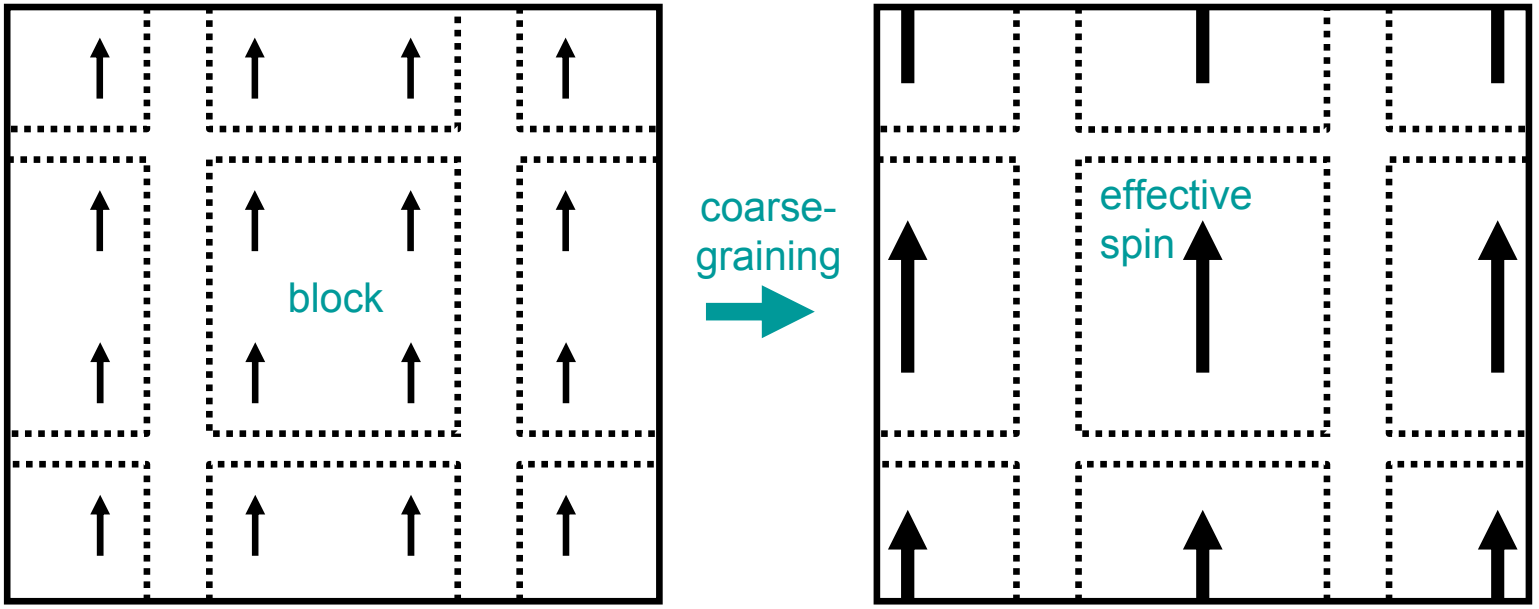
$$\langle T_N|\tilde{T}_{N-1}\rangle$$

- Reduces to a sequence of MPS contractions with an MPO. Can truncate to a new MPS with similar algorithms to those discussed.
- This method can be used to efficiently evaluate H_ℓ and N_ℓ required for the variational minimization.

Real space renormalization methods

- A final approach we shall discuss is the so-called multi-scale entanglement renormalization ansatz (MERA).
- Nicely combines condensed matter and quantum information ideas.

Kadanoff's spin blocking (1966)

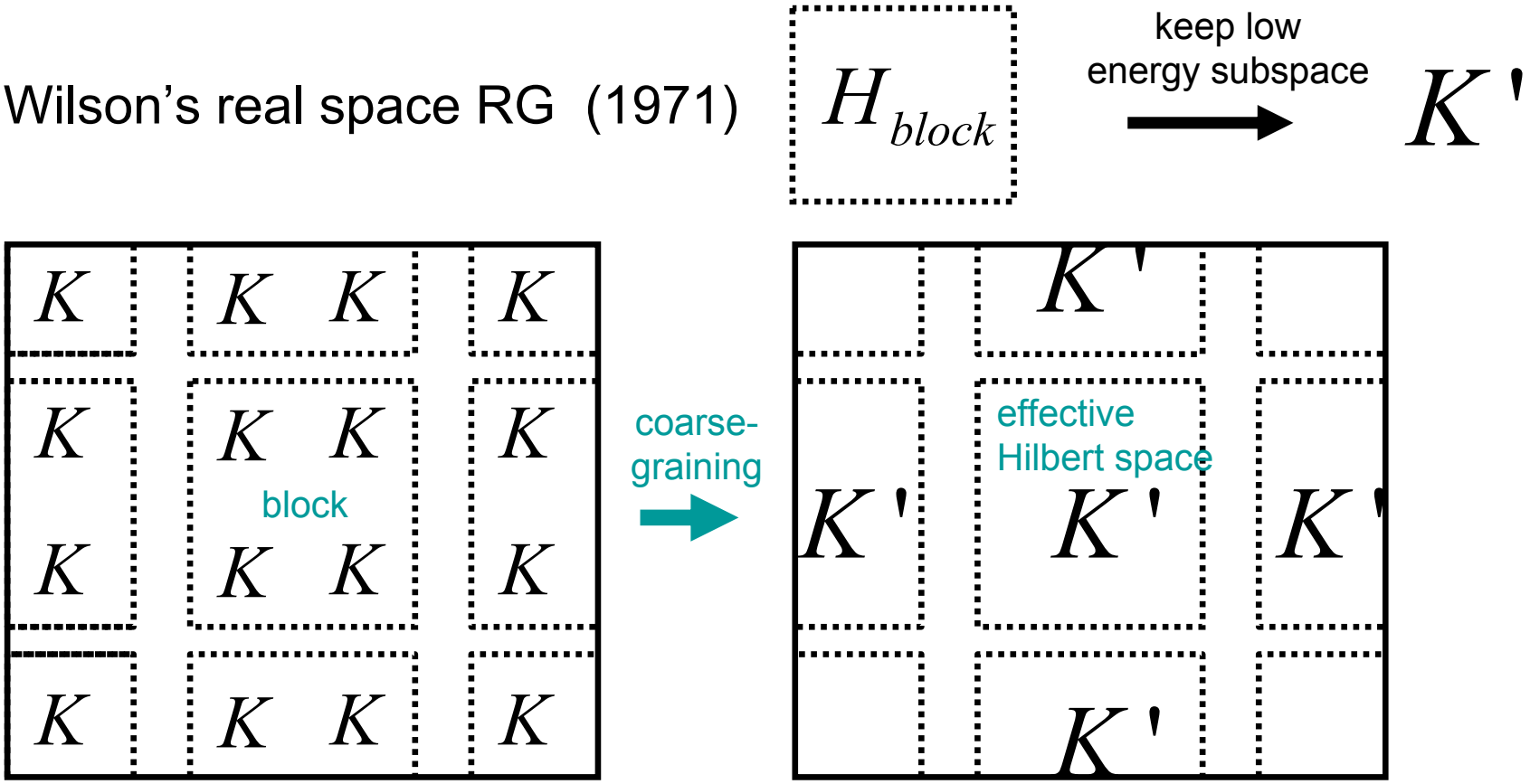


leading intuition: critical system ⟶ scale invariance

How to coarse-grain? - Wilson

- Physically intuitive to use the low-energy eigenstates of a block to define a coarse-graining projection.

Wilson's real space RG (1971)

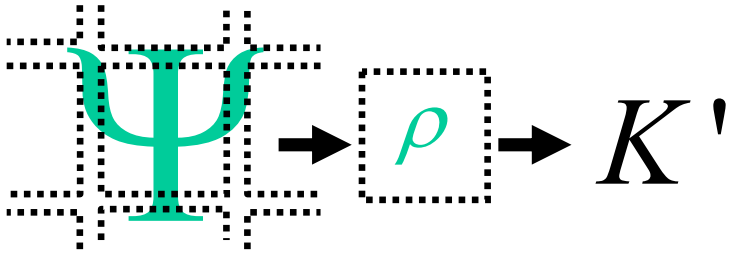


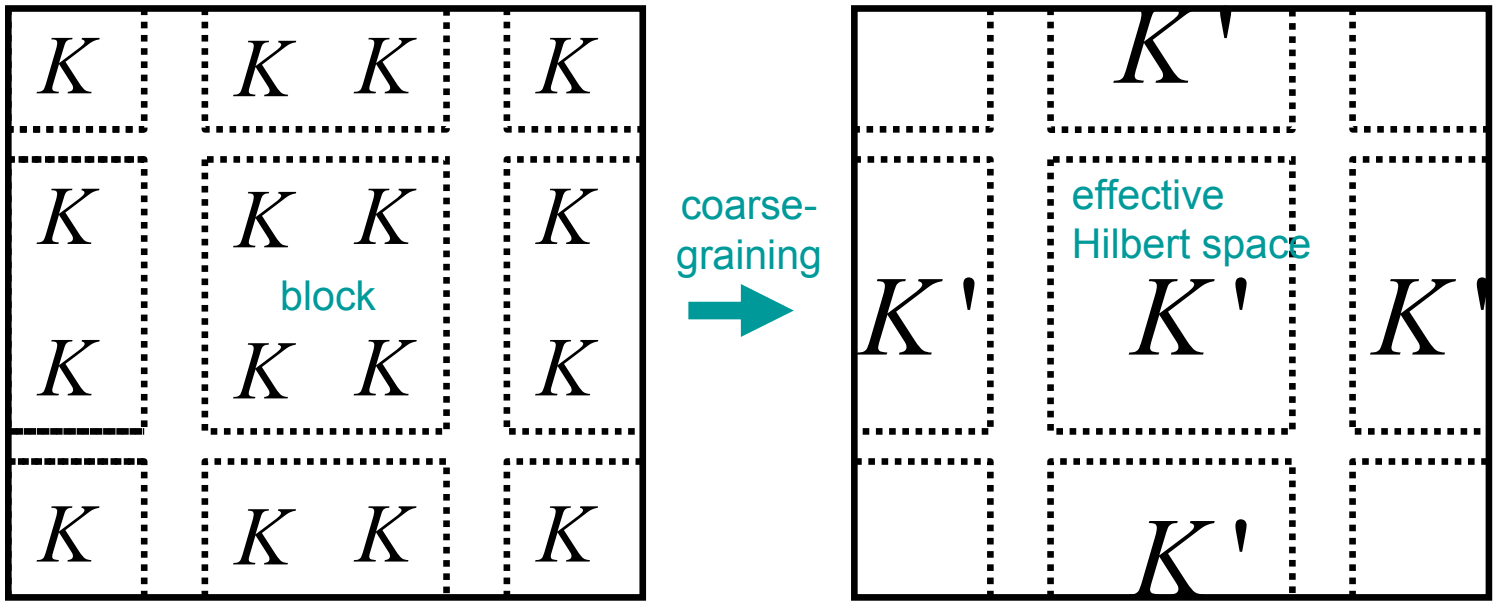
leading intuition: ground state ⟶ low energy

How to coarse-grain? - White

- Dramatic improvements in 1D where found when the density matrix itself was used to define the coarse-graining – so called DMRG:

White's density matrix RG (1992)



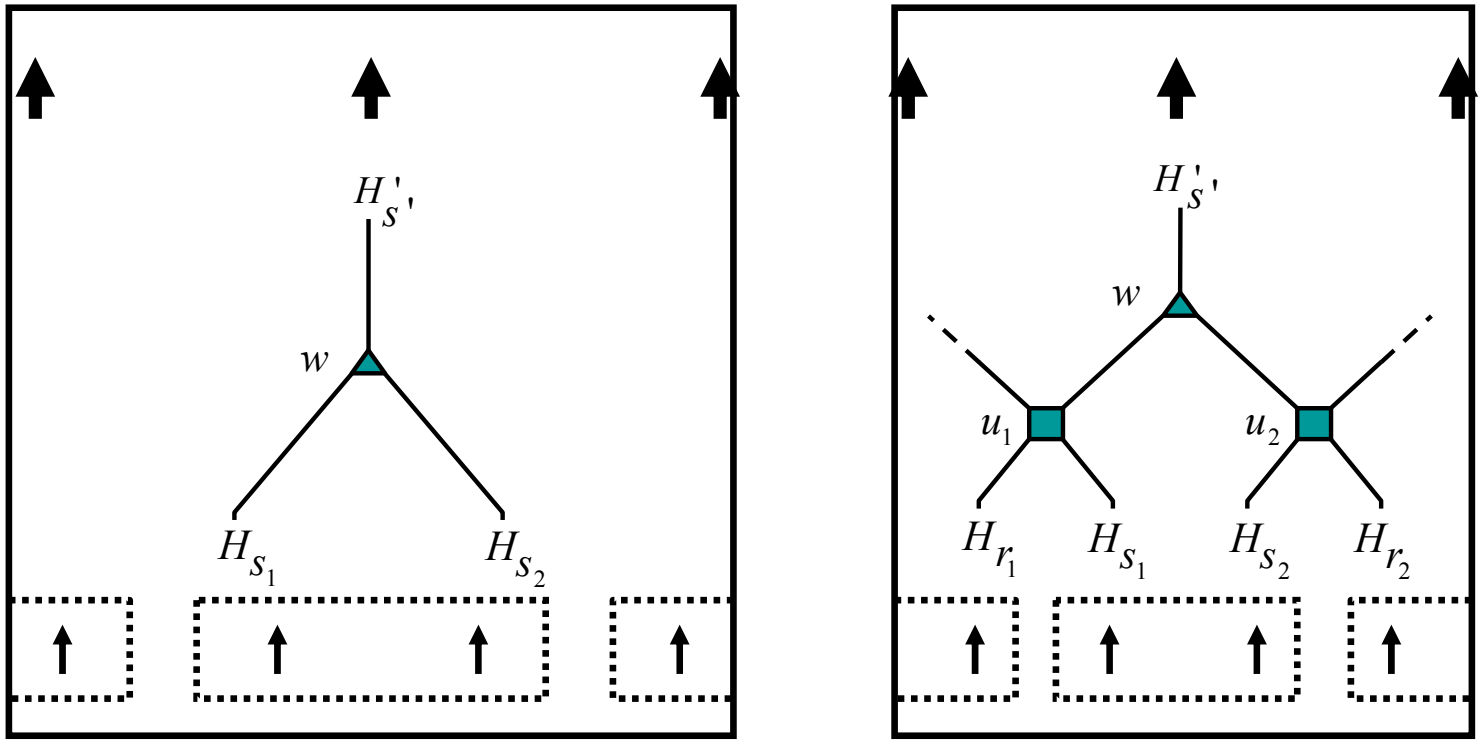


leading intuition: target the local support of the global ground state

Entanglement renormalization

- Recent advances use quantum information concepts precisely in the form of a tensor network approximation:

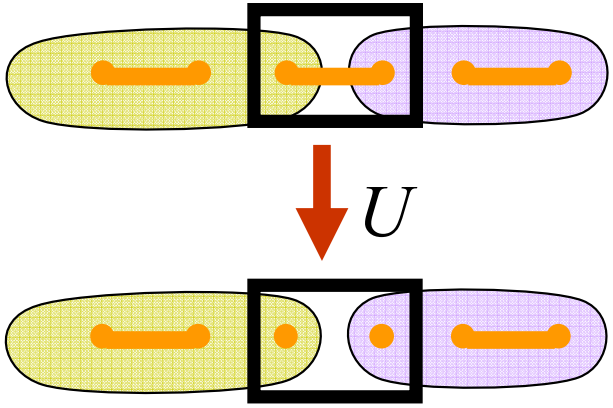
Vidal's Entanglement RG (2005)



leading intuition: attempt to disentangle the block before projecting it

Entanglement renormalization cont.

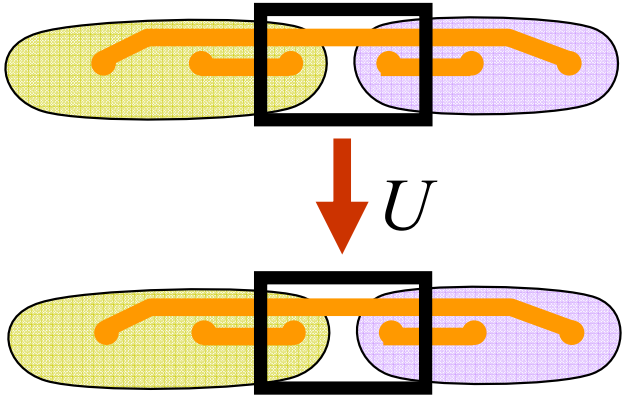
- We can illustrate the purpose of this new step with cartoon examples:



completely disentangled

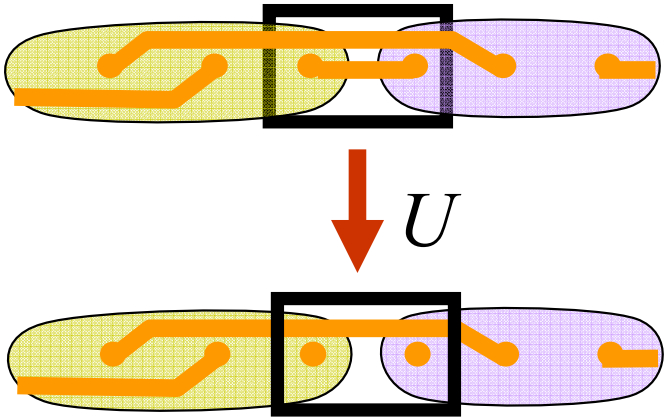
Here the dots connected by lines signify entangled pairs.

A unitary is applied between the outer spins of the two subsystems.



no disentanglement

An appropriately chosen unitary can disentangle pairs only between the outermost spins.



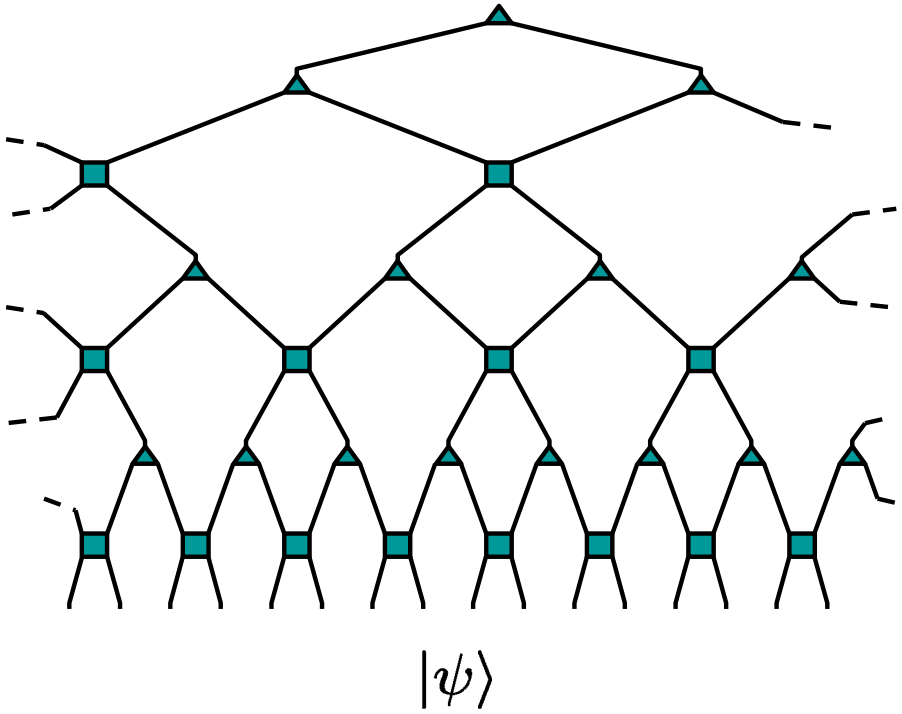
partially disentangled

Any long-ranged entangled pairs cannot be disentangled by a local unitary.

The MERA tensor network

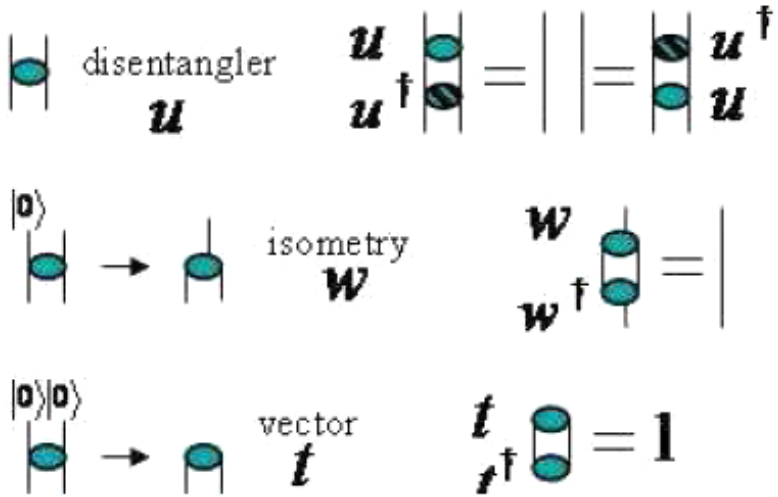
- Attempt to “disentangle” as much as possible at each level, and hope to remove longer-ranged entanglement at larger scales:

The 1D case:



$|\psi\rangle$

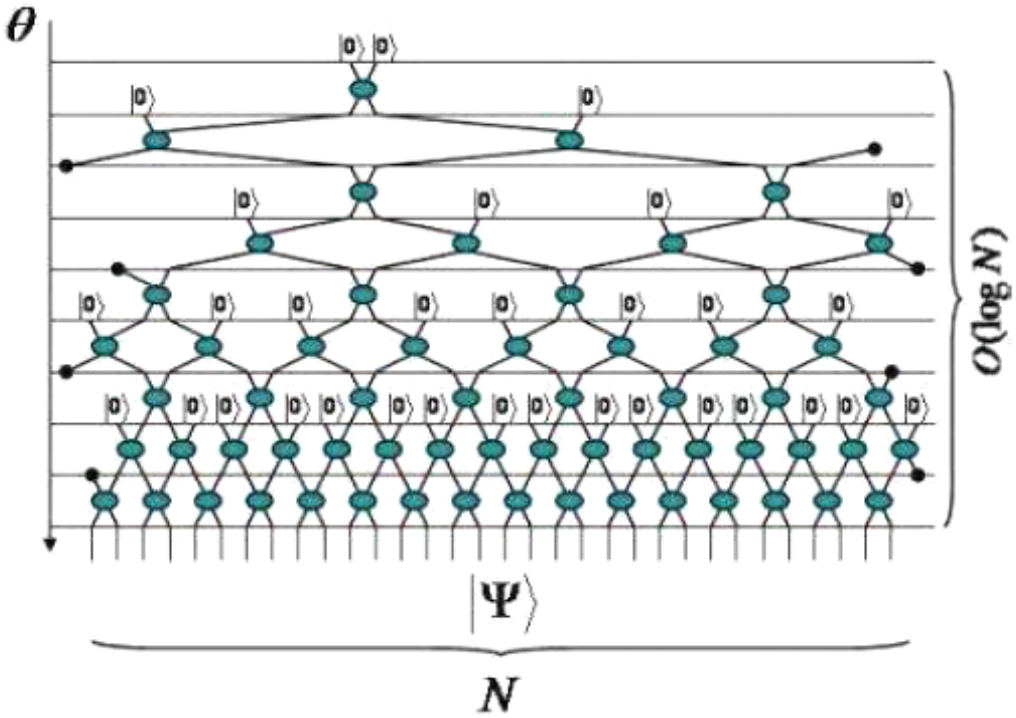
Tensor components have very special properties:

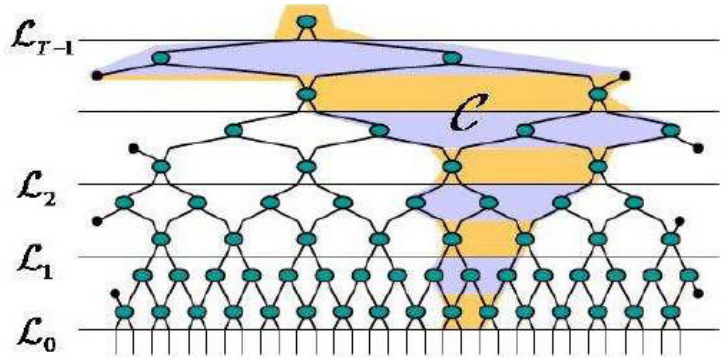


- The MERA hierarchical tensor network aims to completely disentangle a many-body quantum state $|\psi\rangle$ to a product state.

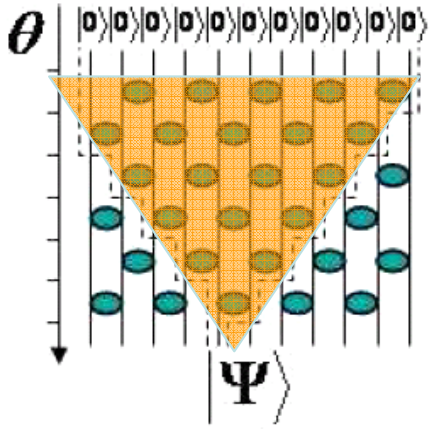
MERA as a quantum circuit

- The MERA tensor network can be viewed as a peculiar quantum circuit in which a trivial product state is unitarily mapped to a highly non-trivial many-body state:





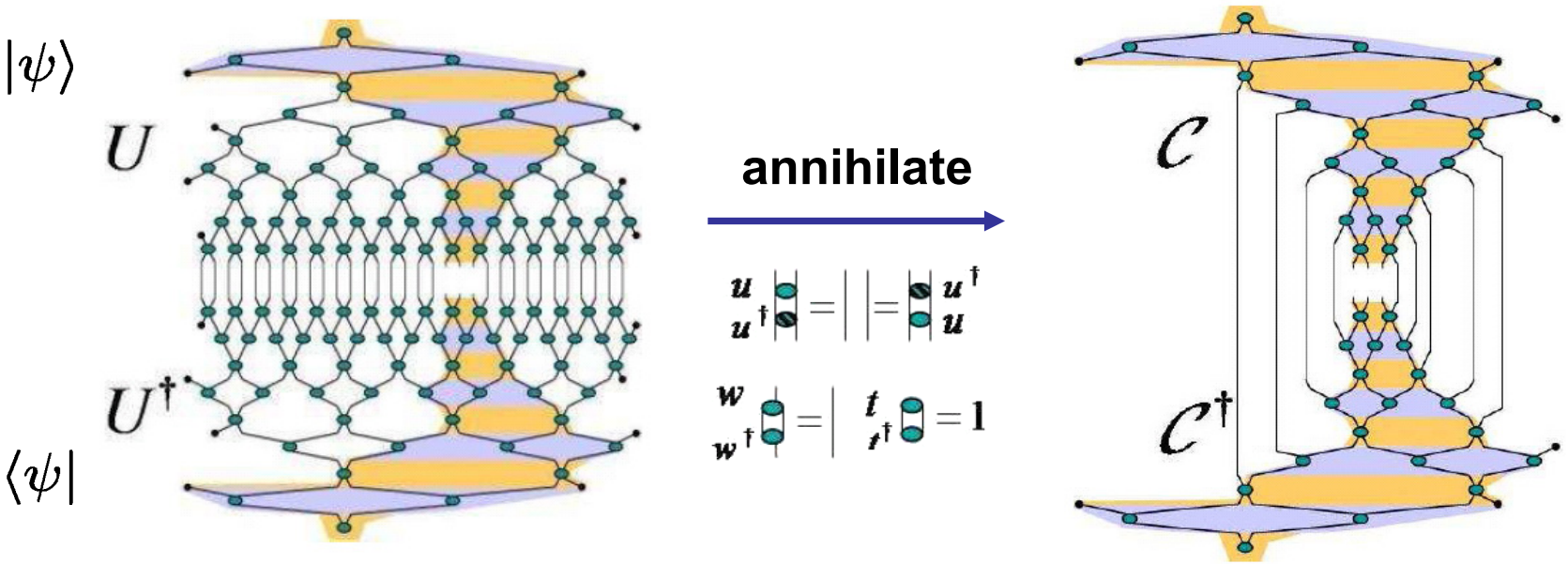
Causal cone has a bounded width due to the isometries.



Contrast this to a simple circuit composed of layers of nearest-neighbour gates. The causal cone spreads back over the entire system.

Efficient contraction of MERA

- The structure of MERA and isometric + unitary properties of the tensors permits reduced density matrices to be computed efficiently:



- Can use these properties to perform variational minimization of the MERA circuit. The scale invariant structure permits violations of the area law and is thus a promising approach to critical systems.

Conclusions and outlook

- **Strongly correlated systems**
  - Remarkably we seem to have found good ways of encoding the physically relevant “corner” of the Hilbert space.
  - In 1D MPS have proven to be extremely accurate:
    - For ground and excited state variational calculations (DMRG)
    - For real and imaginary time-evolution (TEBD)
- **Extensions**
  - Can apply TEBD to incoherent evolution of mixed and thermal states.
  - Can readily extend TEBD to networks with limited tree-width.
- **Generalizations**
  - The PEPS construction naturally generalizes DMRG to 2D systems.
  - Finally the MERA approach provides a physically intuitive renormalization algorithm which can handle a wider – area law violating – class of states.