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Tensor network simulations of strongly correlated quantum systems

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http://www.comlab.ox.ac.uk/activities/quantum/course/

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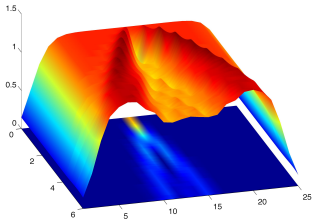
Overview

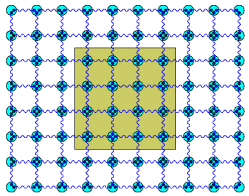
Part I – *Quantum many-body systems*

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



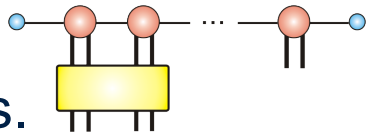
Part II – *Tensor network formalism*

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



Part III – *Extensions and generalizations*

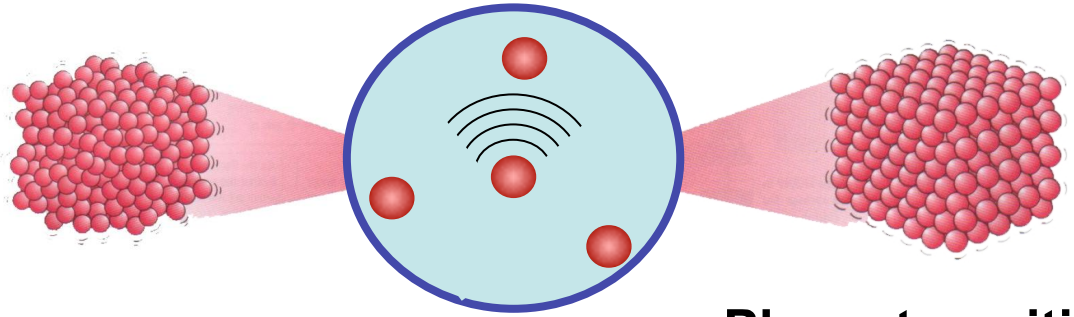
- Simulating tree and network geometries.
- Evolving with mixed states, thermal states and operators.
- Going to 2D systems and beyond.

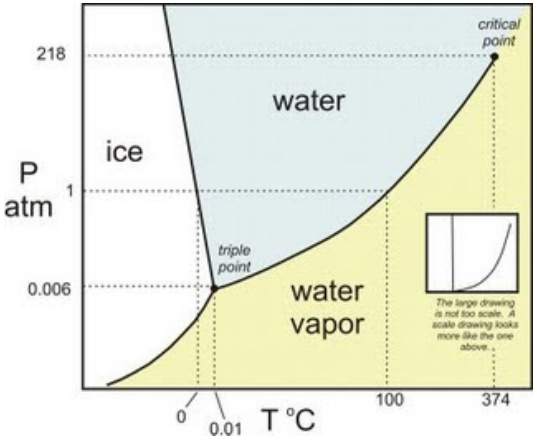


Part I – The many body problem

Consequences of strong correlations …

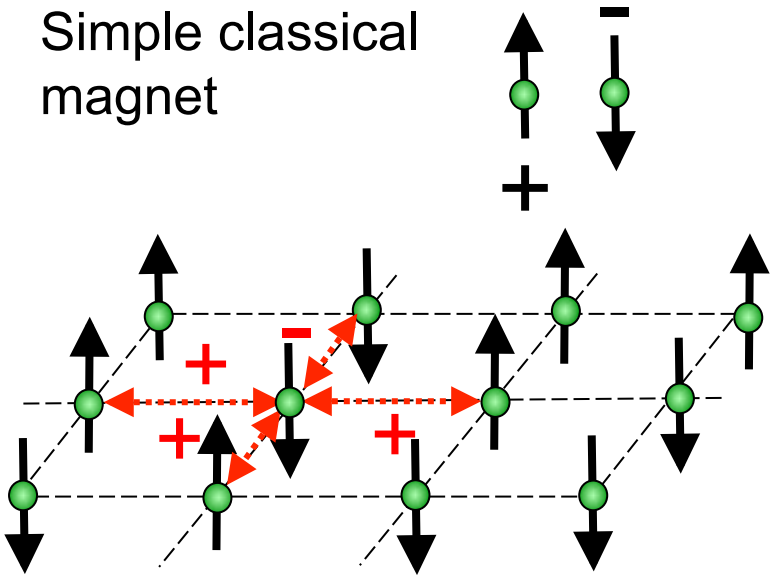
Interplay between interactions and external influences:

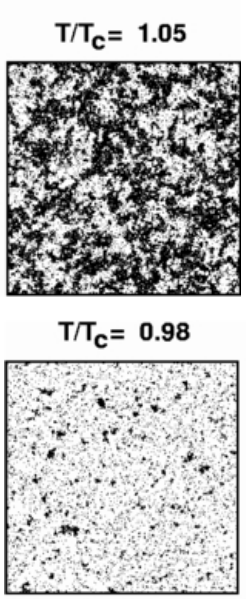


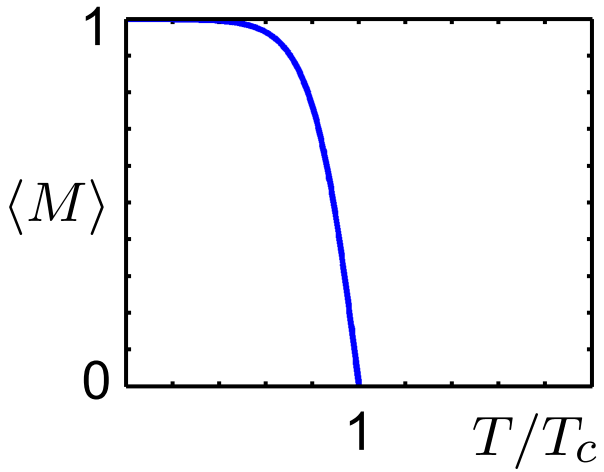


Phase transitions

Simple classical magnet







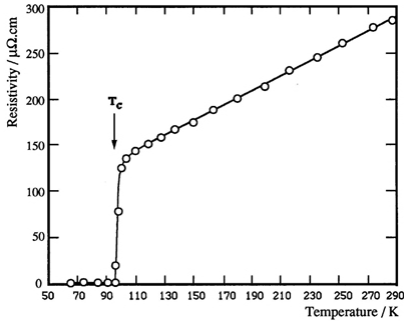
Quantum many body systems

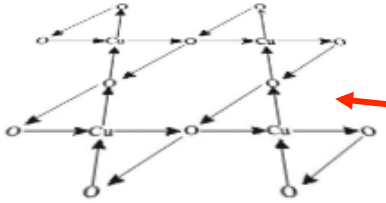
- Major interest in many-body problem focuses on lattice systems.

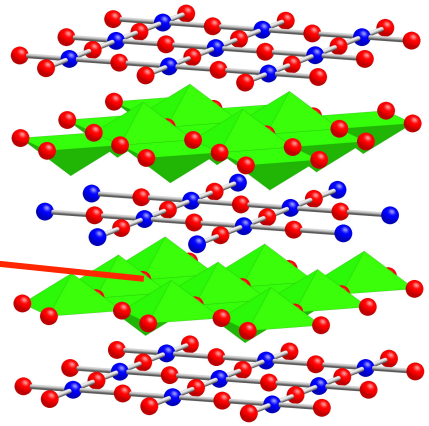
  Understanding quantum properties of electrons in materials:

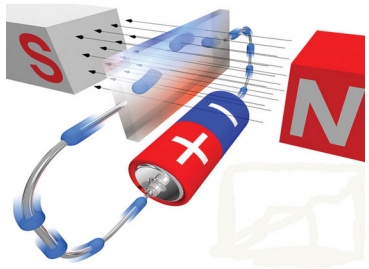
- **High-temperature superconductivity**

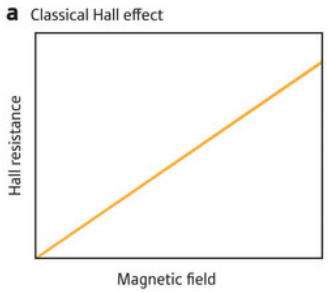
What is the physical mechanism behind it?

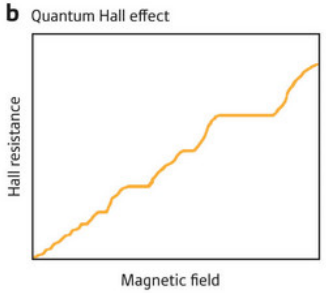










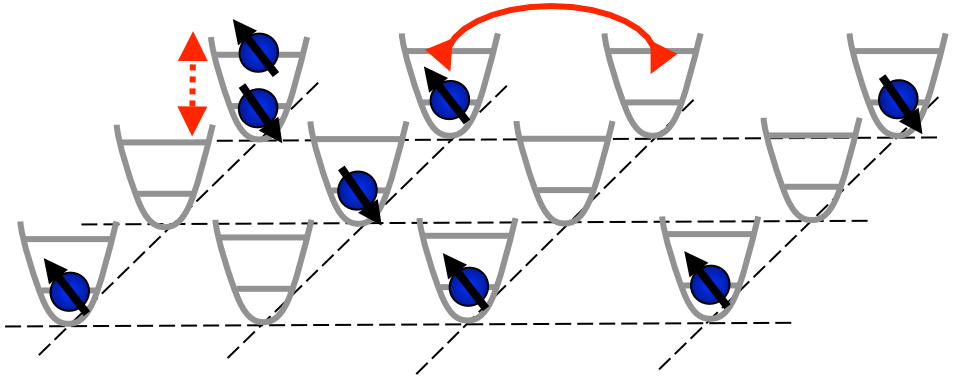


- **Quantum Hall effect**

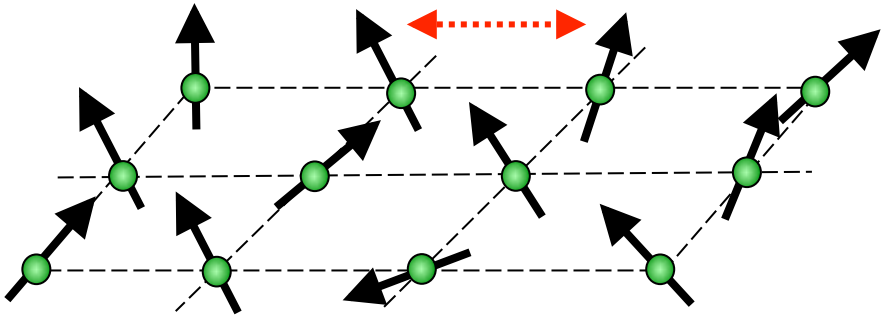
  What are the topological properties of fractional QH states?

Quantum lattice models

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



Hubbard model in 2D



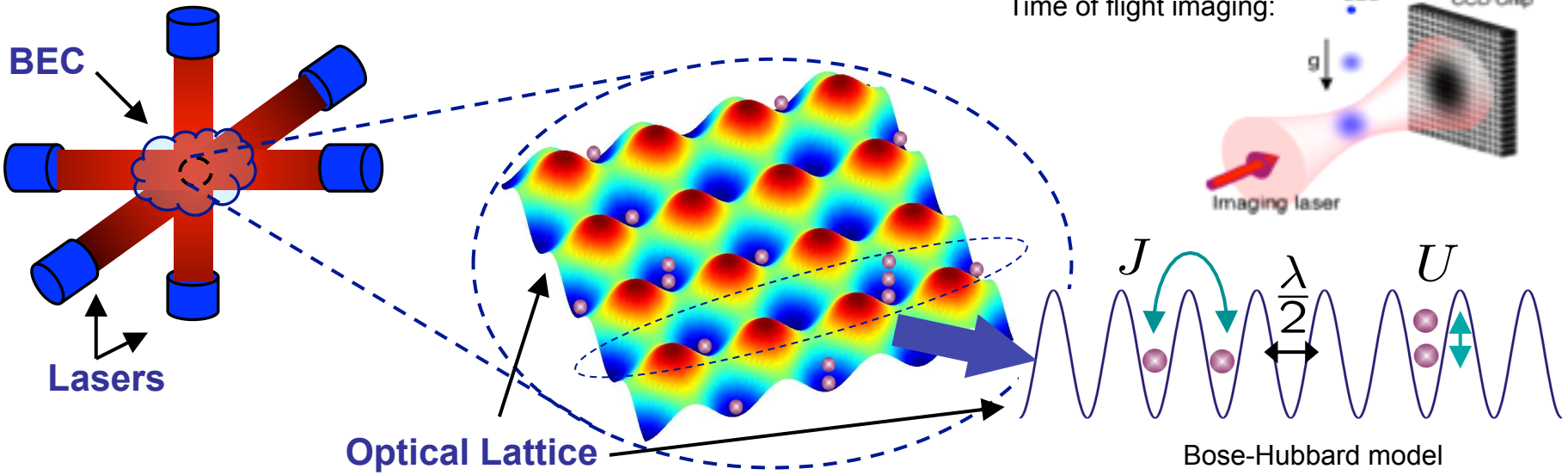
Quantum magnets $H = -\sum_{\langle jk \rangle} \sigma_j^z \sigma_k^z - B \sum_j \sigma_k^x$

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

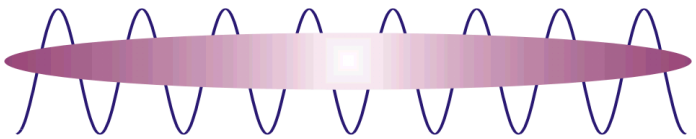
Quantum “wire”

Cold atoms in optical lattices

- Simple models now physically realizable – quantum simulators



Superfluid : $J \gg U$

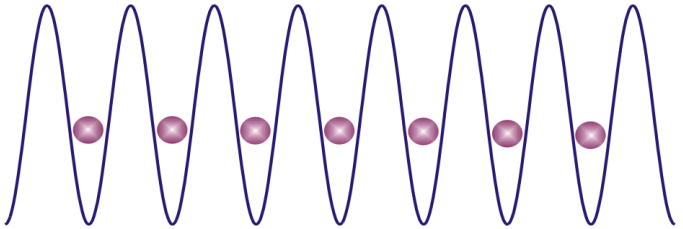


Atoms delocalised over the lattice

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

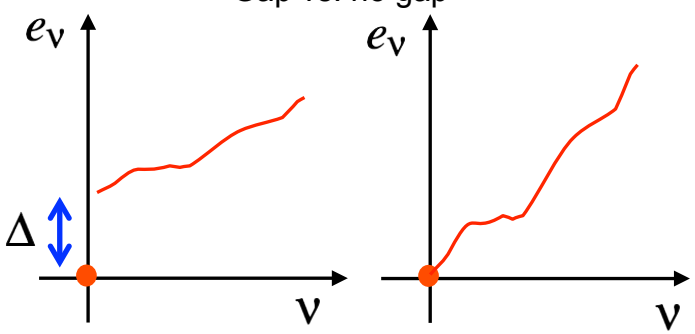
Real eigenvalue - energy

Complex vector

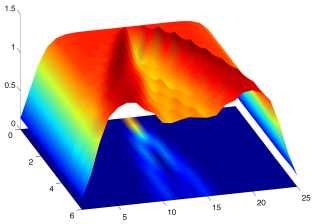
$$\begin{pmatrix} h_{00} & h_{01} & \cdots \\ h_{01}^* & h_{11} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix} = e_\nu \begin{pmatrix} c_0 \\ c_1 \\ \vdots \end{pmatrix}$$

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

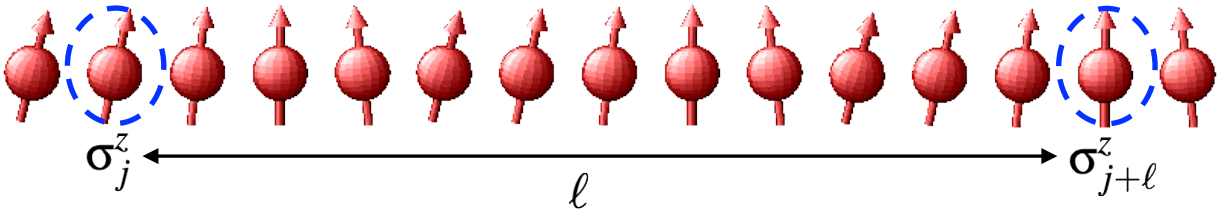
$$|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$$

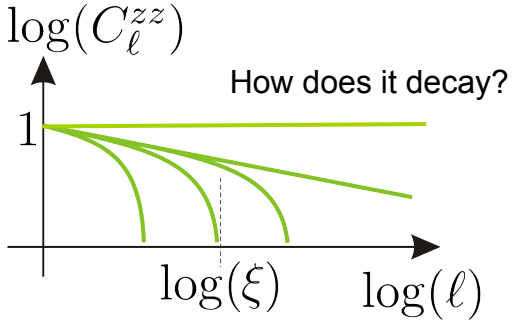
Understanding and manipulating coherent dynamics of quantum systems becoming more important.

Excitations and correlations

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

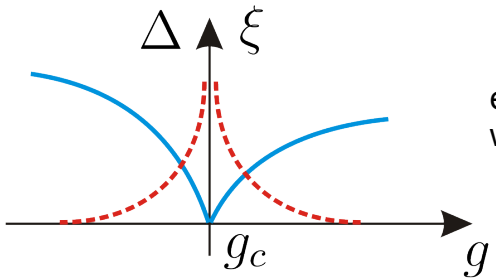
$$C^{zz}_{\ell} = \langle\phi_0|\sigma^z_j\sigma^z_{j+\ell}|\phi_0\rangle - \langle\phi_0|\sigma^z_j|\phi_0\rangle\langle\phi_0|\sigma^z_{j+\ell}|\phi_0\rangle$$





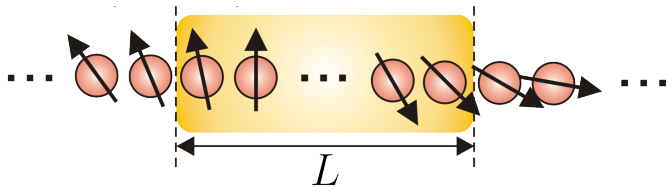
- How does the gap Δ and correlation length ξ depend on an external parameter, like a magnetic field?

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

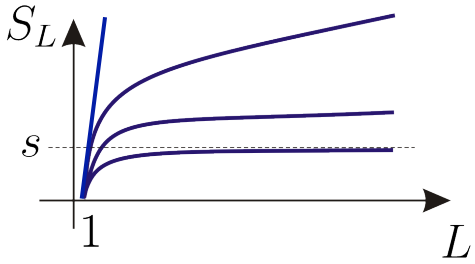


e.g. the Ising model with a transverse field

- Entanglement properties of $|\phi_0\rangle$



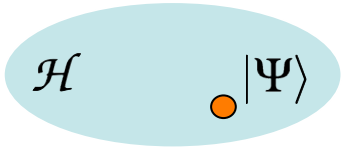
How entangled is a block of **L** spins to the rest of the system?



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**

cfgs = **1024**

But can we solve a more useful ***"small"*** system?

10 x **10**

NO !

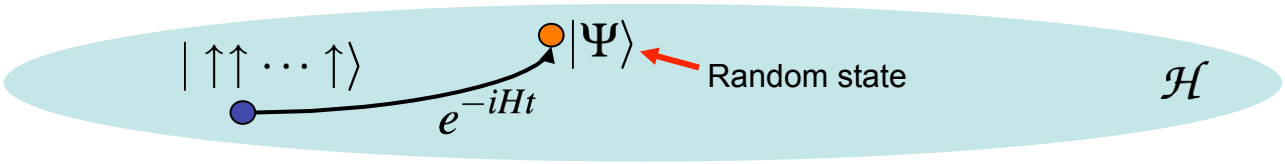
cfgs = **1,267,650,600,228,229,401,496,703,205,376**

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.

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

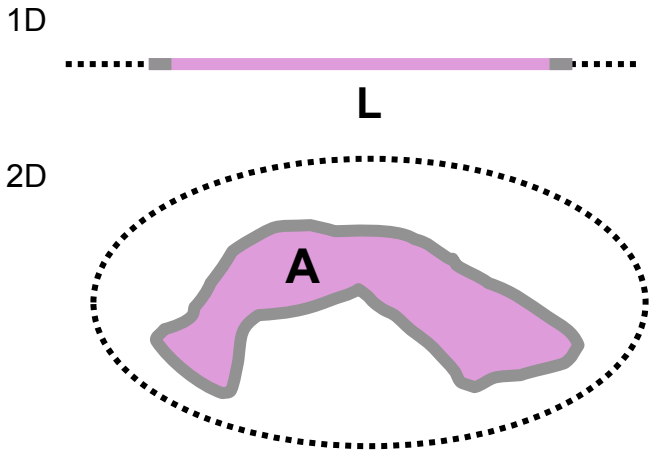
These properties put serious constraints on the states which are accessible and in fact shows that almost all states in are non-physical



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”

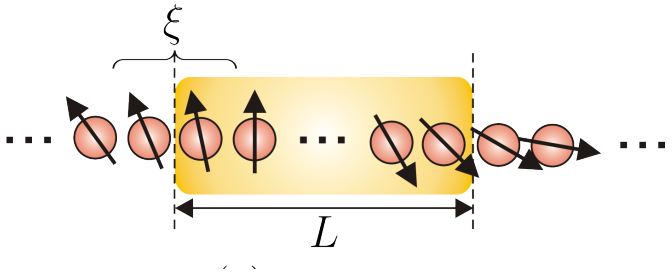
- Conclusion: the fraction of states in this exponentially large Hilbert space that are physical is in fact exponentially small.

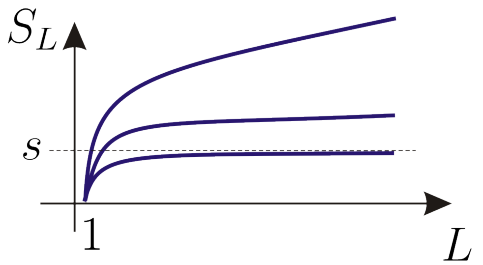


- Ground state and low-lying excitations have very little entanglement …

“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

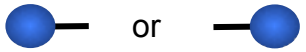
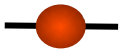
- Interested in quantum lattice problems – numerous applications.
- Simulation of quantum many-body system appears to be exponentially difficult …
- but, nature prefers local few-body interactions,
- so physical states occupy only a small part of the Hilbert space,
- and such systems display an “area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

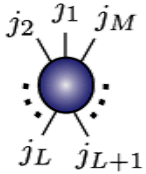
Tensors, contractions and diagrams

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

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

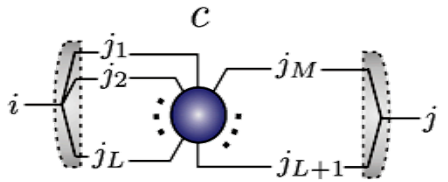
(a)

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



(b)

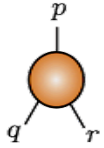
$$C_{ij} =$$



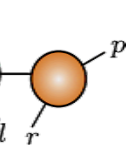
(c)

$$A_{ijkl} =$$

$$B_{pqr} =$$



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

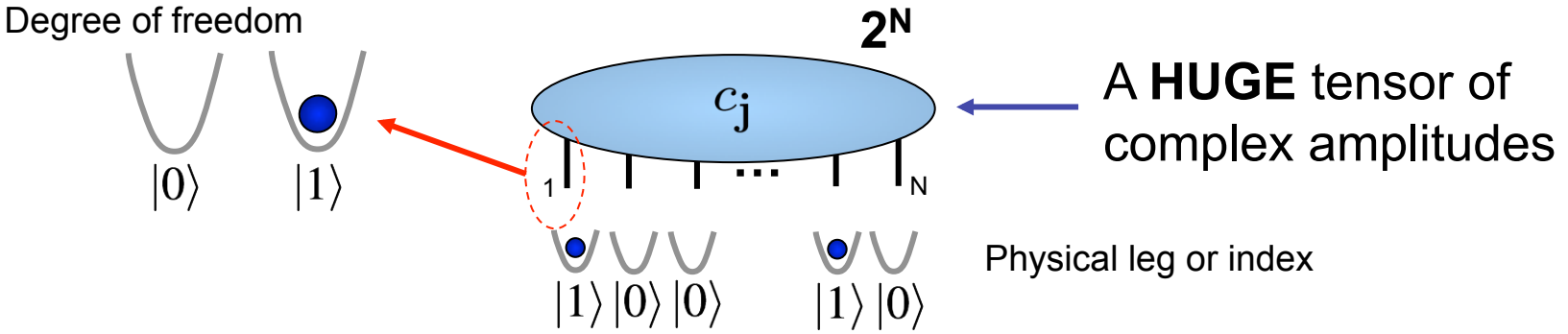


- The essential mathematical content of tensor methods actually boils down to using standard methods from linear algebra of matrices.

Aim of tensor methods in a nutshell

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

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



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

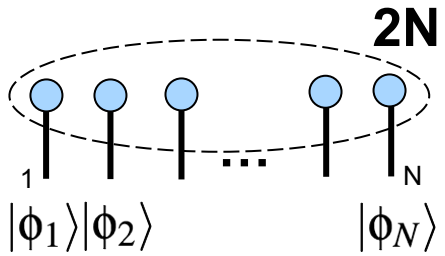
Primary aim = encode with a polynomial number of parameters.

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

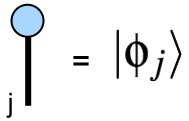
- The simplest approach possible is to describe each site (physical leg) by its own **independent** tensor



Equivalent to a product state approximation.

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

Rank 1 tensor gives an state for each site

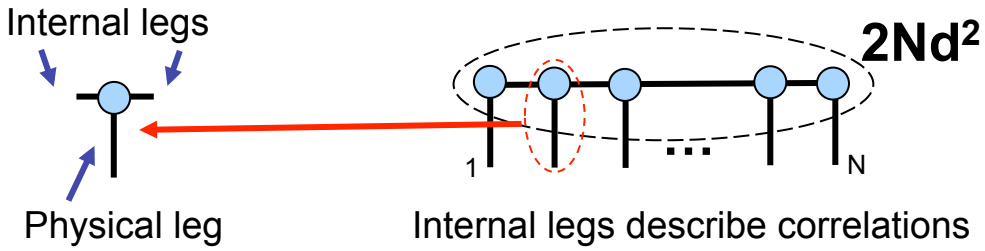


This approach is a very common technique called **mean-field theory**.

[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**.



Internal legs describe correlations

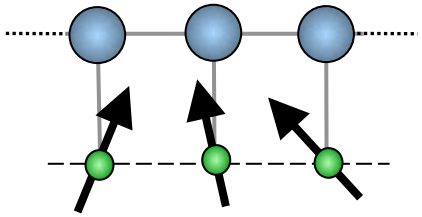
Contract all internal legs to form a comb network.

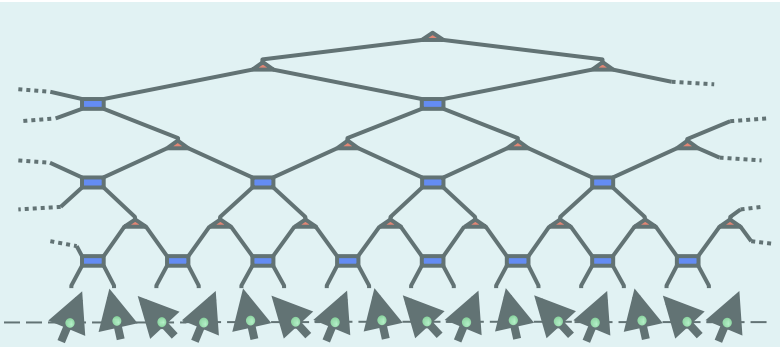
Manifestly 1D network geometry.

A zoo of tensor networks

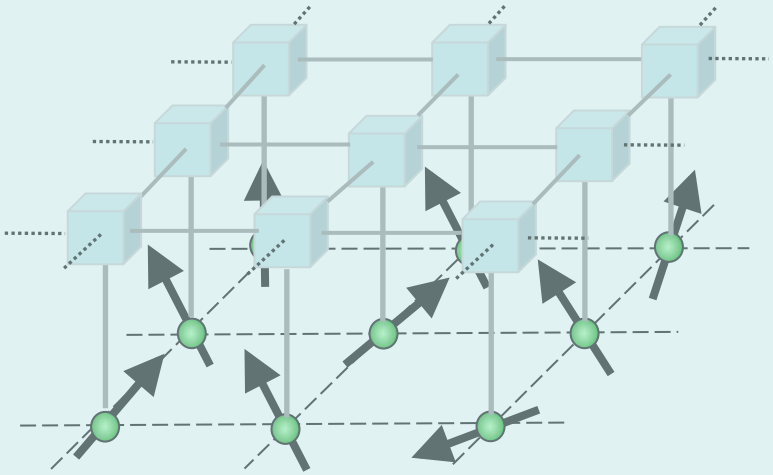
Can physically motivate a variety of tensor networks structures:

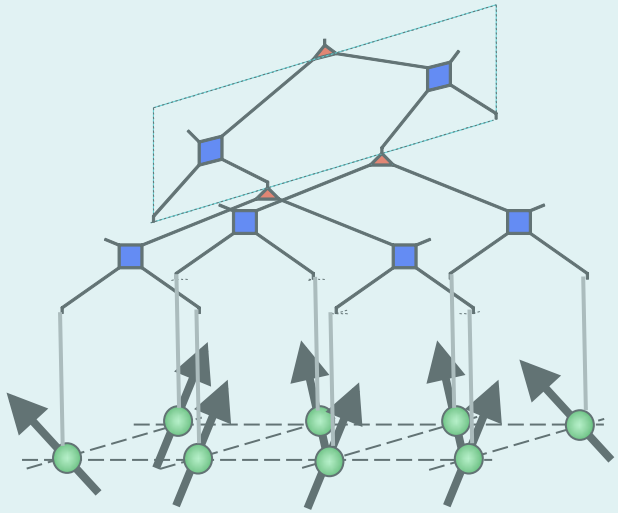
1-D





2-D



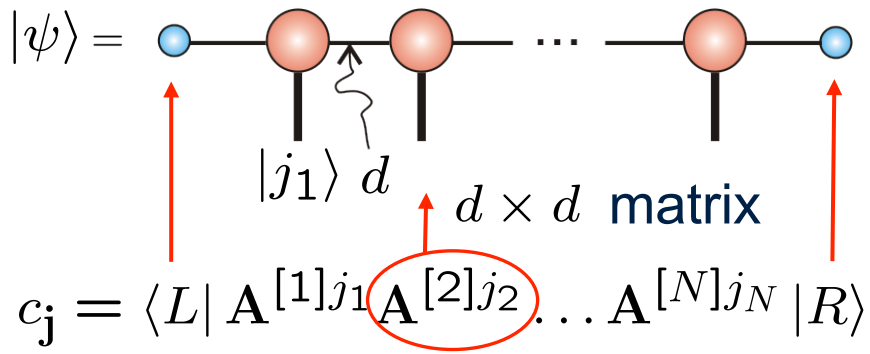


All aim to provide accurate near-lossless compression of physical states.

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:

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



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) $d = 1$ $\quad |\psi\rangle = |\phi\rangle \otimes |\phi\rangle \otimes \cdots$

A **1 x 1** "matrix" for each local state $\quad \mathbf{A}^{\uparrow} = \alpha \quad \mathbf{A}^{\downarrow} = \beta$ $\quad |\phi\rangle = \alpha |\uparrow\rangle + \beta |\downarrow\rangle$

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: $\mathbf{A}^{\uparrow} = \sigma^{+}$ $\mathbf{A}^{\downarrow} = \sigma^{-}$ 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:

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

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

Use matrices: $\mathbf{A}^{\uparrow} = \frac{1}{2}(\mathbb{1} + \sigma^{z})$ $\mathbf{A}^{\downarrow} = \frac{1}{2}(\mathbb{1} - \sigma^{z})$ 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:

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

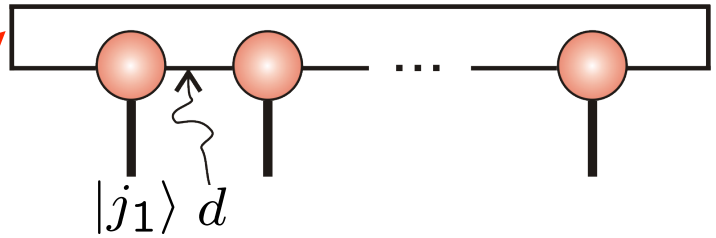
Boundary vectors select the bottom left state.

Translational invariance and PBC

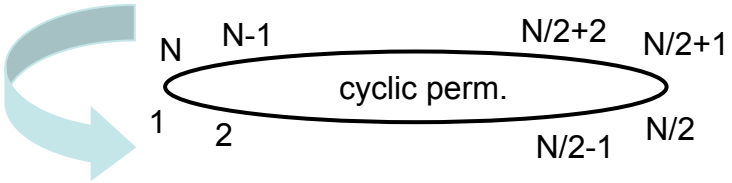
- We could have formulated our comb-like tensor network slightly differently by joining the two boundary legs together as:

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

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).



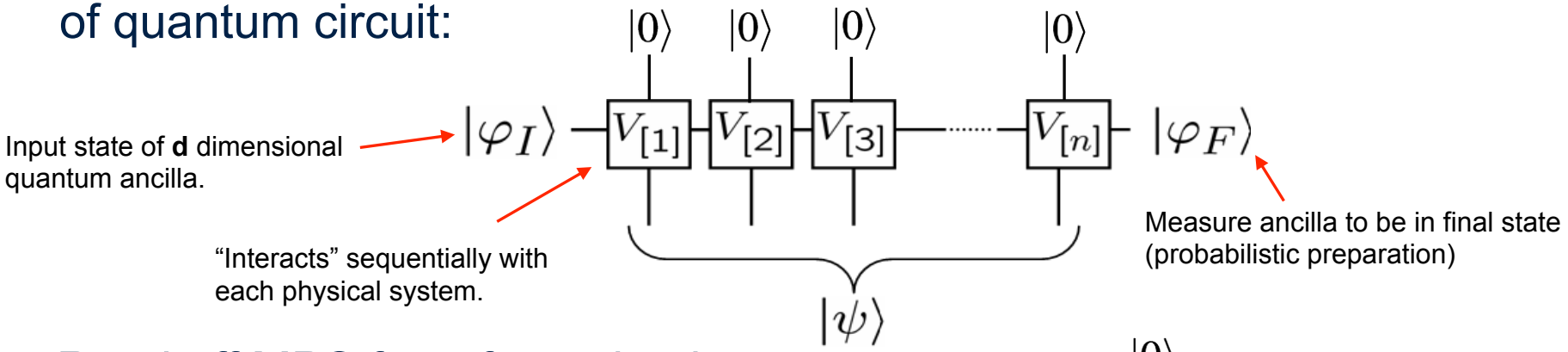
Given identical **A** matrices for all sites then the state is manifestly translationally invariant.

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 …

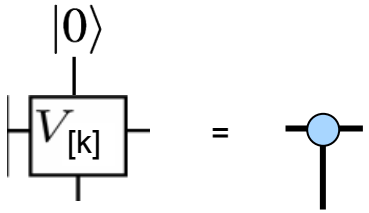
Sequential generation of an MPS

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



- Read off MPS form from circuit:

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

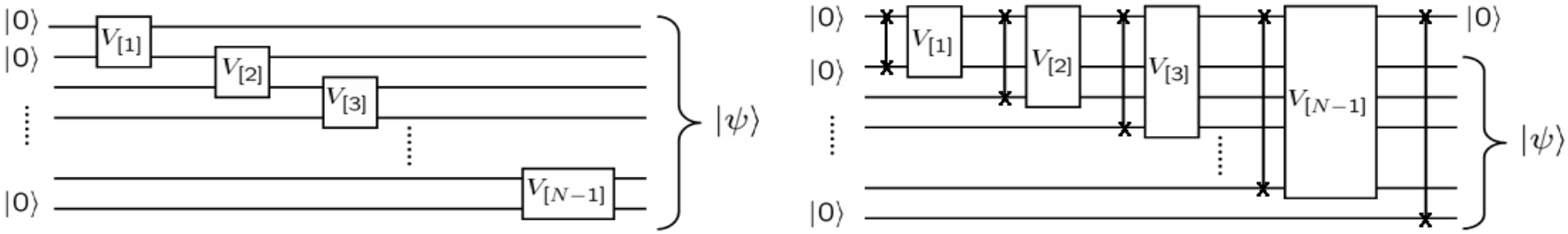


- Can enforce w.l.o.g. unitary interactions **V** and decoupling of the ancilla at the end, i.e. no measurement so deterministic preparation.

- 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:

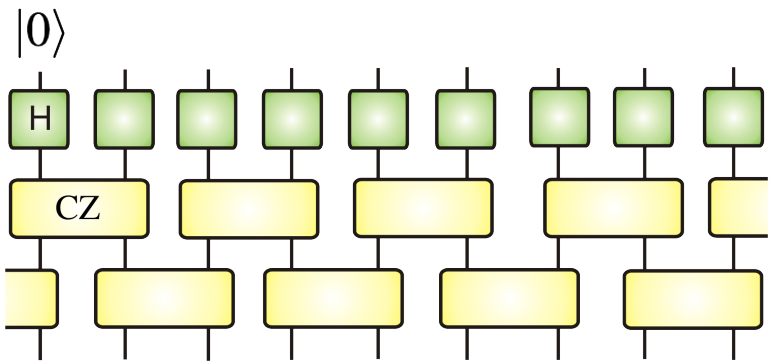


- Such states are in fact **d** = 2 MPS since the circuit is equivalent to a sequential preparation with a qubit ancilla.

Another example – **1D cluster state**

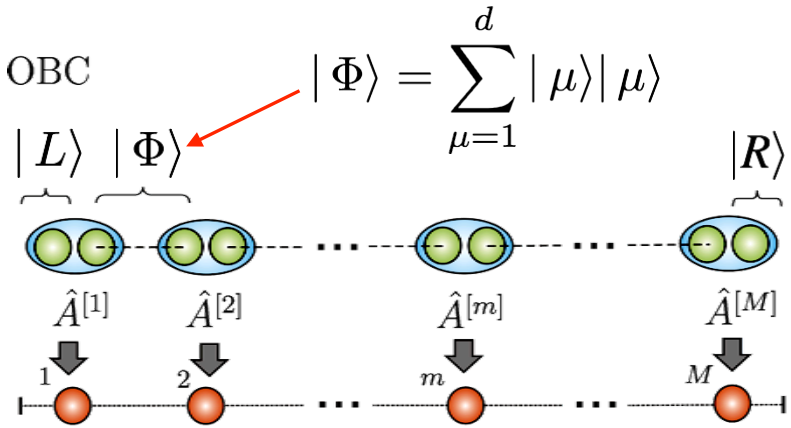
Can rearrange circuit as a staircase thus it has **d** = 2. Read-off matrices.

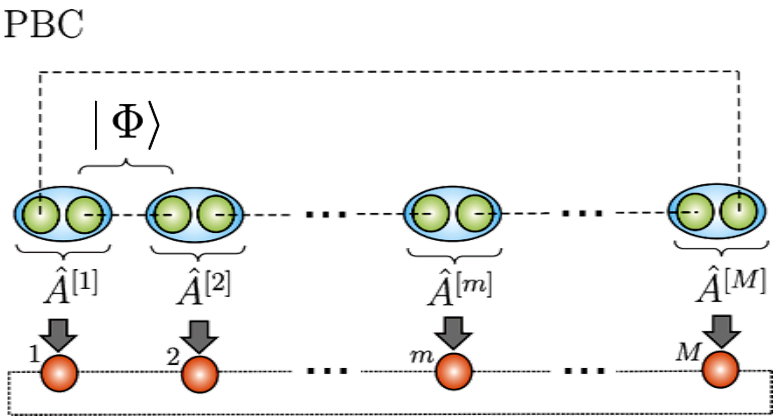
Exercise for the audience …



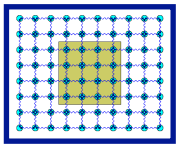
MPS from Projected Entangled Pairs

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

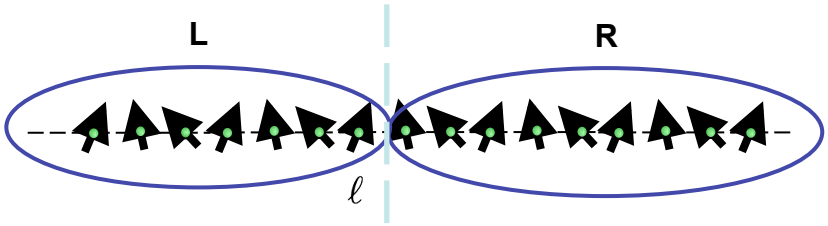


- Shows that MPS obey an area law by construction. The entanglement of any block limited by the ancillae dimension d

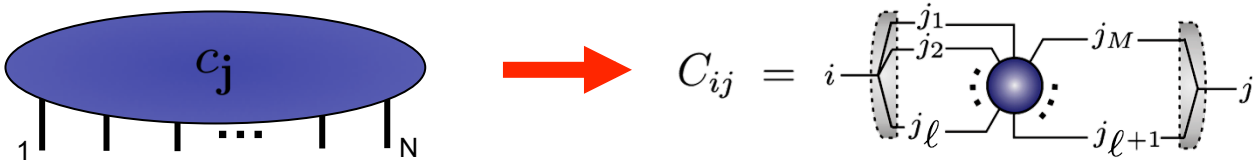
Schmidt decomposition

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

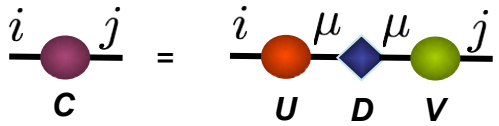
Suppose we split the system into two pieces after site ℓ :



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:

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

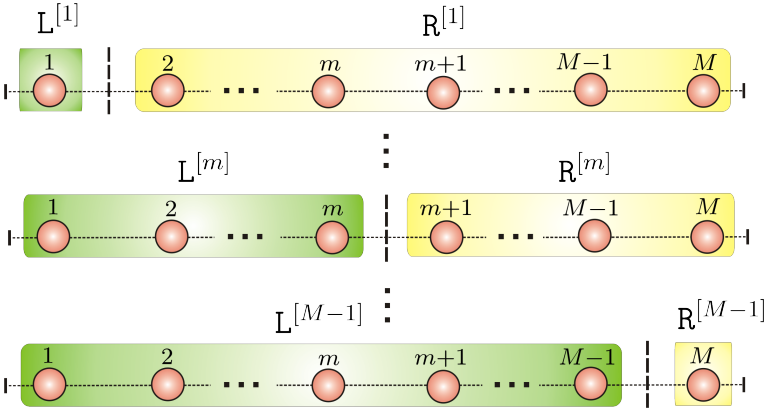
$$|\mathrm{L}^{[2]}_{\mu_2}\rangle = \sum_{i_2} \sum_{\mu_1=1}^{r_1} A^{[2]i_2}_{\mu_1\mu_2} |\mathrm{L}^{[1]}_{\mu_1}\rangle |i_2\rangle$$

$$\vdots$$

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

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

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



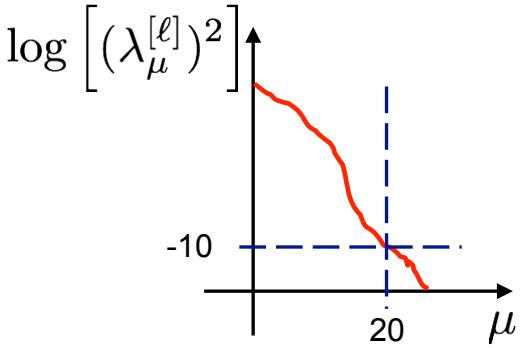
Recursively expand *left* Schmidt states.

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

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.

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