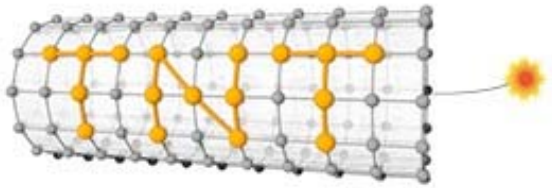

Tensor Network Theory

An introduction to DMRG and MPS methods

Quantum and Kinetic Problems: Modeling, Analysis, Numerics and Applications
IMS Singapore

Dieter Jaksch

University of Oxford

Special thanks to: Stephen Clark, University of Bristol

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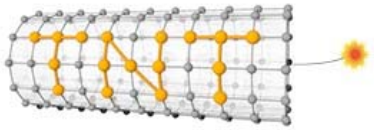


Outline of lectures

- Lecture 1

Introduction to strong correlations, many-body problem, recap on essential linear algebra we will need later.

- Lecture 2

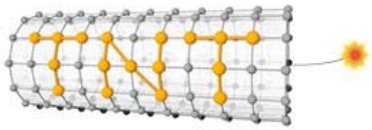
Tensors and contractions, product states and variational principle, matrix product states (MPS), and their entanglement properties.

- Lecture 3

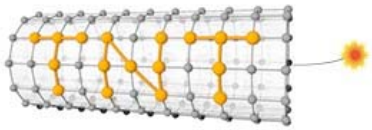
The “calculus” of MPS, algorithms for their variational optimisation, and algorithms for time-evolution of MPS.

- Lecture 4

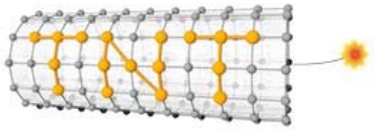
Moving to finite temperatures, renormalisation approaches to tensor networks, extension to 2D with projected entangled pairs.



Lecture 2



1: Tensors and contractions



Tensors

For us a “tensor” is nothing more than a multi-dimensional array of complex numbers. The number of indices an array has is called its “rank”. Simplest tensors includes the very familiar …

rank 0 = scalars

$$a$$

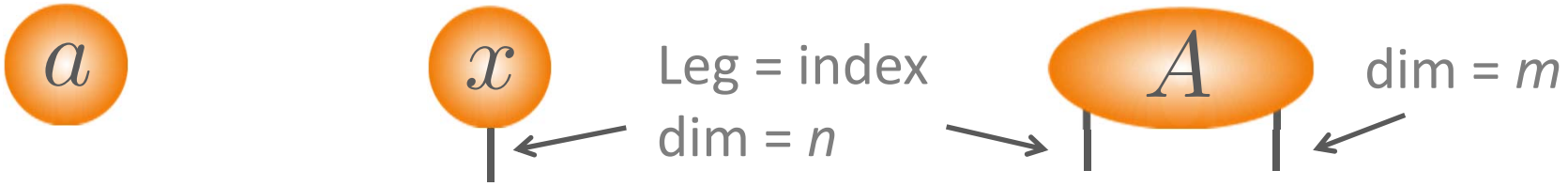
rank 1 = vectors

$$\vec{x} \rightarrow \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}$$

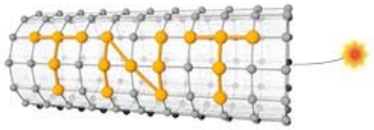
rank 2 = matrices

$$\mathbf{A} \rightarrow \begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n} \\ A_{21} & A_{22} & \cdots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \cdots & A_{mn} \end{pmatrix}$$

Introduce a diagrammatic notation – “blobs and sticks”:

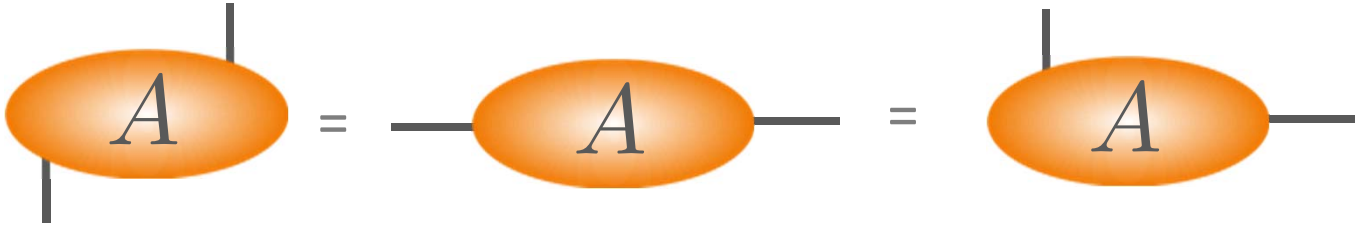


Each leg of a tensor has a certain dimension, i.e. range of the index.



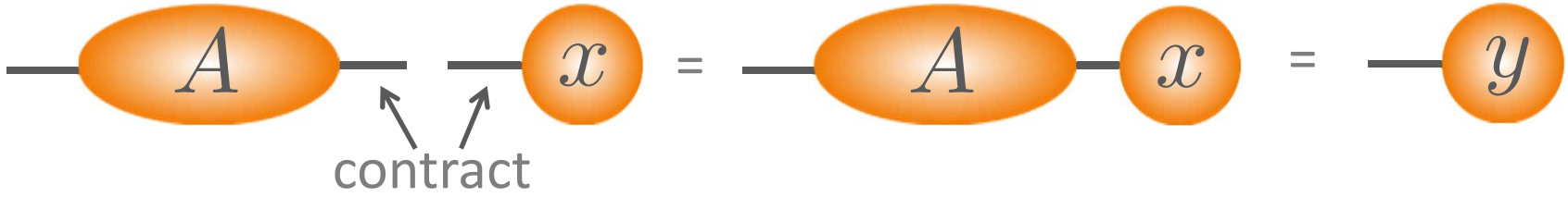
Tensors

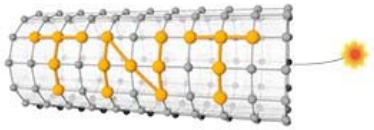
We won't be too concerned about how we precisely draw tensors:



However, we need to keep track of which leg is which and may label them or introduce a convention. For example:

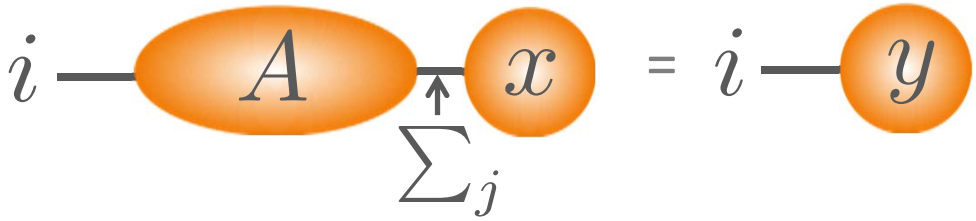
Contraction: We can join tensors together by "contracting" legs together which are of the same dimension:





Tensors

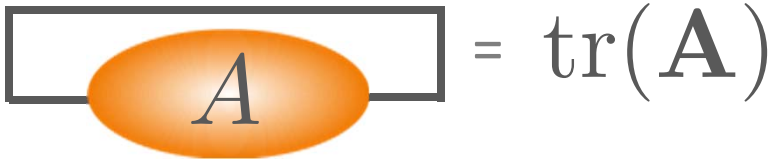
Contraction means multiply elements and sum. So in terms of tensor elements this contraction is simply:

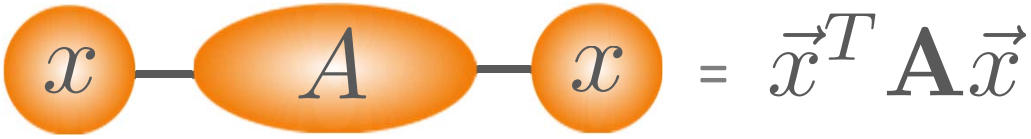


$$\sum_j A_{ij} x_j = y_i$$

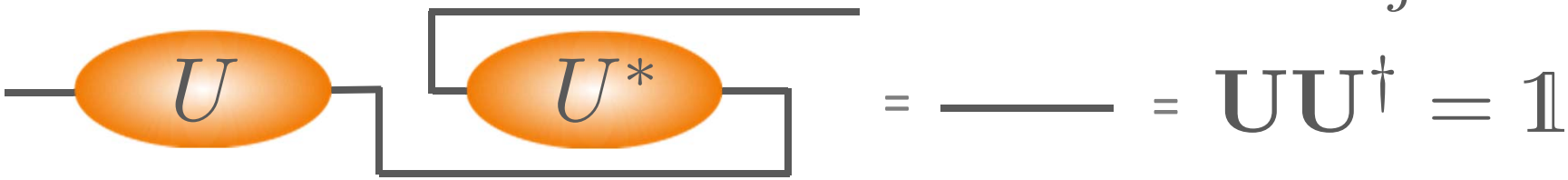
or $\mathbf{A}\vec{x} = \vec{y}$

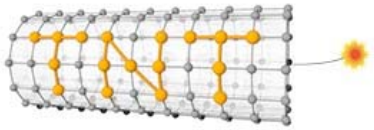
i.e. it reduces to matrix-vector multiplication. Likewise other linear algebra operations have diagrams:





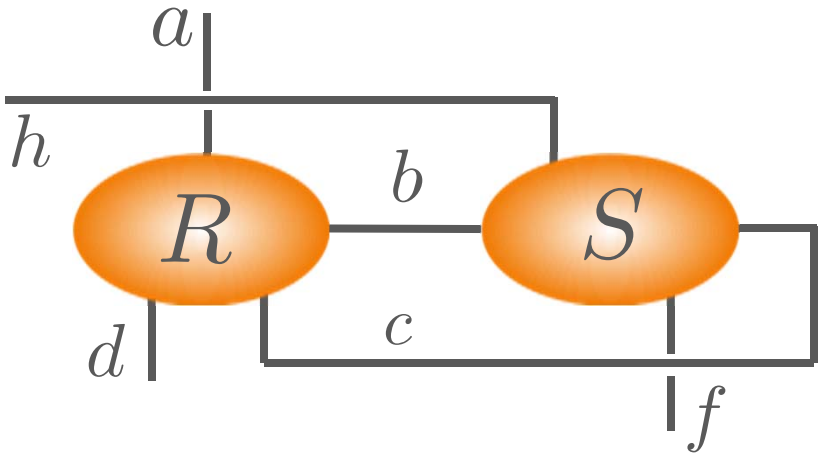
$= A_{ij}$





Tensors

All of this generalises naturally to higher rank tensors. Consider the contraction of two rank-4 tensors:



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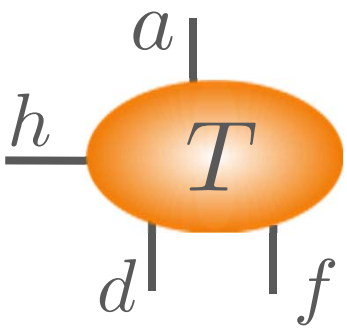


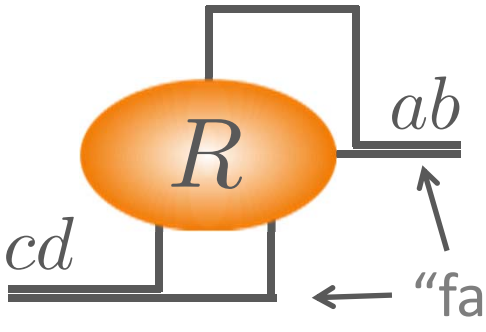
or explicitly …

$$T_{adfh} = \sum_{bc} R_{abcd} S_{bcfh}$$

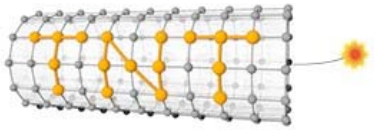
We will also often “reshape” tensors to lower or higher rank by combining or splitting legs.

Reshape rank-4 tensor into a matrix:

MATLAB command `reshape(…)`

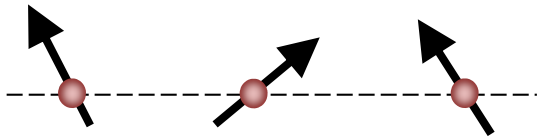


← “fat” indices



Tensors

Quantum states give a concrete (very relevant) example of higher rank tensors. Take three spin-$^1/_2$ particles:



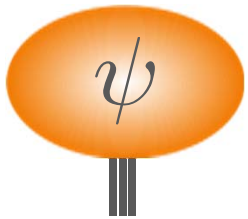
$$|\psi\rangle = c_1|\uparrow\uparrow\uparrow\rangle + c_2|\downarrow\uparrow\uparrow\rangle + c_3|\uparrow\downarrow\uparrow\rangle + c_4|\downarrow\downarrow\uparrow\rangle + c_5|\uparrow\uparrow\downarrow\rangle + c_6|\downarrow\uparrow\downarrow\rangle + c_7|\uparrow\downarrow\downarrow\rangle + c_8|\downarrow\downarrow\downarrow\rangle$$

Conventionally we represent this state as a vector, but can reshape:

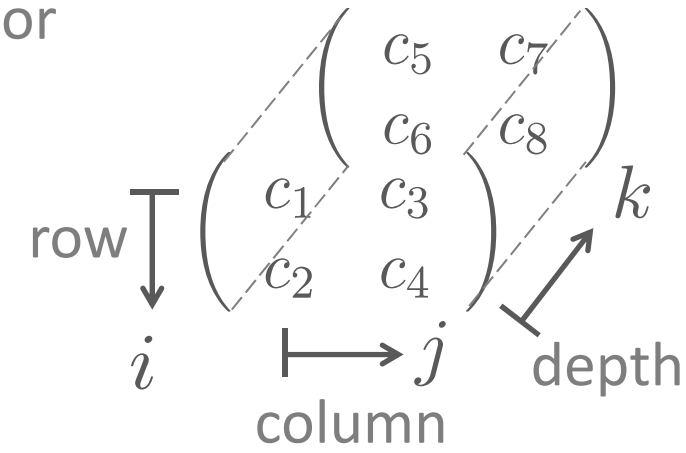
$2^3 \times 1$ vector

$$\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ c_7 \\ c_8 \end{pmatrix}$$

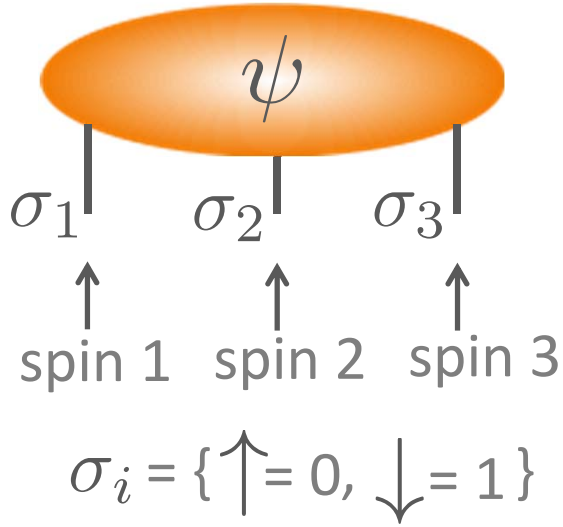
rank-1 tensor



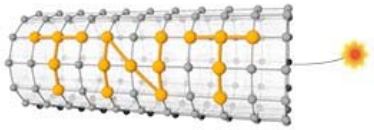
$2 \times 2 \times 2$ array



rank-3 tensor



$\sigma_i = \{\uparrow = 0, \downarrow = 1\}$

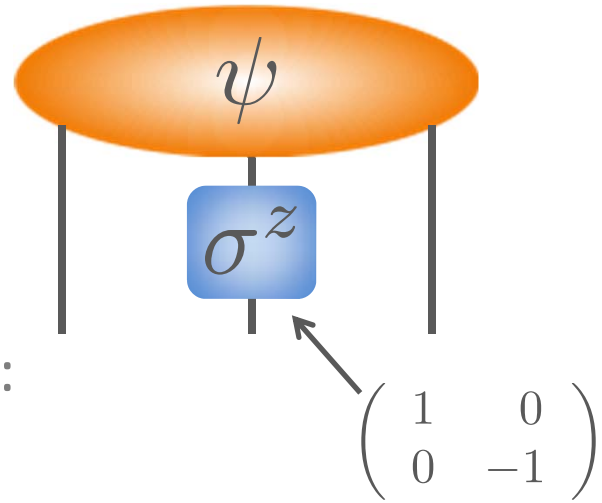


Tensors

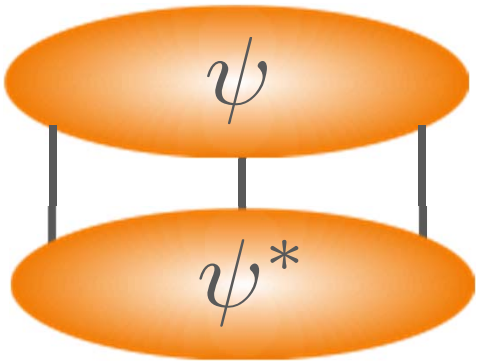
A tensor representation exposes each degree of freedom. Many QM calculations have simple diagrams …

apply operator on spin 2:

$$\mathbb{1} \otimes \sigma^z \otimes \mathbb{1} |\psi\rangle =$$

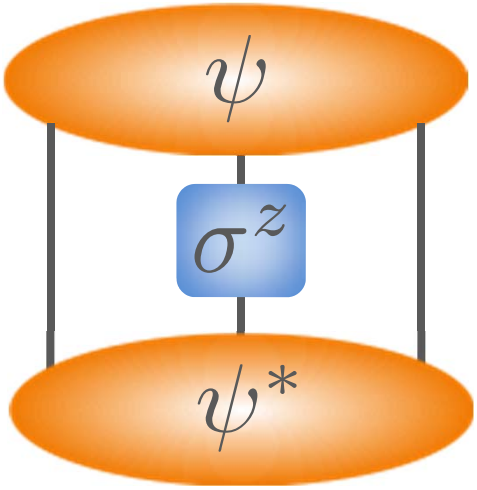


compute norm:



$= \langle\psi|\psi\rangle$

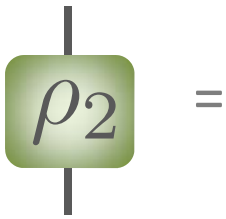
compute expectation value:



$= \langle\psi|\mathbb{1} \otimes \sigma^z \otimes \mathbb{1}|\psi\rangle$

compute reduced density matrix:

$$\rho_2 = \mathrm{tr}_{13}(|\psi\rangle\langle\psi|) =$$



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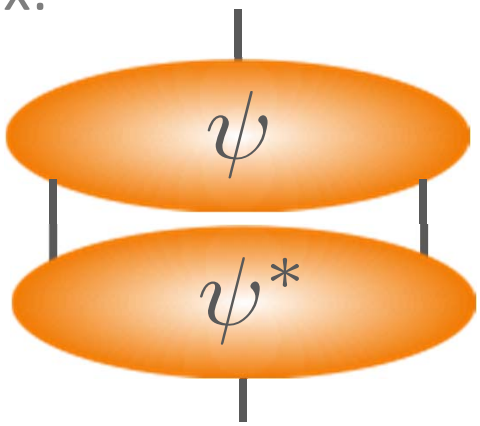
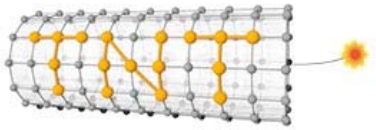
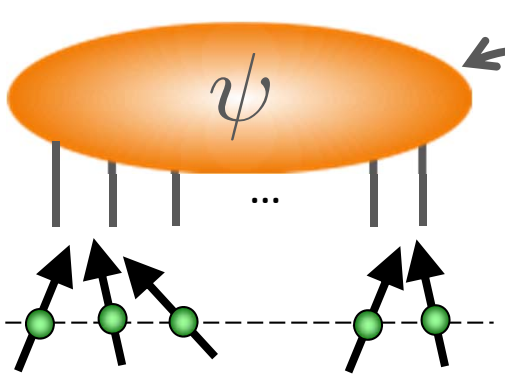




Our problem restated …

What about *N* spins? Now represented by a rank-*N* tensor:



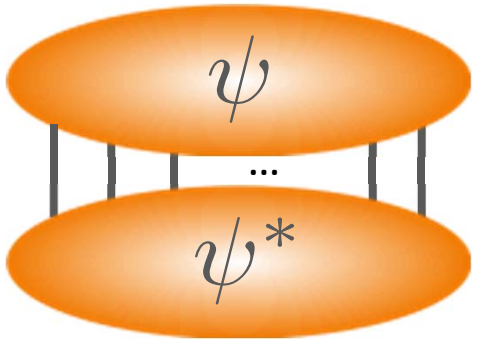
$$|\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots,\sigma_N} \psi_{\sigma_1,\sigma_2,\ldots,\sigma_N} |\sigma_1,\sigma_2,\ldots,\sigma_N\rangle$$

tensor contains 2^N complex numbers!

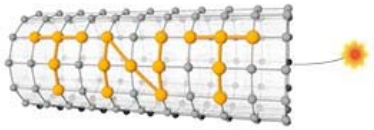
Since ψ is a **structureless** tensor any calculation we perform is forced to operate on exponentially many elements …

The *"curse of dimensionality"* again

Even computing the norm is $\mathcal{O}(2^N)$

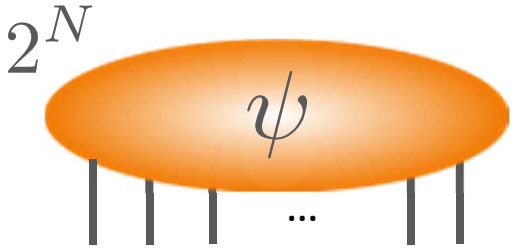


Punch line – we have to factorise this tensor into a network of smaller tensors with a physically motivated structure …



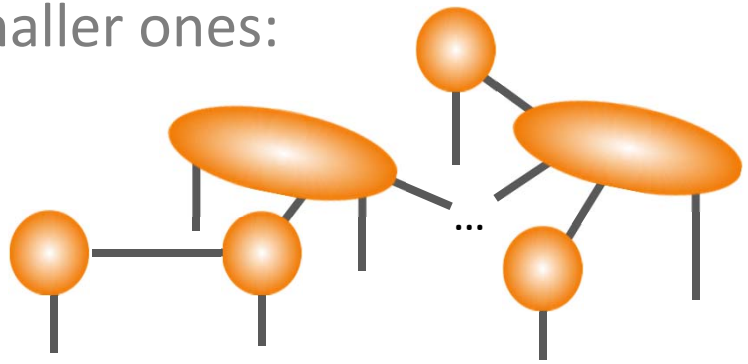
Our approach …

We are confronted with an intractable problem because our tensor for an arbitrary state is *structureless* = exponentially large.



Physical states have structure (see shortly) – so we want to break-up this tensor into a network of smaller ones:

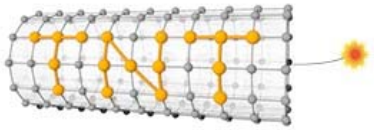
Contract pieces together to build a state:



Can we accurately encode physical states into such networks with only a number of parameters that grows only polynomially with *N*?

But even with this we also need to be able to:

- find and time evolve our representation **efficiently**
- and then be able to **efficiently** calculate observables from it

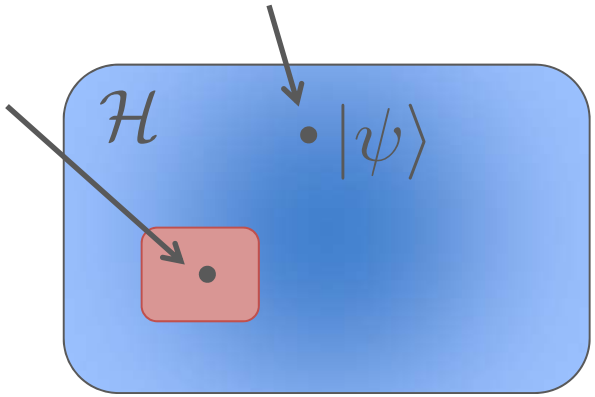


Physical states

One might question whether our goal is even possible in principle – why should we be able to encode states so compactly?

Random states in Hilbert space are clearly not compressible.

However, we're interested in *physical* states, i.e. those arising as stationary states of lattice Hamiltonians with short-range 2-body interactions, like:



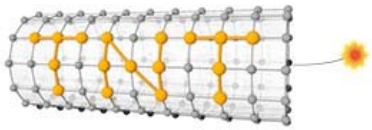
$$\hat{H} = J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + B \sum_i \sigma_i^x$$

Since $\hat{H}$ is specified by a polynomial number of parameters in *N* a thermal states appears efficient:

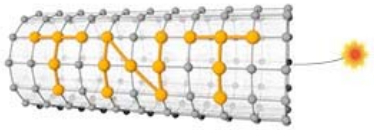
$$\rho_\beta = \frac{1}{Z} e^{-\beta \hat{H}}$$

Alas, we can't efficiently evolve or compute observables from this.

We'll characterise physical states in more detail later …



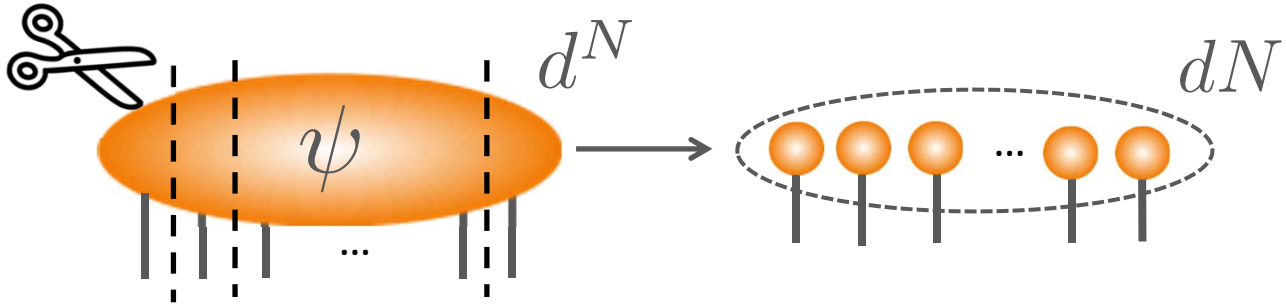
2: Product states



Simplest tensor network

Let's start by taking to approach to its most extreme limit:

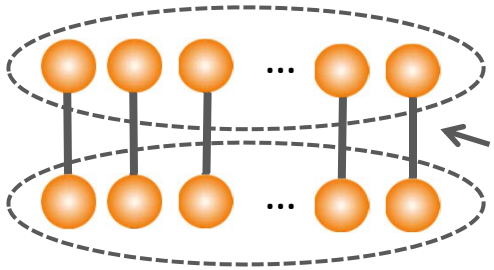
Slice up tensor into *N* pieces:



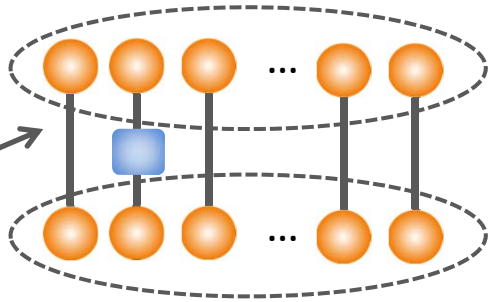
Since  = $|\varphi_j\rangle$ this gives $|\psi\rangle = |\varphi_1\rangle \otimes |\varphi_2\rangle \otimes \cdots \otimes |\varphi_N\rangle$

This is a *product* state – it clearly **cannot** be exact. Parameter counting shows that we have gone from d^N to just dN amplitudes.

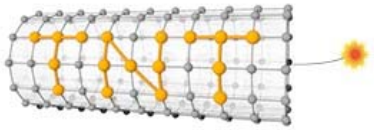
Yet, this quantum state origami makes calculations trivially easy:



usually normed = 1

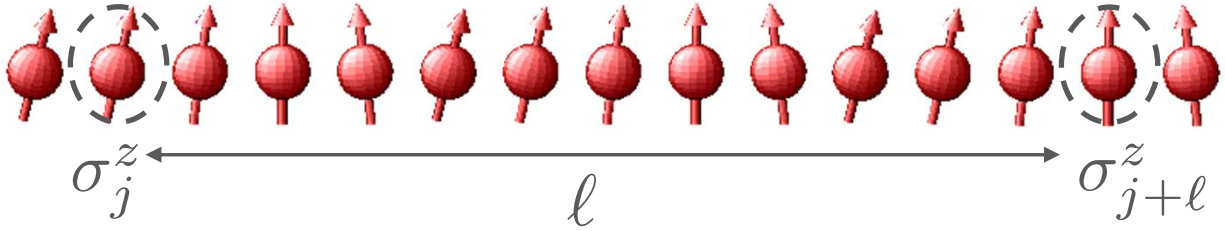


$\langle\psi|\psi\rangle = \prod_j \langle\varphi_j|\varphi_j\rangle$ $\quad$ $\langle\sigma_2^z\rangle = \langle\varphi_2|\sigma_2^z|\varphi_2\rangle \prod_{j\neq 2}\langle\varphi_j|\varphi_j\rangle$



Product state ansatz

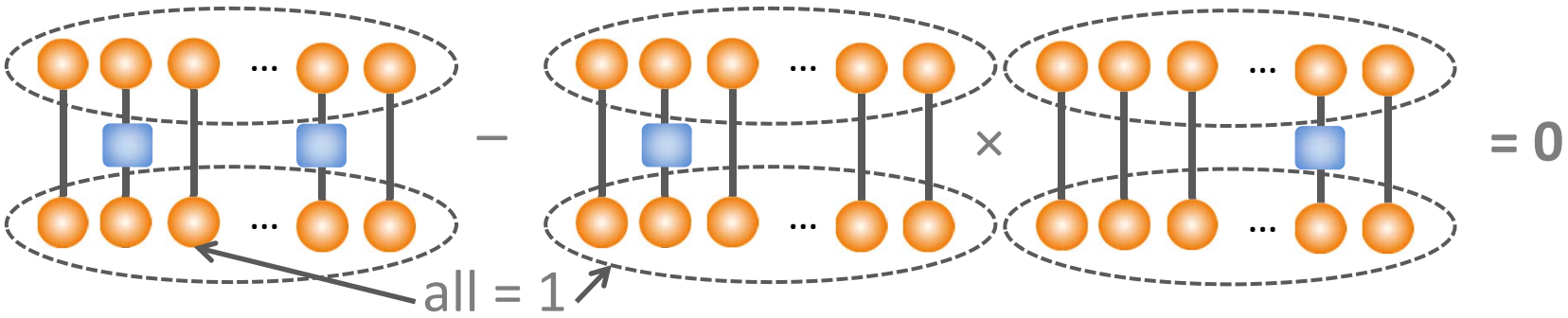
However, this also shows that product states are very crude.
Consider long-ranged correlations along a spin-chain:

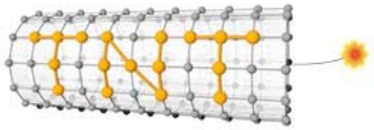


We quantify the quantum correlation by computing:

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

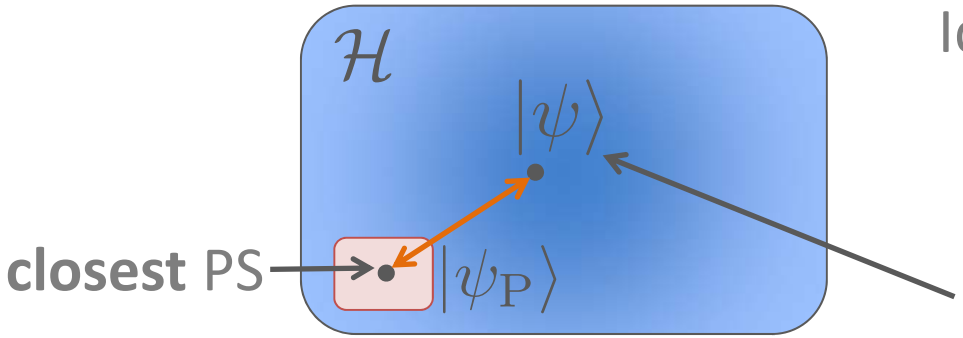
But for product states this can never be anything but zero …





Computing the ground state

Product states are a very commonly used approximation. So how do we find the "best" or "closest" such state to the exact ground state?



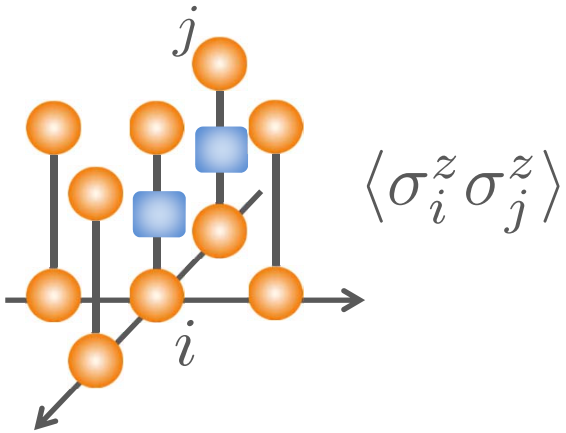
Ideally we would want to find:

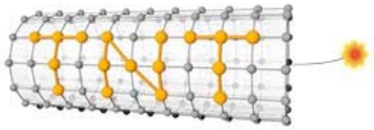
$$\min \left| \left| |\psi\rangle - |\psi_{\mathrm{P}}\rangle \right| \right|_2$$

The problem is we **don't** know the exact GS. But we do know the Hamiltonian it comes from. For example an Ising spin system:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + B \sum_j \sigma_j^z$$

and we can easily compute its expectation value for PS independent of dimension:

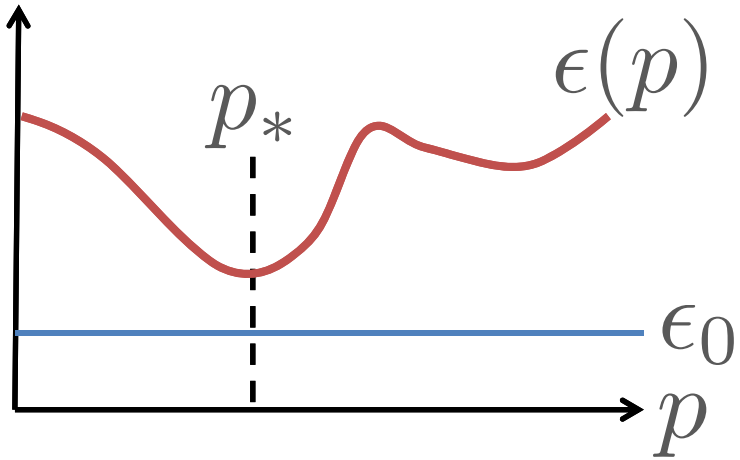




Variational principle

For this reason our strategy for finding the best product state approximation will be to apply the variational principle:

Compute: $\epsilon(p) = \dfrac{\langle\psi(p)|\hat{H}|\psi(p)\rangle}{\langle\psi(p)|\psi(p)\rangle} \geq \epsilon_0$ upper-bounds exact GS energy

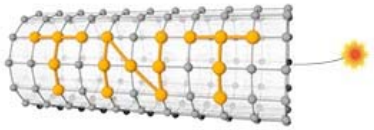


Then minimise over parameter(s):

$$\epsilon_{\text{est}} = \epsilon(p_*) = \min_p \epsilon(p)$$

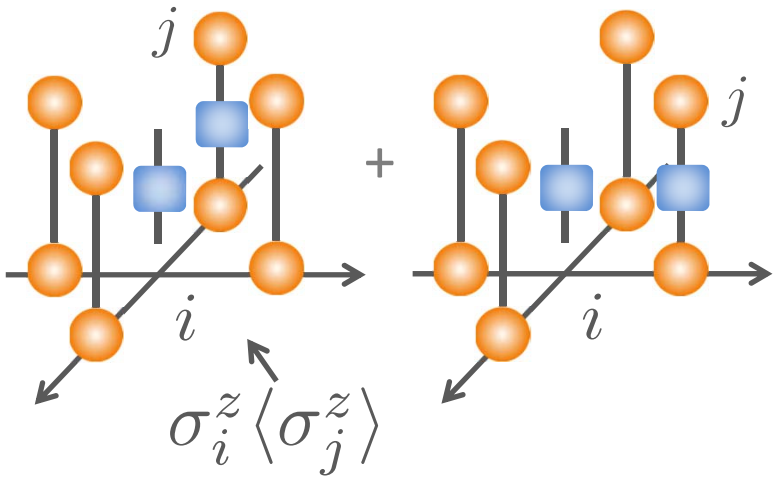
to get the "best" estimate.

This is a powerful principle we will exploit frequently for other more complex tensor networks. Let's see how it works here:



Mean-field theory

Assume translational invariance – we need only solve for one site by finding an effective Hamiltonian and Norm:

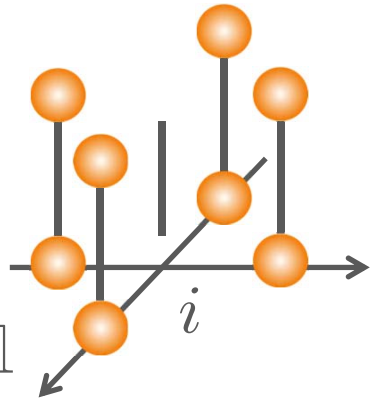


sum up averaged n.n. terms:

n.n.

$$\hat{H}_{\text{eff}} = -zJ\langle\sigma^z\rangle\sigma^z + B\sigma^z$$

Formally we have a local generalised eigenvalue problem, but …

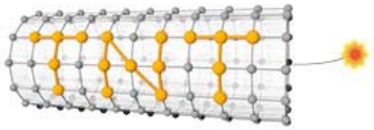


$$\hat{N}_{\text{eff}} = \mathbb{1}$$

So in this case it reduces to a standard eigenvalue problem:

which is then iterated.

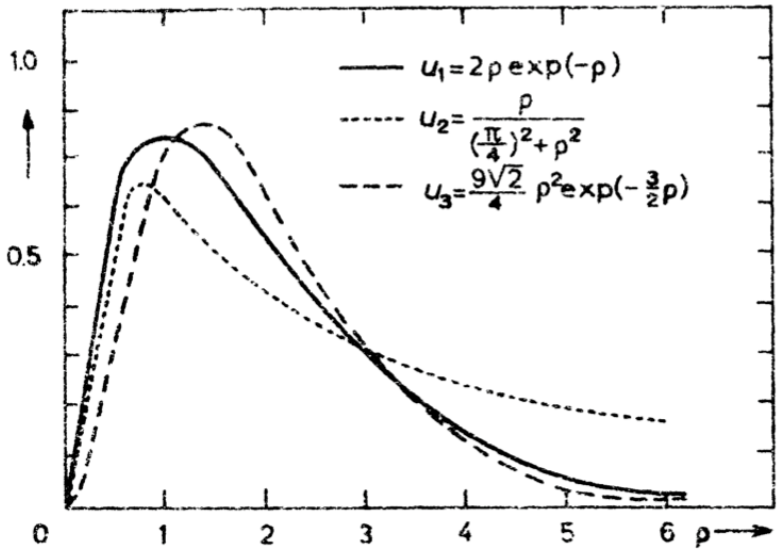
For obvious reasons this approach is called “mean-field” theory and we have seen this for two particles in two boxes.



Aside: lower energy = better?

Not quite. The variational principle is subtle. Consider three simple trial wave-functions for "simple hydrogen":

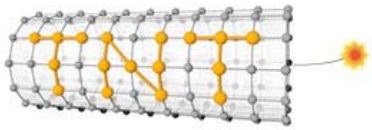
$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0 r}$$



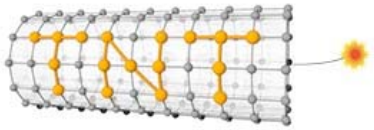
[See QM by A. Messiah page 768]

		1	2	3
$u(b, \varrho)$	=	$\varrho\, e^{-b\varrho}$	$\frac{\varrho}{b^2 + \varrho^2}$	$\varrho^2 e^{-b\varrho}$
N^2	=	$1/4b^3$	$\pi/4b$	$3/4b^5$
$E(b)/E_H$	=	$b^2 - 2b$	$(\pi - 8b)/2\pi b^2$	$\frac{1}{3}b^2 - b$
b_{min}	=	1	$\frac{1}{4}\pi$	$\frac{3}{2}$
E_{var}	=	$-E_H$	$-0.81\, E_H$	$-0.75\, E_H$
$\frac{E_{var} - E_0}{E_1 - E_0}$	=	0	0.25	0.33
$(u/N)_{var}$	=	$2\varrho\, e^{-\varrho}$	$\varrho[(\frac{1}{4}\pi)^2 + \varrho^2]^{-1}$	$\frac{1}{4} \times 9\sqrt{2}\, \varrho^2 e^{-\frac{3}{2}\varrho}$
$\langle r \rangle_{var}$	=	$1.5\, a_0$	∞	$1.66\, a_0$
$\varepsilon = 1 - \lvert\langle \Psi_0 \rvert \Psi_{var} \rangle\rvert^2$	=	0	0.21	0.05

Having a lower energy **only** tells us that a given ansatz estimates **energy** better – it's no guarantee it does anything else better.

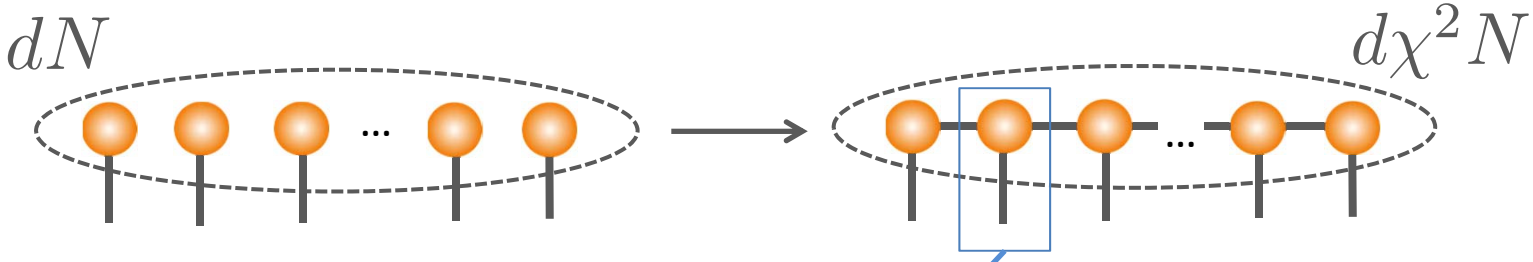


3: Matrix Product States

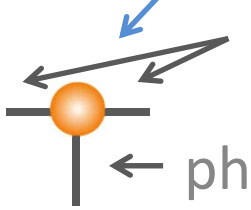


Matrix Product States

While useful product states miss out a lot of physics. Can we build a proper tensor network from them? Yes, lets add some new links:



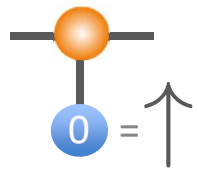
Except the boundaries we now have rank-3 tensors at each site:

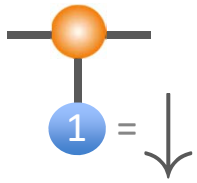


internal legs dim = χ

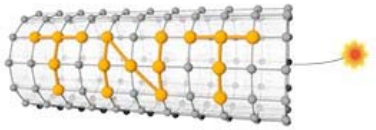
physical leg dim = d

For fixed χ we still only have a polynomial number of parameters. We can interpret each rank-3 tensor as a matrix indexed by the physical leg. For spins we would have:

$\mathbf{A}^{\uparrow}$ = 

$\mathbf{A}^{\downarrow}$ = 

Both are $(\chi \times \chi)$ matrices.



Matrix Product States

By explicitly writing out all the contractions we arrive at:

$$|\psi\rangle = \sum_{\sigma_1,\sigma_2,\ldots,\sigma_N} \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_N}|\sigma_1,\sigma_2,\ldots,\sigma_N\rangle$$

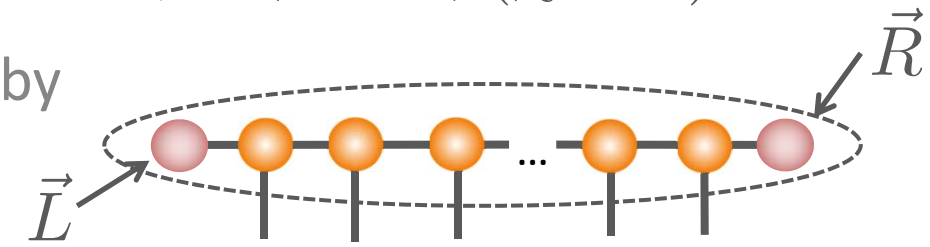
A matrices are different on every site

The amplitudes of the state are therefore parameterised by products of matrices which are collapsed to a scalar (hence the name MPS):

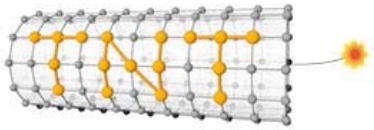
$$\psi_{\underbrace{\sigma_1,\sigma_2,\ldots,\sigma_N}_{\vec{\sigma}}} = \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_{N-1}}\mathbf{A}^{\sigma_N}$$

$$(1\times\chi)\quad(\chi\times\chi)\quad(\chi\times\chi)\quad(\chi\times 1)$$

We can make all A tensors rank-3 by introducing "internal" boundary vectors giving instead:



$$\psi_{\sigma_1,\sigma_2,\ldots,\sigma_N} = \vec{L}^{\dagger}\mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_{N-1}}\mathbf{A}^{\sigma_N}\vec{R}$$



Example MPS

Note that product states are just MPS with $\chi = 1$:

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

$$\downarrow$$

$$|\varphi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle \longrightarrow \begin{array}{l} \mathbf{A}^{\uparrow} = \alpha \\ \mathbf{A}^{\downarrow} = \beta \end{array}$$

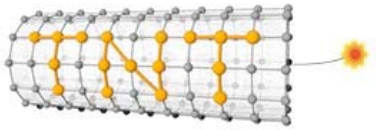
However, the purpose of introducing "internal" legs was to allow for correlations. Some simple examples show we now get this once $\chi > 1$

AF-GHZ state: $|\Psi_{\mathrm{GHZ}}\rangle = |\uparrow\downarrow\uparrow\cdots\downarrow\rangle + |\downarrow\uparrow\downarrow\cdots\uparrow\rangle$

Set all **A** tensors to : $\mathbf{A}^{\uparrow} = \sigma^{+} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $\mathbf{A}^{\downarrow} = \sigma^{-} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

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

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



Example MPS

The AF-GHZ state is then obtained by using: $\vec{L} = \vec{R} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$|\Psi_{\rm GHZ}\rangle = \overbrace{\vec{L}^\dagger \sigma^+ \sigma^- \vec{R}}^{=1} |\uparrow\downarrow\uparrow\cdots\downarrow\rangle + \overbrace{\vec{L}^\dagger \sigma^- \sigma^+ \vec{R}}^{=1} |\downarrow\uparrow\downarrow\cdots\uparrow\rangle$$

This state has *infinite-ranged* correlations since $C^{zz}_\ell = (-1)^\ell \ \forall \ell.$

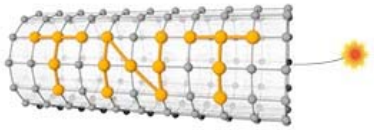
W state: $|\Psi_{\rm W}\rangle = |\downarrow\uparrow\uparrow\cdots\uparrow\rangle + |\uparrow\downarrow\uparrow\cdots\uparrow\rangle + \cdots + |\uparrow\uparrow\uparrow\cdots\downarrow\rangle$

Set all **A** tensors to : $\mathbf{A}^\uparrow = \mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \mathbf{A}^\downarrow = \sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$

Since $(\mathbf{A}^\downarrow)^2 = 0$ only *N* + 1 products of matrices are non-zero:

$$\mathbf{A}^\uparrow \mathbf{A}^\uparrow \mathbf{A}^\uparrow \cdots \mathbf{A}^\uparrow = \mathbb{1} \quad \text{and} \quad \mathbf{A}^\downarrow \mathbf{A}^\uparrow \mathbf{A}^\uparrow \cdots \mathbf{A}^\uparrow = \sigma^-$$

+ translates



Example MPS

The W state is then obtained by using: $\vec{L} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \quad \vec{R} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$$|\Psi_{\mathrm{W}}\rangle = \overbrace{\vec{L}^{\dagger}\vec{R}}^{=0}|\uparrow\uparrow\uparrow\cdots\uparrow\rangle + \overbrace{\vec{L}^{\dagger}\sigma^{-}\vec{R}}^{=1}|\downarrow\uparrow\uparrow\cdots\uparrow\rangle + \ldots$$

Another perspective: view the rank-3 tensors as a matrix of states:

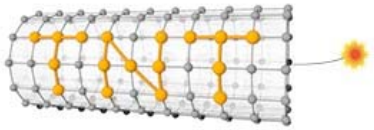
$$A^{\sigma}_{\alpha,\beta} \qquad \mathbf{A}^{\sigma} \qquad \mathbf{A} \qquad \mathbf{A}$$

α — β, σ $=$ $\begin{pmatrix} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} & \\ & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \end{pmatrix}$ $=$ $\begin{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} & 0 \\ \begin{pmatrix} 0 \\ 1 \end{pmatrix} & \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{pmatrix}$ $=$ $\begin{pmatrix} |\uparrow\rangle & 0 \\ |\downarrow\rangle & |\uparrow\rangle \end{pmatrix}$

Matrix multiplication (contraction) yields Kronecker product of states:

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

Full state is then just: $|\Psi_{\mathrm{W}}\rangle = \vec{L}^{\dagger}\mathbf{A}\mathbf{A}\cdots\mathbf{A}\vec{R}$ a useful trick.



Adding two MPS

Consider two MPS of dimension χ_1 and χ_2 respectively:

$$|\psi\rangle = \sum_{\vec{\sigma}} \mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_N}|\vec{\sigma}\rangle \qquad |\phi\rangle = \sum_{\vec{\sigma}} \mathbf{B}^{\sigma_1}\mathbf{B}^{\sigma_2}\cdots\mathbf{B}^{\sigma_N}|\vec{\sigma}\rangle$$

We can form the MPS of their superposition by embedding their matrices in the bulk into a large matrix:

$$|\theta\rangle = \alpha|\psi\rangle + \beta|\phi\rangle \rightarrow \quad \mathbf{C}^{\sigma} = \mathbf{A}^{\sigma} \oplus \mathbf{B}^{\sigma} = \begin{pmatrix} \mathbf{A}^{\sigma} & 0 \\ 0 & \mathbf{B}^{\sigma} \end{pmatrix}$$

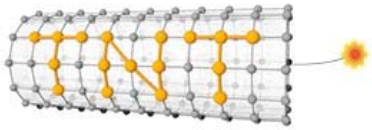
and boundaries (vectors) as:

$$\mathbf{C}^{\sigma_1} = \begin{pmatrix} \alpha\mathbf{A}^{\sigma_1} & \beta\mathbf{B}^{\sigma_1} \end{pmatrix}$$

$$\mathbf{C}^{\sigma_N} = \begin{pmatrix} \mathbf{A}^{\sigma_N} \\ \mathbf{B}^{\sigma_N} \end{pmatrix}$$

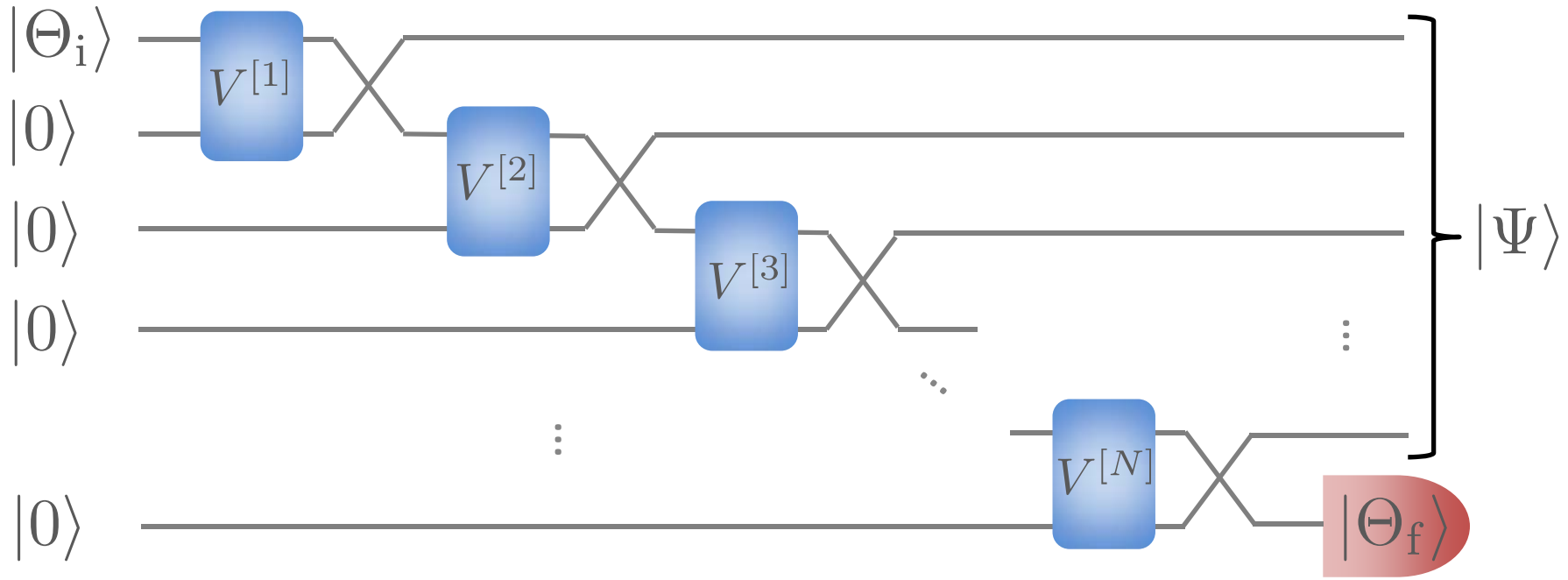
This MPS for $|\theta\rangle$ therefore has dimension $\chi_3 = \chi_1 + \chi_2$, i.e. it has enlarged, but it is also usually sub-optimal (see later).

Thus the family of MPS with a dimension χ do not form a subspace.

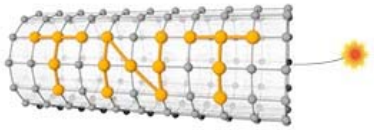


Sequential generation

What about MPS with larger χ? Consider the following quantum circuit for *N d*-level systems and one χ-level ancilla:

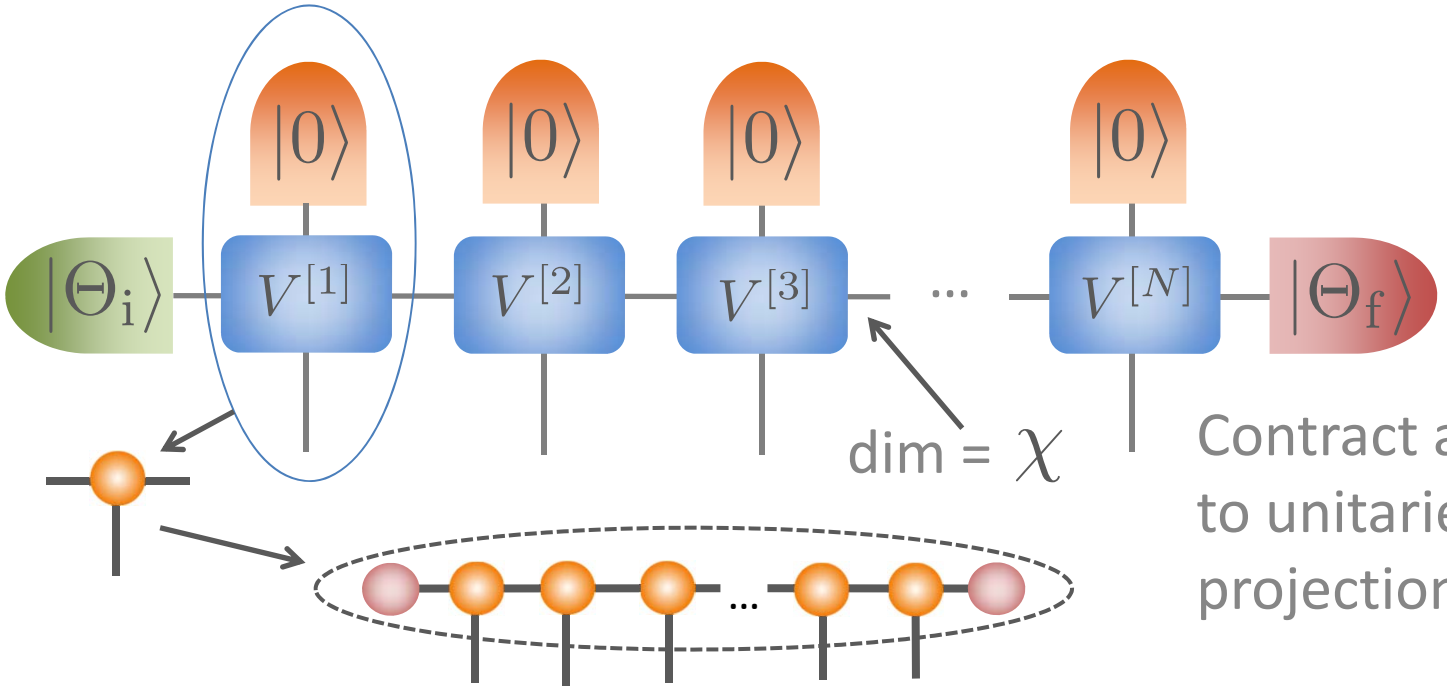


The ancilla interacts via a unitary gate $V^{[j]}$ sequentially with each *d*-level system in turn giving a "staircase circuit". We then project out the ancilla in the state $|\Theta_f\rangle$ leaving the *N d*-level systems in some state $|\Psi\rangle$. This state is a χ dimensional MPS …



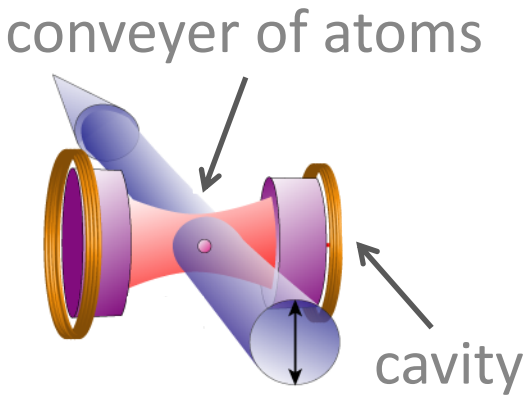
Sequential generation

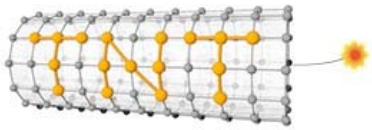
We can see this by rearranging the circuit into a tensor network:



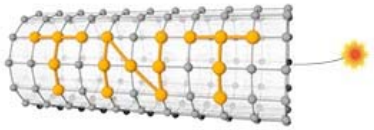
Contract all the inputs to unitaries and projection of ancilla

Ancilla carries correlations from one site to the next. It's ability to do so is heavily influenced by its dimension. This process can even give a physical construction of MPS:





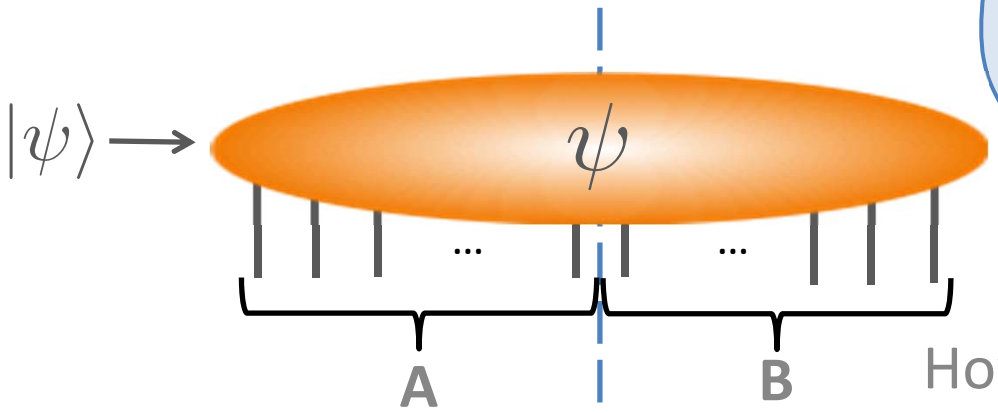
4: Entanglement properties

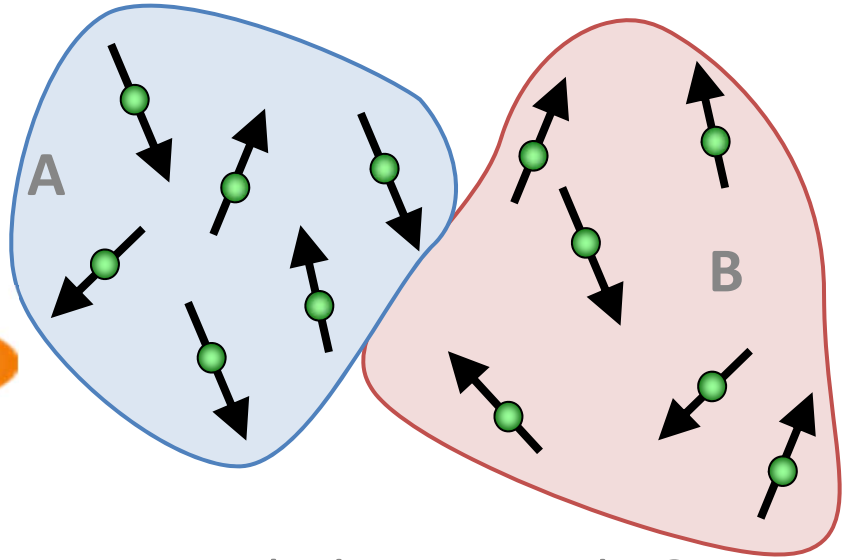


Entanglement

To fully understand MPS, i.e. where it will work and fail, we need to unravel its correlations in terms of entanglement. Take a system of spins in some state $|\psi\rangle$ …

Let's split the system into two:

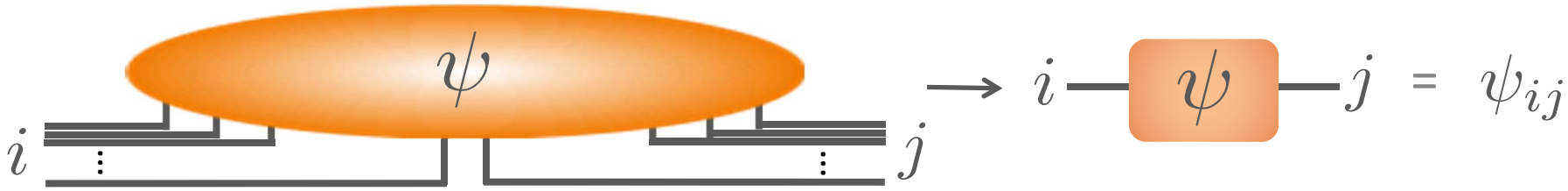


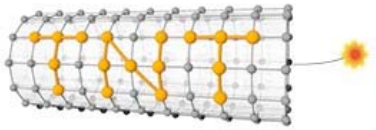


How entangled are **A** and **B**?

First, reshape tensor into a matrix:

$$|\psi\rangle = \sum_{ij} \psi_{ij} |i\rangle_A |j\rangle_B$$



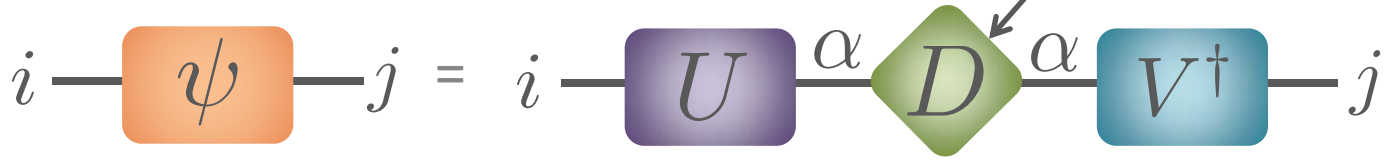


Entanglement

Remember *D* is diagonal

$$D_{\alpha\alpha} = \lambda_\alpha$$

Now SVD this matrix:



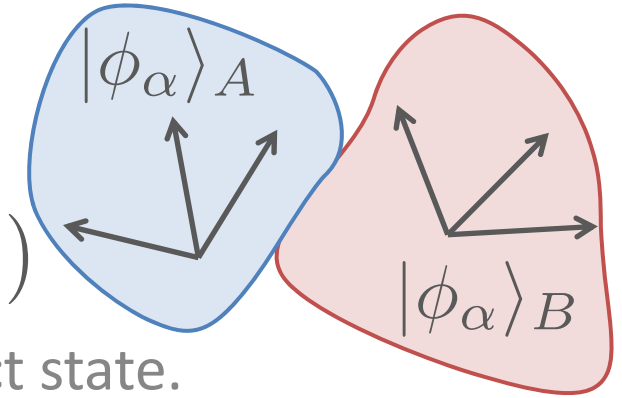
This operation "Schmidt decomposes" the state:

$$|\psi\rangle = \sum_{ij} \left(\sum_{\alpha=1}^{r} U_{i\alpha} D_{\alpha\alpha} (V^\dagger)_{\alpha j} \right) |i\rangle_A |j\rangle_B$$

$$|\psi\rangle = \sum_{\alpha=1}^{r} \lambda_\alpha \left(\sum_i U_{i\alpha} |i\rangle_A \right) \left(\sum_j (V^\dagger)_{\alpha j} |j\rangle_B \right)$$

$$|\psi\rangle = \sum_{\alpha=1}^{r} \lambda_\alpha |\phi_\alpha\rangle_A |\phi_\alpha\rangle_B$$

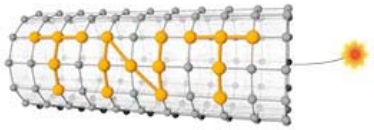
Schmidt bases =



λ_α = Schmidt coefficients $\sum_{\alpha=1}^{r} \lambda_\alpha^2 = 1$

Schmidt rank = $r = \min\left(\dim(A), \dim(B)\right)$

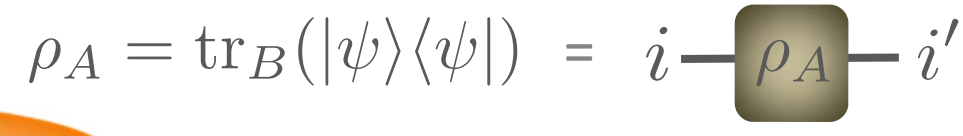
Any state with *r* > 1 is entangled = *not* a product state.

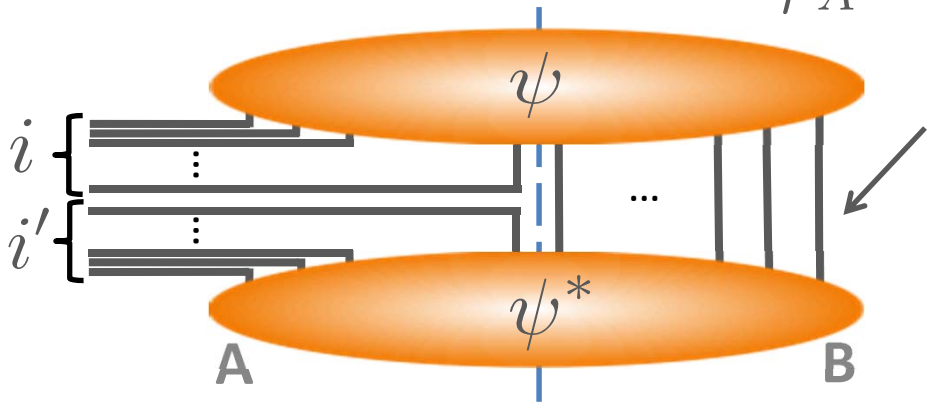


Entanglement

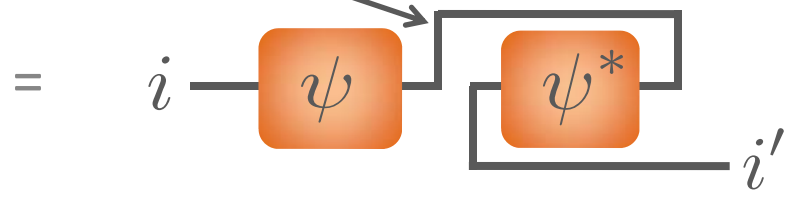
How are quantum correlations between **A** and **B** exposed? Compute reduced density operators:

$$\rho_A = \mathrm{tr}_B(|\psi\rangle\langle\psi|)$$

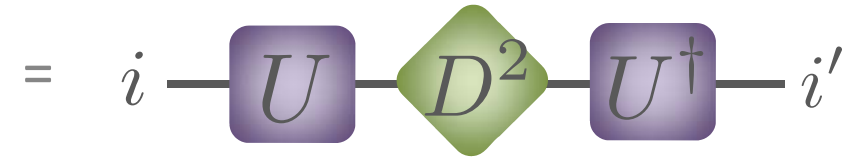




trace out **B**



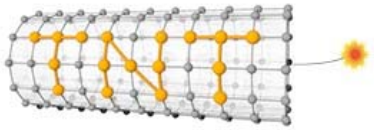
A's Schmidt basis diagonalises ρ_A:



When $r > 1$ ρ_A is mixed (despite $|\psi\rangle$ being pure). The more uncertain ρ_A the more entangled $|\psi\rangle$ is. Quantify this via an entropy:

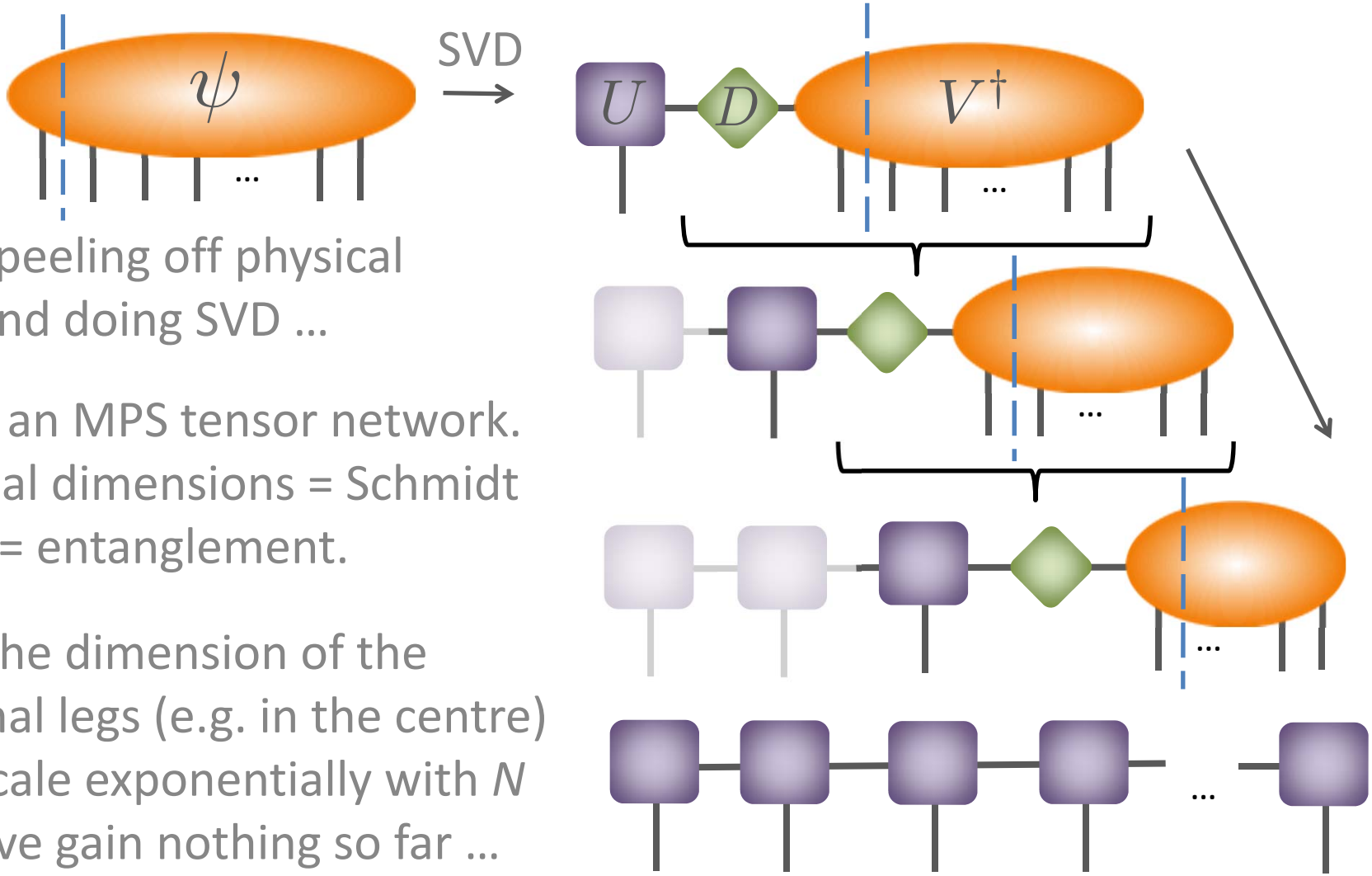
von Neumann entropy: $S(\rho) = -\mathrm{tr}(\rho \log(\rho))$

Shannon entropy of λ_α^2: $S(\rho_A) = S(\rho_B) = -\sum_{\alpha=1}^{r} \lambda_\alpha^2 \log(\lambda_\alpha^2)$



Exact MPS for any state

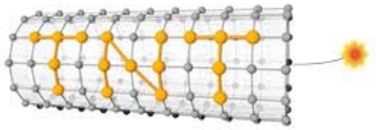
If we allow the dimension χ of an MPS to vary as needed then **any** state can be represented exactly. Take an arbitrary state $|\psi\rangle$:



Keep peeling off physical legs and doing SVD …

Yields an MPS tensor network. Internal dimensions = Schmidt ranks = entanglement.

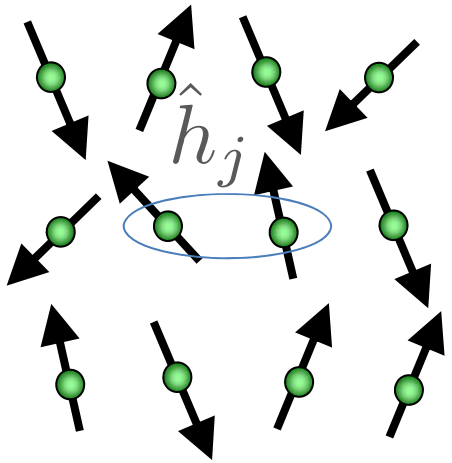
But, the dimension of the internal legs (e.g. in the centre) can scale exponentially with *N* – we've gain nothing so far …



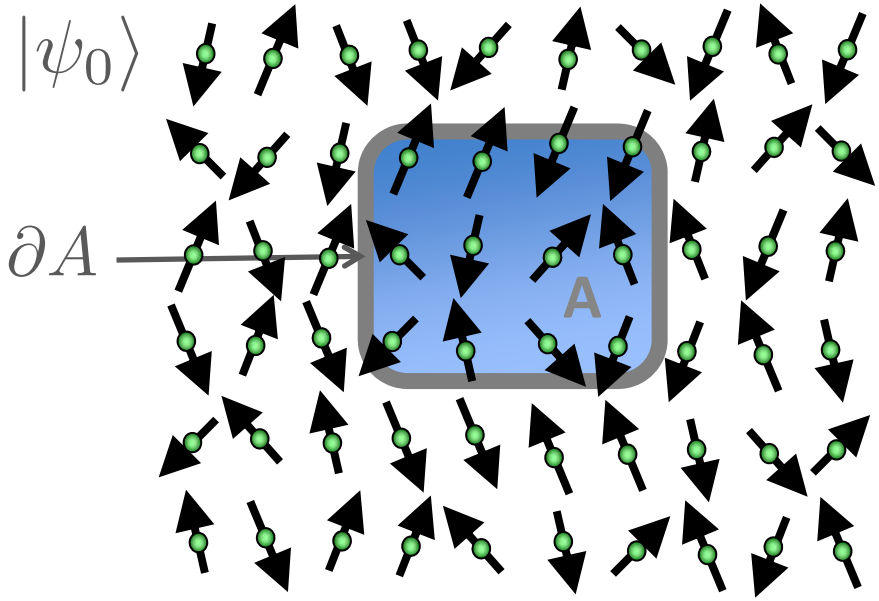
Physical states/boundary laws

We now come to an important observation about physical states. Suppose we have a Hamiltonian of the form:

$$\hat{H} = \sum_j \hat{h}_j$$



where $\hat{h}_j$ acts only on a finite number of sites or spins (usually 2) that are geometrically local (usually nearest-neighbour) then …

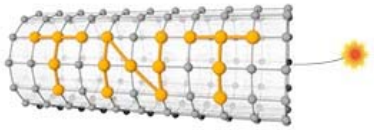


Pick any region **A** then we find that for the ground state $|\psi_0\rangle$:

$$S(\rho_A) \sim |\partial A|$$

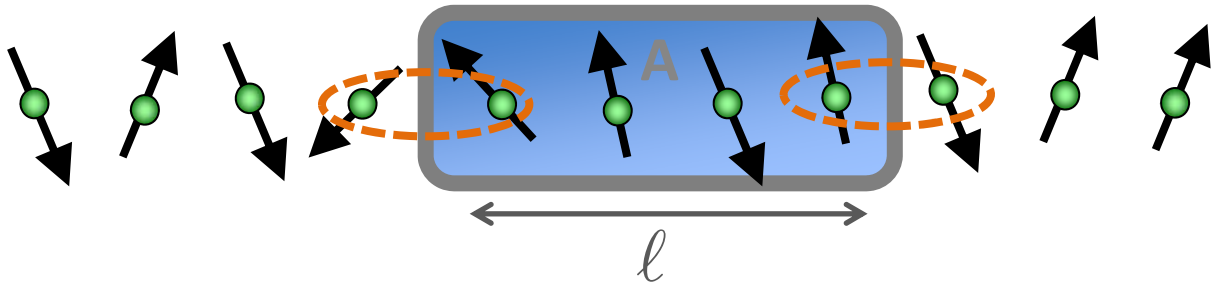
The entanglement between **A** and the rest scales with the boundary

Contrast this to entropies in stat. mech. which scale with $|A|$.



Physical states/boundary laws

Intuitively a boundary law means that entanglement, and so correlations, between a region and the rest is concentrated at their interface. In 1D this is particularly constraining …



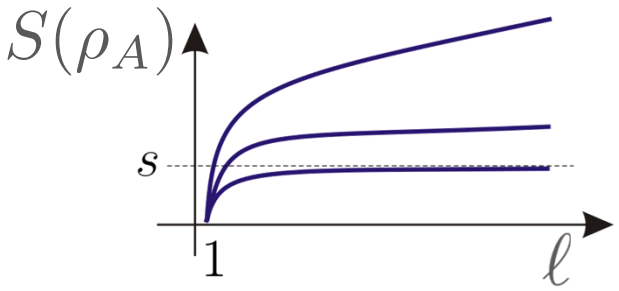
Obeying the boundary law means that $S(\rho_A) \sim \text{const.}$ for any ℓ.

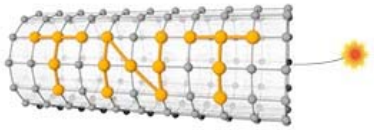
Beyond numerical evidence the boundary law has been proven for:

- Any gapped 1D Hamiltonian with unique GS.
- For gapped free bosonic/fermionic models in any dimension.

Even critical gapless systems in 1D, which violate the boundary-law, do so "gently" as:

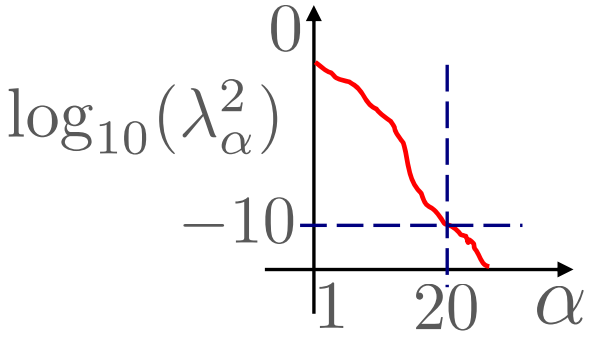
$$S(\rho_A) \sim \log(\ell)$$





Physical states/boundary laws

A consequence of the boundary law is that the Schmidt coefficients for such states decay very quickly with the index α :



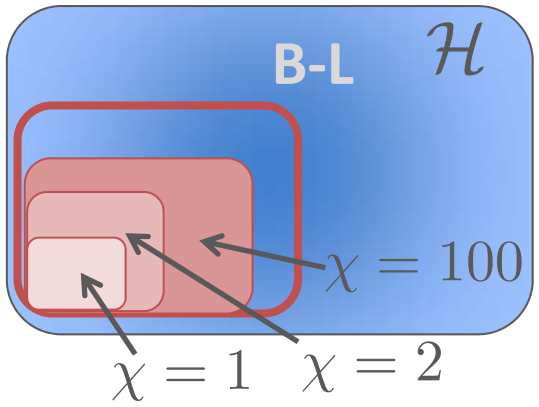
This indicates that in 1D GS and low-lying excitations are only very weakly entangled with only a few relevant degrees of freedom.

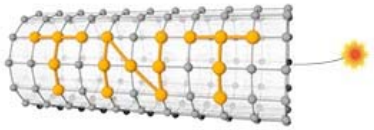
We can truncate the rank *r* for every bipartition without any significant loss of accuracy:

$$\| |\psi\rangle - |\psi_\chi\rangle \|_2^2 \leq 2 \sum_{j=1}^{N-1} \left[\sum_{\alpha=\chi+1}^{r_j} (\lambda_\alpha^{[j]})^2 \right]$$

The *locality* of physical states means they occupy an exponentially small "corner" of the many-body Hilbert space:

Tensor-networks try to encode this corner …

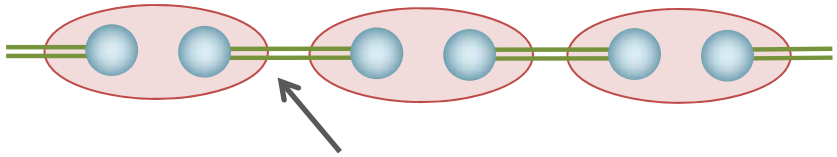




Projected entangled pairs

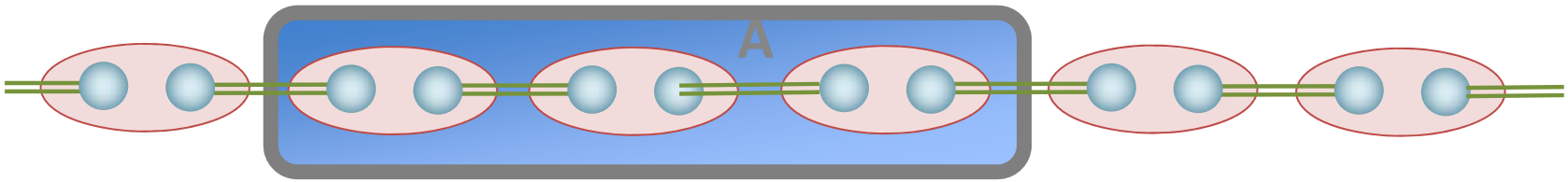
The connection between MPS and the boundary law is best exposed by considering the projected entangled pairs construction:

Introduce a pair of χ-level ancilla for each physical site:



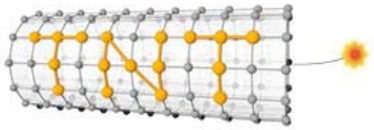
Maximally entangle neighbouring ancilla: $|\Phi\rangle = \frac{1}{\sqrt{\chi}} \sum_{j=1}^{\chi} |j\rangle|j\rangle$

Resulting state exactly embodies the boundary law. Bipartition the system anywhere:



we will always cut through two bonds so $S(\rho_A) = 2\log(\chi)$ and so is constant.

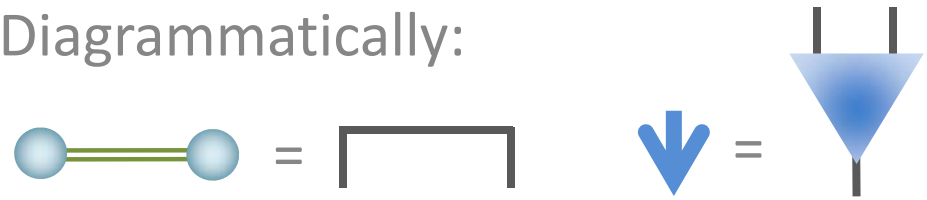
This state is a bit artificial, but it can be used to generate MPS …

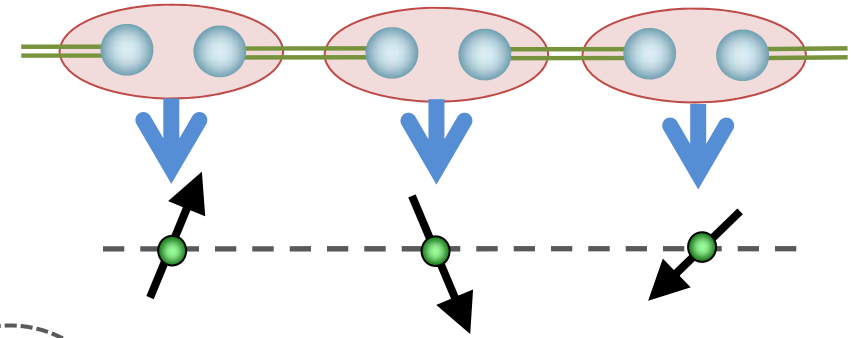


Projected entangled pairs

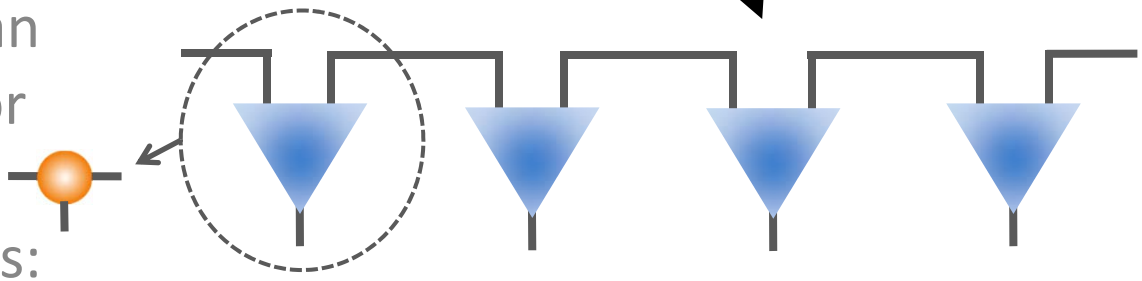
Let us apply a *projector* which maps $\mathbb{C}^\chi \otimes \mathbb{C}^\chi \mapsto \mathbb{C}^d$ the on-site pair of ancilla to the proper physical site:

Diagrammatically:

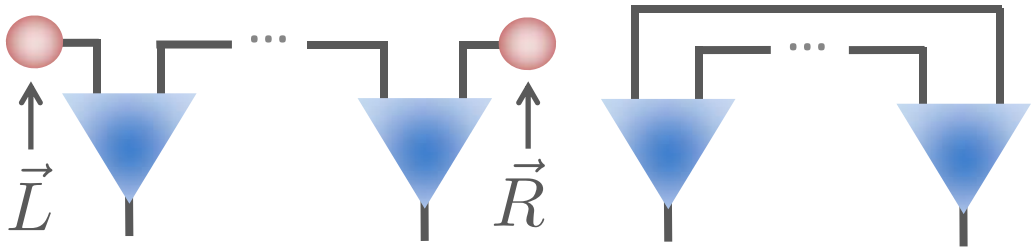




Putting this together we can identify our rank-3 **A** tensor as the projector glued together by entangled pairs:



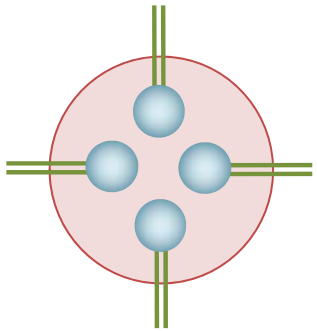
What about boundaries?

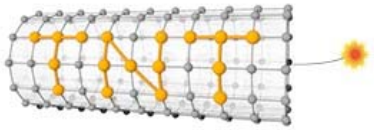


OBC as before $= \vec{L}^\dagger \mathbf{A}\mathbf{A}\cdots\mathbf{A}\vec{R}$

PBC new option $= \mathrm{tr}(\mathbf{A}\mathbf{A}\cdots\mathbf{A})$

Can generalise to 2D (see later):

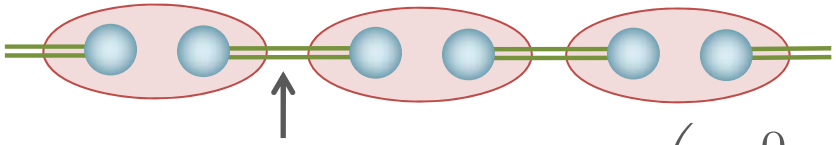




AKLT example

The PEPS construction can give exact ground state. Here is a famous example for a spin-1 chain:

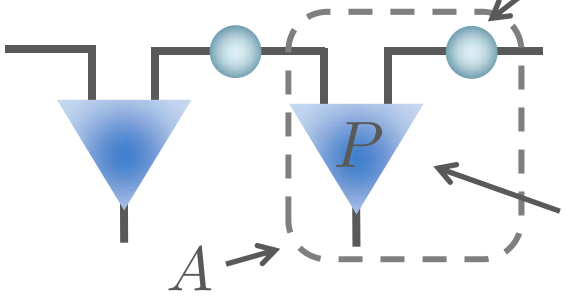
$$\hat{H} = \sum_j \mathbf{S}_j \cdot \mathbf{S}_{j+1} + \tfrac{1}{3}(\mathbf{S}_j \cdot \mathbf{S}_{j+1})^2$$



$$|\Phi\rangle = \tfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

is a sum of projectors of spin 1 pairs into spin 2 subspace, so

$$\hat{H}|\psi_0\rangle = 0$$



GS given by the projection of shared singlets into the triplet subspace:

$$\mathbf{P}^+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \mathbf{P}^0 = \tfrac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \mathbf{P}^- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

Merge (and normalise): $|\Psi_{\mathrm{AKLT}}\rangle = \sum_{\vec{\sigma}} \mathrm{tr}(\mathbf{A}^{\sigma_1}\mathbf{A}^{\sigma_2}\cdots\mathbf{A}^{\sigma_N})|\vec{\sigma}\rangle$

MPS with tensors: $\mathbf{A}^+ = \sqrt{\tfrac{2}{3}}\sigma^+ \quad \mathbf{A}^0 = -\sqrt{\tfrac{1}{3}}\sigma^z \quad \mathbf{A}^- = -\sqrt{\tfrac{2}{3}}\sigma^-$

First exactly solved system with characteristics of a Haldane phase, e.g. gapped GS with finite correlation length (see problem class).