Matrix-product states (MPS)

Recap

$*$ MPS many-body state

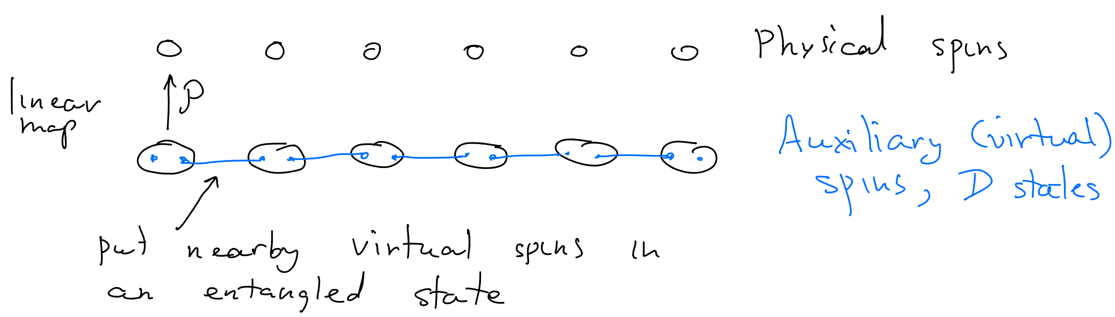
$$|\Psi\rangle = \sum_{\sigma_1 \ldots \sigma_N} \mathrm{Tr}\left[A^{[1]}_{\sigma_1} A^{[2]}_{\sigma_2} \ldots A^{[N]}_{\sigma_N} \right] |\sigma_1 \ldots \sigma_N\rangle$$

$A^{[i]}_{\sigma_i}$ – matrix (d for each site – # spin states)
size $D \times D$ $\Rightarrow$ D – bond dimension

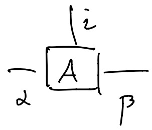
D determines maximum entanglement of $|\Psi\rangle$

$*$ Different choices of $A^{[\,]}$ define a manifold of MPS with fixed bond dimension

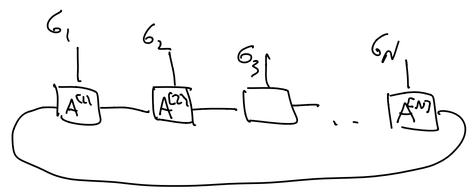
$*$ Can think of MPS via auxiliary spins



Graphical representation of MPS



A is a 3-legged tensor

$\langle \sigma_1 \ldots \sigma_N | \psi \rangle =$ 

A tensor network

* Connected lines assume contraction
* Above picture for periodic B.C.
* If state is translationally invariant, all $A^{[i]}$ may be chosen the same

* We've discussed that MPS can approximate gapped ground states (tensor-network algorithms)
  Can view MPS with bond dimension D as a variational manifold

* Also, MPS can give <u>exact</u> ground states

MPS: exact ground state
AKLT model '87

Ref: Review by U. Schöllwock '10

* Consider spin-1 chain

$$H = \sum H_{i,i+1}$$

$$H_{i,i+1} = \vec{S}_i \cdot \vec{S}_{i+1} + \frac{1}{3}(\vec{S}_i \cdot \vec{S}_{i+1})^2 + \frac{2}{3}$$ SU(2)-symmetric

* Lets show that ground state is exact MPS with bond dimension $D=2$
* Can compute certain correlation functions analytically

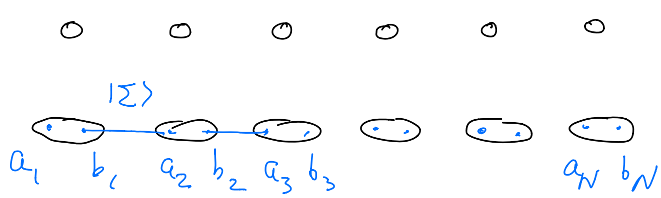
* Note that

$$H_{i,i+1} = \Pi_{2,i,i+1}$$ – projector onto 5-dim. spin-2 subspace of spins $i, i+1$

* Idea: Construct $|\psi_{AKLT}\rangle$: annihilated by each $\Pi_{2,i,i+1}$

Would have zero energy → ground state

* Virtual spins-$\frac{1}{2}$ $(D=2)$



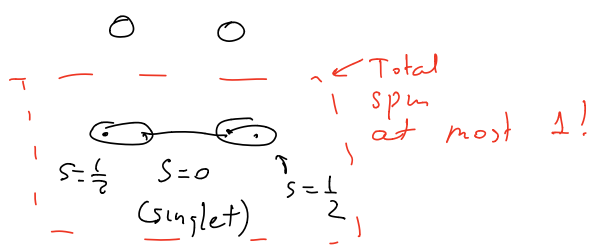
* Put neighboring virtual spins to a singlet state

$$|\Sigma^{[i]}\rangle = \sum_{b_i, a_{i+1} = \uparrow,\downarrow} \Sigma_{ba} |b_i\rangle\langle a_{i+1}|$$

$$\Sigma = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

* Then, will project onto state with spin 1 to get our physical spin

* Easy to see that such a state would be annihilated by $\Pi_{2\,i,i+1}$



* Lets represent such state in MPS form:

* State of virtual spins:

$$|\psi_\Sigma\rangle = \sum_{\{a\},\{b\}} \Sigma_{b_1 a_2} \Sigma_{b_2 a_3} \cdots \Sigma_{b_N a_1} \cdot |a_1\rangle \otimes |a_2\rangle \cdots \otimes |b_1\rangle \cdots \otimes |b_N\rangle$$

* Linear map $P_i : \frac{1}{2} \oplus \frac{1}{2} \rightarrow 1$

M^{σ}_{ab} : $|\sigma\rangle = +, 0, -$

$$|\uparrow\uparrow\rangle \rightarrow |+\rangle$$
$$\frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \rightarrow |0\rangle$$

$|\downarrow\downarrow\rangle \to |-\rangle$

$$M^+ = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \qquad M^- = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \qquad M^0 = \begin{bmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

* Then : state of physical spins

$$|\Psi_{AKLT}\rangle = \sum_{\{\sigma\},\{a\},\{b\}} M^{\sigma_1}_{a_1 b_1} \cdots M^{\sigma_N}_{a_N b_N} |\vec{\sigma}\rangle (\langle\vec{a}| \otimes \langle\vec{b}|) \Psi_\Sigma\rangle =$$

$$= \sum_{\{\sigma\},\{a\},\{b\}} M^{\sigma_1}_{a_1 b_1} \Sigma_{b_1 a_2} M^{\sigma_2}_{a_2 b_2} \Sigma_{b_2 a_3} \cdots \Sigma_{b_{N-1} a_N} M^{\sigma_N}_{a_N b_N} \times$$

$$\times \Sigma_{b_N a_1} |\vec{\sigma}\rangle =$$

$$= \sum_{\{\vec{\sigma}\}} \mathrm{Tr.}(M^{\sigma_1} \Sigma M^{\sigma_2} \cdots M^{\sigma_N} \Sigma) |\sigma_1 \ldots \sigma_N\rangle$$

* Define $\bar{A}^\sigma = M^\sigma \Sigma$ ($\bar{A}$, bar because still have to set normalization)

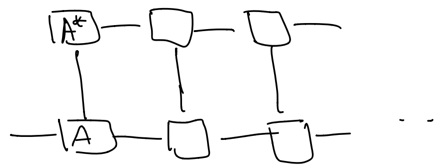
$$\bar{A}^+ = \begin{bmatrix} 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 \end{bmatrix} \qquad \bar{A}^0 = \begin{bmatrix} -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}, \quad \bar{A}^- = \begin{bmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{bmatrix}$$

* How to normalize? Turns out need to just rescale by $2/\sqrt{3}$:

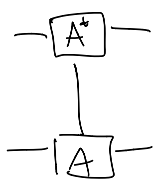
$$A^+ = \begin{bmatrix} 0 & \sqrt{\frac{2}{3}} \\ 0 & 0 \end{bmatrix} \qquad A^0 = \begin{bmatrix} -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{1}{\sqrt{3}} \end{bmatrix} \qquad A^- = \begin{bmatrix} 0 & 0 \\ -\sqrt{\frac{2}{3}} & 0 \end{bmatrix}$$

* To normalize, check overlap $\langle \psi_{AKLT} | \psi_{AKLT} \rangle$

Use graphical notation

$\langle \psi_{AKLT} | \psi_{AKLT} \rangle =$ 

Define transfermatrix

$E \equiv$  $= \sum_s A^{*s} \otimes A^s$

Explicitly, for AKLT

$$E = \begin{bmatrix} 1/4 & 0 & 0 & \frac{1}{2} \\ 0 & -1/4 & 0 & 0 \\ 0 & 0 & -1/4 & 0 \\ \frac{1}{2} & 0 & 0 & 1/4 \end{bmatrix}$$

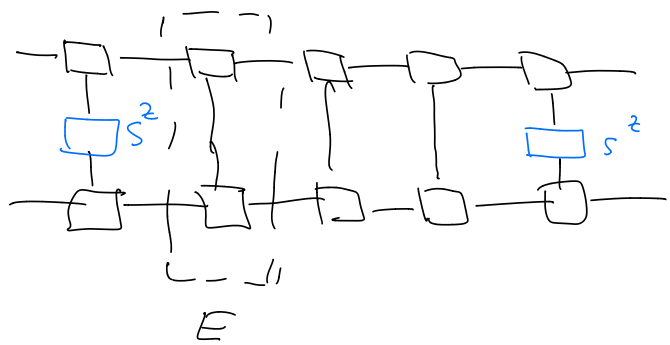
Eigenvalues: $\lambda_1 = 1$, $\lambda_2 = \lambda_3 = \lambda_4 = -\frac{1}{3}$ Normalized ✓

* We used MPS to find an exact ground state of a certain model.

Reverse also possible: for a given MPS, can construct a local Hamiltonian for which it would be an exact ground state

* MPS also useful to find correlations

$\langle S_i^z S_j^z \rangle$ – ?



$$= E^{i-1} \sum_{\sigma_i} A^{*\sigma_i} S^z_{\sigma_i} \otimes A^{\sigma_i} \ldots E^{j-i-1} \ldots \sum_{\sigma_j} A^* S^z A \times$$

$$\times E^{N-j-1}$$

E^i – becomes a projector onto leading eigenvector

Can express the correlators via eigenvectors of E and action of $A^* \cdot S^z \otimes A$ on them!

$$\langle S_i^z S_j^z \rangle \sim \left(-\tfrac{1}{3}\right)^{i-j}$$

* General recipe for computing correlations via MPS