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Tutorial 9 (AKLT model[1])
The AKLT state has historically played an important role as analytically tractable, exact ground state in MPS form of a spin-1 model. In this tutorial we will construct this quantum state, which is sometimes deemed as the simplest non-trivial MPS. We start from the following Hamiltonian, which acts on spin-1 particles arranged on a one-dimensional lattice with periodic boundary conditions:

$$H = \sum_{j=1}^{L} P_j, \qquad P_j = \frac{1}{2}\vec{S}_j \cdot \vec{S}_{j+1} + \frac{1}{6}(\vec{S}_j \cdot \vec{S}_{j+1})^2 + \frac{1}{3}I,$$

where $\vec{S} = (S^x, S^y, S^z)$ collects the following "spin-1 operators":

$$S^x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^y = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \quad \text{and} \quad S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The notation $\vec{S}_j$ means that $\vec{S}$ acts on the j-th particle, and $\vec{S}_j \cdot \vec{S}_{j+1} = S^x_j\, S^x_{j+1} + S^y_j\, S^y_{j+1} + S^z_j\, S^z_{j+1}$. It turns out that P_j is a projector, i.e., it is Hermitian and $P_j^2 = P_j$, and thus has eigenvalues 0 and 1. Since the Hamiltonian is a sum of positive semidefinite terms, its smallest possible eigenvalue is 0. The AKLT state is constructed as eigenstate of H with eigenvalue 0, and is thus a ground state (which turns out to be unique).

The basis states for a spin-1 particle are $|\hat{1}\rangle$, $|\hat{0}\rangle$ and $|-\hat{1}\rangle$. It is possible to combine two qubits to represent a spin-1 particle, via

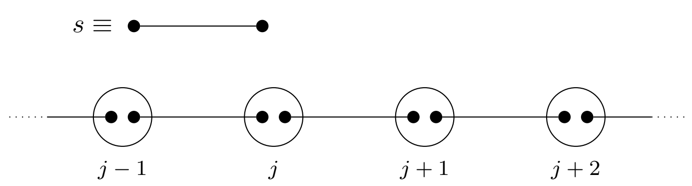
$$|\hat{1}\rangle = |00\rangle\,, \quad |\hat{0}\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \quad \text{and} \quad |-\hat{1}\rangle = |11\rangle\,.$$

(a) Write down an operator $\mathcal{P}$ that maps states from this two-qubit subspace to the spin-1 space. Then define the degree-three tensor M such that $\mathcal{P} = \sum_{\sigma\in\{1,0,-1\}} \sum_{a,b\in\{0,1\}} m_{\sigma ab}\, |\hat{\sigma}\rangle\, \langle ab|$, where $|\hat{\sigma}\rangle\, \langle ab| \equiv |\hat{\sigma}\rangle \circ |ab\rangle$ denotes the outer product of $|\hat{\sigma}\rangle$ and $|ab\rangle$.

(b) As shown in the diagram below, the AKLT construction puts adjacent qubits of two neighboring sites into a so-called "singlet state":

$$s = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle).$$

Assemble the matrix G such that $s = \sum_{a,b} g_{ba}\, |b\rangle\, |a\rangle$. Use it to write an expression for a state ψ with L lattice sites and periodic boundary conditions, where each site is in the state shown in the diagram.



(c) Project the state into the spin-1 subspace, $\hat{\psi} = \prod_{j=1}^{L} \mathcal{P}_j\, \psi$, and find the left-orthonormal MPS tensors A such that

$$\hat{\psi} = \sum_{\sigma\in\{1,0,-1\}^L} \mathrm{tr}\,[A^{\sigma_1} A^{\sigma_2} \cdots A^{\sigma_L}]\, |\sigma\rangle\,.$$

Solution

(a) We can write down the general form for $\mathcal{P}$ as

$$\mathcal{P} = |\hat{1}\rangle\, \langle 00| + |\hat{0}\rangle \left(\frac{\langle 01| + \langle 10|}{\sqrt{2}}\right) + |-\hat{1}\rangle\, \langle 11|$$

[1]Original AKLT papers: I. **A**ffleck, T. **K**ennedy, E. H. **L**ieb, H. **T**asaki: *Rigorous results on valence-bond ground states in antiferromagnets*, Phys. Rev. Lett. 59, 799 (1987) and I. **A**ffleck, T. **K**ennedy, E. H. **L**ieb, H. **T**asaki: *Valence bond ground states in isotropic quantum antiferromagnets*, Commun. Math. Phys. 115, 477–528 (1988)

Now we can bring it into the desired form by comparing coefficients.

$$\mathcal{P} = \sum_{\sigma} \sum_{a,b} m_{\sigma ab} \left|\hat{\sigma}\right\rangle \left\langle ab\right| ,$$

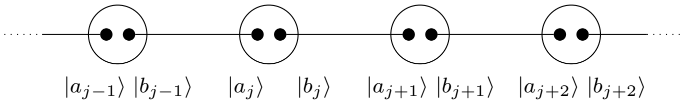
where

$$m_{\hat{1}ab} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad m_{\hat{0}ab} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & 0 \end{pmatrix}, \quad m_{-\hat{1}ab} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

(b) By once more comparing coefficients we find

$$G = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}.$$

We will denote the states of specific qubits as



written as

$$\left|\vec{a}\right\rangle \left|\vec{b}\right\rangle = \left|a_1 b_1 a_2 b_2 \dots a_L b_L\right\rangle .$$

Then we can rewrite ψ as

$$\psi = \sum_{\vec{a}\vec{b}} g_{b_1 a_2} g_{b_2 a_3} \cdots g_{b_L a_1} \left|\vec{a}\right\rangle \left|\vec{b}\right\rangle$$

with respect to periodic boundary conditions.

(c)

$$\begin{aligned} \hat{\psi} &= \prod_{j=1}^{L} \mathcal{P} \sum_{\vec{a}\vec{b}} g_{b_1 a_2} g_{b_2 a_3} \cdots g_{b_L a_1} \left|\vec{a}\right\rangle \left|\vec{b}\right\rangle \\ &= \sum_{\vec{\sigma}} \sum_{\vec{a}\vec{b}} m_{\sigma_1 a_1 b_1} g_{b_1 a_2} m_{\sigma_2 a_2 b_2} g_{b_2 a_3} \cdots m_{\sigma_L a_L b_L} g_{b_L a_1} \left|\vec{\sigma}\right\rangle \\ &= \sum_{\vec{\sigma}} \mathrm{Tr}\left[M_{\sigma_1} G M_{\sigma_2} G \cdots M_{\sigma_L} G\right] \left|\vec{\sigma}\right\rangle \\ &= \sum_{\vec{\sigma}} \mathrm{Tr}\left[\tilde{A}_{\sigma_1} \tilde{A}_{\sigma_2} \cdots \tilde{A}_{\sigma_L}\right] \left|\vec{\sigma}\right\rangle , \end{aligned}$$

which is in MPS form with

$$\begin{aligned} \tilde{A}_{\hat{1}} &= M_{\hat{1}} G = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}}, \\ 0 & 0 \end{pmatrix} \\ \tilde{A}_{\hat{0}} &= M_{\hat{0}} G = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}, \\ \tilde{A}_{-\hat{1}} &= M_{-\hat{1}} G = \begin{pmatrix} 0 & 0 \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}. \end{aligned}$$

We still need to check, if this actually gives rise to a left-orthonormal MPS, i.e., if

$$\sum_{\sigma} \tilde{A}_{\sigma}^{\dagger} \tilde{A}_{\sigma} = I.$$

Therefore, we compute

$$\tilde{A}_{\hat{1}}^{\dagger} \tilde{A}_{\hat{1}} + \tilde{A}_{\hat{0}}^{\dagger} \tilde{A}_{\hat{0}} + \tilde{A}_{-\hat{1}}^{\dagger} \tilde{A}_{-\hat{1}} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2} \end{pmatrix} + \begin{pmatrix} \frac{1}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix} + \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 0 \end{pmatrix} = \frac{3}{4} I.$$

Thus we need to renormalise the MPS by setting

$$A_{\sigma} = \sqrt{\frac{4}{3}} \tilde{A}_{\sigma}.$$

Finally the MPS corresponding to the AKLT state is given as

$$\psi = \sum_{\vec{\sigma}} \mathrm{Tr}\left[A_{\sigma_1} \cdots A_{\sigma_L}\right].$$