

The AKLT state

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In this problem, we consider a spin-1 interacting Hamiltonian whose ground state can be *exactly* described by an MPS with a remarkably small bond dimension, $\chi = 2$. Affleck, Kennedy, Lieb, and Tasaki introduced the model in 1987, and it is known in the literature as the AKLT model.

To this end, let us consider a chain made of N spin-1 particles, which are therefore characterized by a local Hilbert space of dimension $d = 3$, spanned by the computational basis $\{|-j\rangle, |0_j\rangle, |+j\rangle\}$. It will be convenient, for this problem, to impose periodic boundary conditions, *i.e.* $N + 1 \equiv 1$. It will turn out to be convenient to actually parametrize each spin-1 particle, say the particle sitting at site j in the lattice, by a *pair* of spin-1/2 particles. In other words, we will see each particle j as a *compound* object, made by the virtual pair (L_j, R_j) , in which L_j denotes the “left” spin-1/2 component, and R_j denotes the “right” spin-1/2 component. Let us denote, for both L_j and R_j , the two states in the computational basis as $|\uparrow_j\rangle$ and $|\downarrow_j\rangle$; so that, for instance, the configuration in which both L_j and R_j are in the “up” state will be denoted with $|\uparrow_j\uparrow_j\rangle$.

Q. 1 Is the mapping from the spin-1/2 pair to the spin 1 object one-to-one?

Q. 2 Given the answer to the previous point, we will use the following mapping

$$|+_j\rangle \equiv |\uparrow_j\uparrow_j\rangle, \quad |-_j\rangle \equiv |\downarrow_j\downarrow_j\rangle, \quad |0_j\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow_j\downarrow_j\rangle + |\downarrow_j\uparrow_j\rangle), \quad (1)$$

what is the physical motivation behind this choice?

Q. 3 Rewrite the mapping in Eq. (1) in terms of a *projection operator*, $\hat{P}_j$, projecting the *full* virtual Hilbert space at site j into the physical, spin-1, Hilbert space at site j .

Q. 4 Given $\hat{P}_j$, consider its matrix elements, $P_{ab}^{(j)s} \equiv \langle s_j | \hat{P}_j | a_j b_j \rangle$, with $s_j \in \{+_j, 0_j, -_j\}$ and $a_j, b_j \in \{\uparrow_j, \downarrow_j\}$. Show that we have

$$P_{ab}^{(j)+} = \delta_{a_j\uparrow_j}\delta_{b_j\uparrow_j}, \quad P_{ab}^{(j)0} = \frac{1}{\sqrt{2}}(\delta_{a_j\uparrow_j}\delta_{b_j\downarrow_j} + \delta_{a_j\downarrow_j}\delta_{b_j\uparrow_j}), \quad P_{ab}^{(j)-} = \delta_{a_j\downarrow_j}\delta_{b_j\downarrow_j}. \quad (2)$$

Given the mapping just described, we now aim to create a non-trivial MPS state, which later will be shown to be the ground state of a physically meaningful interacting Hamiltonian for the spin-1 DOFs. Towards this goal, and working directly on the virtual degrees of freedom, we want to impose the constraint that the *right* spin at site j , R_j , is paired into a singlet with the *left* spin at site $j + 1$, L_{j+1} , thus creating a correlation between different sites. Concretely, we require that they form the following state

$$|\omega\rangle_{R_j, L_{j+1}} = \frac{1}{\sqrt{2}} \left(|\uparrow\rangle_{R_j} |\downarrow\rangle_{L_{j+1}} - |\downarrow\rangle_{R_j} |\uparrow\rangle_{L_{j+1}} \right). \quad (3)$$

Q. 5 Show that Eq. (3) can be recast in the compact form

$$|\omega\rangle_{R_j, L_{j+1}} = \frac{1}{\sqrt{2}} \sum_{b, c=\uparrow, \downarrow} \epsilon_{bc} |b\rangle_{R_j} |c\rangle_{L_{j+1}}, \quad (4)$$

with $\epsilon_{bc} = i\hat{\sigma}^y$ being the fully antisymmetric tensor in 2 dimensions.

So, in total, we have the following configuration:

1. For each site j , we have two virtual degrees of freedom, L_j and R_j .
2. The virtual degrees of freedom *inside* a single site j are projected into the physical Hilbert space via the projector $\hat{P}_j$ or, equivalently, its matrix elements in Eq. (2).
3. The right virtual particle in site j and the left virtual particle in $j+1$ are then forced to be in singlet state by means of the tensor $\frac{1}{\sqrt{2}}\epsilon_{bc}$ appearing in Eq. (3).

Q. 6 Argue that the two constraints written above can be combined into a single condition, for each physical site j , reading

$$A_{ac}^{[j]s} = \frac{1}{\sqrt{2}} \sum_{b=\uparrow, \downarrow} P_{ab}^{(j)s} \epsilon_{bc}. \quad (5)$$

Q. 7 Verify that the quantities $A_{ac}^{[j]s}$ define an MPS ansatz of bond dimension $\chi = 2$ and explicitly derive the following expressions

$$A^+ = \frac{1}{\sqrt{2}} \hat{\sigma}^+, \quad A^0 = -\frac{1}{2} \hat{\sigma}^z, \quad A^- = -\frac{1}{\sqrt{2}} \hat{\sigma}^-, \quad (6)$$

with $\hat{\sigma}_{\pm} \equiv \frac{1}{2} (\hat{\sigma}^x \pm i\hat{\sigma}^y)$.

All in all, we ended up building the following MPS state, for a chain of N spin-1 particles with periodic boundary conditions:

$$|\Phi\rangle_{\text{AKLT}} = \sum_{s_1, s_2, \dots, s_N} \text{Tr} [A^{s_1} \cdot A^{s_2} \dots A^{s_N}] |s_1 s_2 \dots s_N\rangle, \quad (7)$$

and we want to argue that it is a ground state for a meaningful Hamiltonian defined for the N spin 1 particles. To this end, consider the following many-body Hamiltonian

$$\hat{H} = \sum_{j=1}^N \hat{\Pi}_{j, j+1}^{S=2}, \quad (8)$$

where each operators, $\hat{\Pi}_{j, j+1}^{S=2}$, projects into the subspace of total spin $S_{\text{tot}} = 2$ of the two neighboring sites j and $j+1$.

Q. 8 Argue that the spectrum of $\hat{H}$ is *non-negative*.

Q. 9 Use the explicit construction in terms of the virtual spin-1/2 degrees of freedom to deduce that

$$\hat{\Pi}_{j, j+1}^{S=2} |\Phi\rangle_{\text{AKLT}} = 0 \quad \forall j \Rightarrow \hat{H} |\Phi\rangle_{\text{AKLT}} = 0, \quad (9)$$

which in turn implies that $|\Phi\rangle_{\text{AKLT}}$ is a ground state for the Hamiltonian of Eq. (8).

It can be shown that the Hamiltonian of Eq. (8) can be recast (as a bonus question you can try to prove it) in the following more appealing form, involving the spin-1 matrices $\hat{S}_i^\alpha$, with $\alpha = x, y, z$:

$$\hat{H} = \frac{1}{6} \sum_{i=1}^N \left(\left(\vec{S}_i \cdot \vec{S}_{i+1} \right)^2 + 3\vec{S}_i \cdot \vec{S}_{i+1} + 2 \right). \quad (10)$$