Expectation values in MPS: Example of AKLT state

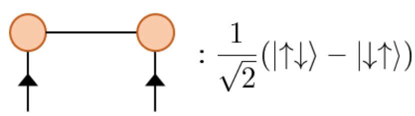
Author: Seung-Sup Lee

Before following this tutorial, it is necessary to solve Exercise (a) of tutorial "Canonical forms of MPS", since we will use the function `canonForm_Ex.m` to bring the MPSs into canonical forms.

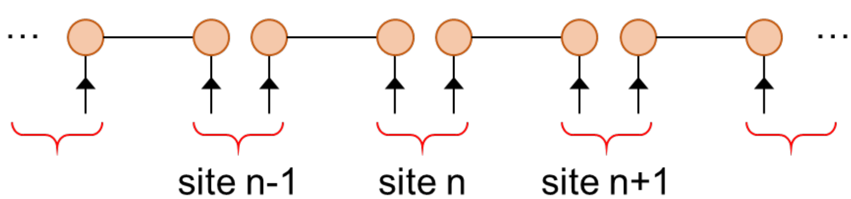
Quick introduction to the Affleck-Kennedy-Lieb-Tasaki (AKLT) state

The AKLT state is one of the most famous MPSs. Ian Affleck, Tom Kennedy, Elliott Lieb, and Hal Tasaki, who devised this state, showed it to be the exact ground state of the spin-1 chain model in which spins interact via the Heisenberg interaction and biquadratic interaction terms [I. Affleck *et al.*, Phys. Rev. Lett. **59**, 799 (1877)]. Despite its simple structure (see below), the AKLT state has rich, interesting physical properties. One such property is **symmetry-protected topological order**: there is a finite energy gap between the AKLT state (ground state) and excited states, and the symmetry of the system is not broken. The AKLT state can be generalized to the ground states of the Haldane phase (named after Duncan Haldane) of the spin-1 chain model. Indeed, Haldane's contribution to the theory of topological phases of matter was the main reason to award him the 2016 Nobel Prize in Physics! In this tutorial, we will use the AKLT state as just an example to practice computing expectation values, without explaining further physical implications. The details of the AKLT state will be covered later in the lecture course. Interested students may refer to the Wikipedia page.

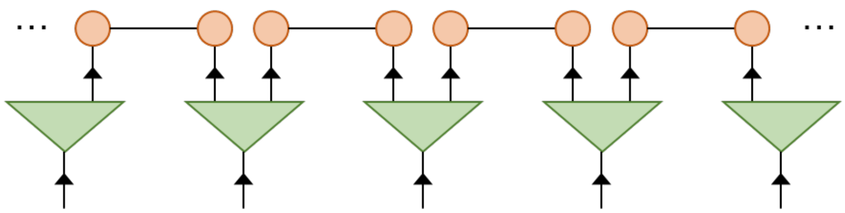
The spin-1 AKLT state can be understood as a product state of valence bonds. First, one associates each spin-1 particle on each physical site with two spin-1/2 (virtual) particles, and each of which forms a spin singlet, i.e, a valence bond, with the virtual particles on its neighboring site. The tensor diagram representation of such spin singlet is:



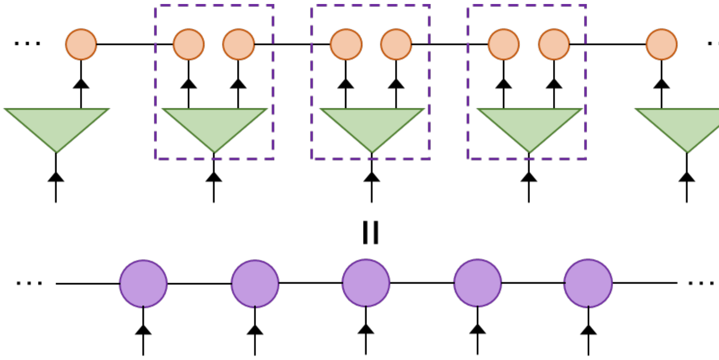
Here all legs have dimension 2. The physical legs (bottom legs) have dimension 2 since they are associated with spin-1/2's. And the horizontal leg connecting vertices is of size 2 since the Schmidt rank (i.e. number of nonzero Schmidt coefficients, or equivalently, of singular values) is 2. Then we arrange the singlets, and associate the right physical leg of one singlet and the left physical leg of the singlet on its right into each physical site.



Each site has two spin-1/2's, so the total spin of the site can be either $S = 0$ or $S = 1$. Then we project the local spaces into the $S = 1$ subspace.



The triangles denote the isometries that map the Hilbert space of one spin-1 into a subspace of the product space of two spin-1/2's. By contracting the tensors associated with the same site (marked by the dashed-line box), we obtain the rank-3 tensors that constitute the AKLT state as an MPS.



By construction, all the tensors here are identical. The left and right legs of each tensor have dimension 2, which corresponds to the Schmidt rank 2 of the spin singlet. The physical (bottom) legs have dimension 3, for the spin-1's, with index values 1, 2, and 3 representing the local spins states $|S_z = +1\rangle$, $|S_z = 0\rangle$, and $|S_z = -1\rangle$, respectively.

Generate the AKLT state

We will generate the AKLT state on a finite chain of length `N`. The tensor at each bulk site (i.e., any site except the left- and rightmost sites) is defined as 3-dimensional array, `AKLT`:

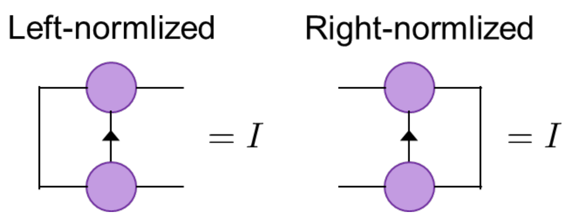
```
clear

AKLT = zeros(2,3,2);
% local spin Sz = -1
AKLT(2,1,1) = -sqrt(2/3);
% local spin Sz = 0
AKLT(1,2,1) = -1/sqrt(3);
AKLT(2,2,2) = +1/sqrt(3);
% local spin Sz = +1
AKLT(1,3,2) = sqrt(2/3);

N = 50; % number of sites
M = cell(1,N); % MPS
M(:) = {AKLT};
```

As we are considering a finite system with open boundary condition, the left- and rightmost legs of the MPS should have dimension 1, to represent a single global quantum state. Therefore, we project the space of the left leg of `M{1}` and the space of the right leg of `M{end}` onto the subspaces of size 1 for each leg. Since the left and right legs have dimension 2, there are $4 = 2 \times 2$ different global states, which are linearly independent. We'll denote them by $|\psi(\alpha, \beta)\rangle$ with $\alpha = 1, 2$ is chosen for the left leg of `M{1}` and $\beta = 1, 2$ for the right leg of `M{end}`. For example, we obtain $|\psi(1, 1)\rangle$ by:

```
M{1} = M{1}(1,:,:);
M{end} = M{end}(:,:,1);
```

[**Warm-up exercise**: Draw the tensor network diagram of the valence bonds and the isometries, for a finite MPS with open boundary condition. Observe that the projection of the leftmost and rightmost legs corresponds to a **boundary condition** which fixes the states of the virtual spin-1/2 particles at the left and right ends.]

Let us check that the bulk tensors are **both left- and right-normalized at the same time**.




```
% check whether left-normalized
T = contract(conj(AKLT),3,[1 2],AKLT,3,[1 2]);
disp(T - eye(size(T))); % all zeros
```

```
     0     0
     0     0
```

```
% check whether right-normalized
T = contract(conj(AKLT),3,[2 3],AKLT,3,[2 3]);
disp(T - eye(size(T))); % all zeros
```

```
     0     0
     0     0
```

Note that the bra tensor is obtained as the complex conjugate of the ket tensor, via `conj`. Of course, `M{1}` is only right-normalized and `M{end}` is only left-normalized, since their left/right legs are projected by boundary condition.

```
T = contract(conj(M{1}),3,[1 2],M{1},3,[1 2]);
disp(T); % not left-normalized
```

```
    0.3333         0
         0    0.6667
```

```
T = contract(conj(M{1}),3,[2 3],M{1},3,[2 3]);
disp(T); % right-normalized
```

```
     1
```

```
T = contract(conj(M{end}),3,[1 2],M{end},3,[1 2]);
disp(T); % left-normalized
```

```
     1
```

```
T = contract(conj(M{end}),3,[2 3],M{end},3,[2 3]);
disp(T); % not right-normalized
```

```
    0.3333         0
         0    0.6667
```

For computing the expectation values, it is convenient to normalize the MPS. (Otherwise, one needs to divide the expectation value with the square of the norm of the MPS.) Let's bring the MPS into its left-canonical form, without loss of generality.

```
% transform into left-canonical form
[M,S] = canonForm_Ex(M,numel(M));
fprintf('Norm of MPS = %.4g\n',S);
```

```
Norm of MPS = 0.7071
```

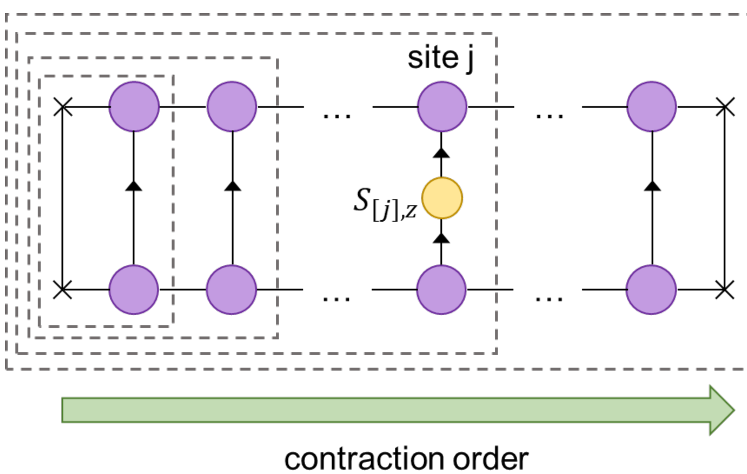
Note that the norm is not unity.

Magnetization

We can compute the local magnetization as the MPS expectation value of the spin-z operator $S_{[j],z}$ acting onto site j. Since we associated the local spin states $|S_z = +1\rangle, |S_z = 0\rangle$, and $|S_z = -1\rangle$ with the indices 1, 2, and 3 within the physical leg space, the spin-z operator can be implemented as:

```
Sz = diag([+1;0;-1]);
```

To compute the expectation value, we contract the tensors from the left:




```
j = 10; % index of site on which Sz operator acts

% T: the contraction of bra/ket/Sz tensors
T = 1; % identity in the dummy leg space for the leftmost leg
% leg order of T and Sz:
%   bottom (towards bras) - top (towards kets)
for it = (1:numel(M))
    T = contract(T,2,1,conj(M{it}),3,1);
    if it == j % contract Sz
```

```
        T = contract(T,3,2,Sz,2,1,[1 3 2]);
        % permute to have leg order left-physical-right
    end
    T = contract(T,3,[1 2],M{it},3,[1 2]);
end

fprintf('Magnetization at site %i = %.4g\n',j,T);
```

```
Magnetization at site 10 = 3.387e-05
```

Exercise (a): Magnetization

In the demonstration above, the code computes the magnetization at only one site, by contracting all the tensors from the left end to the right end. However, as the MPS was already brought into the left-canonical form, one can start from the site j, not from the left end. Keeping this in mind, **compute the magnetization for all chain sites**. And compare the result with the exact analytic result, for all different boundary conditions:

$$\langle\psi(1,1)|S_{[j],z}|\psi(1,1)\rangle = -\langle\psi(2,2)|S_{[j],z}|\psi(2,2)\rangle = \frac{\left(-\frac{1}{3}\right)^{j} - \left(-\frac{1}{3}\right)^{N-j+1}}{\frac{1}{2}\left[1+\left(-\frac{1}{3}\right)^{N}\right]}$$

$$\langle\psi(1,2)|S_{[j],z}|\psi(1,2)\rangle = -\langle\psi(2,1)|S_{[j],z}|\psi(2,1)\rangle = \frac{\left(-\frac{1}{3}\right)^{j} + \left(-\frac{1}{3}\right)^{N-j+1}}{\frac{1}{2}\left[1-\left(-\frac{1}{3}\right)^{N}\right]}$$

Compute the magnetization for all chain sites again, by using the different definition of bulk tensors:

```
AKLT = zeros(2,3,2);
% local spin Sz = -1
AKLT(2,1,1) = -sqrt(2/3); % same
% local spin Sz = 0
AKLT(1,2,1) = -1i/sqrt(3); % changed
AKLT(2,2,2) = +1i/sqrt(3); % changed
% local spin Sz = +1
AKLT(1,3,2) = sqrt(2/3); % same
```

And check the results from different bulk tensors are the same. [**Quick question**: Why do they need to be the same?]

Exercise (b): Spin-spin correlation

Compute the correlation function between the spin-z operators at nearest-neighbor sites j and $j+1$. Compare this with the exact analytic result:

$$\langle\psi(1,1)|S_{[j],z}S_{[j+1],z}|\psi(1,1)\rangle = \langle\psi(2,2)|S_{[j],z}S_{[j+1],z}|\psi(2,2)\rangle = \frac{\left(-\frac{2}{9}\right) - 2\left(-\frac{1}{3}\right)^{N}}{\frac{1}{2}\left[1+\left(-\frac{1}{3}\right)^{N}\right]}$$

$$\langle\psi(1,2)|S_{[j],z}S_{[j+1],z}|\psi(1,2)\rangle = \langle\psi(2,1)|S_{[j],z}S_{[j+1],z}|\psi(2,1)\rangle = \frac{\left(-\frac{2}{9}\right) + 2\left(-\frac{1}{3}\right)^{N}}{\frac{1}{2}\left[1-\left(-\frac{1}{3}\right)^{N}\right]}$$