Expectation values in the AKLT state

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Generate the AKLT state

We will generate the AKLT state on a finite chain of length L. 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(2,2,3);
% local spin S_z = +1
AKLT(1,2,1) = sqrt(2/3);
% local spin S_z = 0
AKLT(1,1,2) = -1/sqrt(3);
AKLT(2,2,2) = +1/sqrt(3);
% local spin S_z = -1
AKLT(2,1,3) = -sqrt(2/3);

L = 50; % number of sites
M = cell(1,L); % 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,:);
```

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 3],AKLT,3,[1 3]);
disp(T - eye(size(T))); % all zeros
```

```
     0     0
     0     0
```

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

```
    0.3333         0
         0    0.6667
```

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

```
     1
```

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

```
     1
```

```
T = contract(M{end},3,[2 3],conj(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(M,numel(M),[],0);
fprintf('Norm of MPS = %.4g\n',S);
```

```
Norm of MPS = 0.7071
```

Note that the norm was not unity. Now the MPS represented by the cell array `M` is normalized.

Magnetization

We can compute the local magnetization as the MPS expectation value of the spin-z operator $S_{[n]z}$ acting onto site $n = 10$. The spin-z operator can be obtained by using `getLocalSpace`:

```
[S,I] = getLocalSpace('Spin',1);
Sz = S(:,:,2); % spin-z
Sz
```

```
Sz = 3×3
     1     0     0
     0     0     0
     0     0    -1
```

Then we contract tensors in a way of "closing the zipper", from left to right. We initialize the contraction result T as 1. Here the spin-z operator is regarded as rank-2. Note that the `updateLeft` function has been slightly updated to treat the case `rankC` = `rankX` = 2; see its documentation for details.

```
T = 1;
n = 10; % index of site on which Sz operator acts
for itN = (1:numel(M))
    if itN == n
        T = updateLeft(T,2,M{itN},Sz,2,M{itN});
    else
        T = updateLeft(T,2,M{itN},[],[],M{itN});
    end
end
fprintf('Magnetization at site %i = %.4g\n',n,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 n, not from the left end. Keeping this in mind, **compute the magnetization for all chain sites**. And compare the results with the exact analytic results, for all different boundary conditions $\alpha, \beta = 1, 2$:

$$\langle \psi(\alpha,\beta) | \widehat{S}_{[n]z} | \psi(\alpha,\beta) \rangle = 2(-1)^{\alpha} \frac{(-1/3)^n - (-1)^{\alpha+\beta}(-1/3)^{L-n+1}}{1+(-1)^{\alpha+\beta}(-1/3)^L}.$$

Exercise (b): Spin-spin correlation

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

$$\langle \psi(\alpha,\beta) | \widehat{S}_{[n+1]z} \widehat{S}_{[n]z} | \psi(\alpha,\beta) \rangle = \frac{(-4/9) - 4(-1)^{\alpha+\beta}(-1/3)^L}{1+(-1)^{\alpha+\beta}(-1/3)^L}.$$

Note that the correlation function does not depend on n.