Exercise 7.1: Matrix product state (MPS) basics

An MPS is just a different representation of $|\psi\rangle = \sum_{j_1,\ldots,j_L \in \{0,1\}} \psi_{j_1,\ldots,j_L} |j_1,\ldots,j_L\rangle$, namely

$$|\psi\rangle = \sum_{j_1,\ldots,j_L} \sum_{\alpha_2=0}^{\chi_2-1} \cdots \sum_{\alpha_L=0}^{\chi_L-1} M^{[1]j_1}_{\alpha_1\alpha_2} M^{[2]j_2}_{\alpha_2\alpha_3} \ldots M^{[L]j_L}_{\alpha_L\alpha_{L+1}} |j_1, j_2, \ldots, j_L\rangle \,. \tag{1}$$

For open boundary conditions [1], α_1 and α_{L+1} are dummy indices with a single entry only ($\chi_1 = \chi_{L+1} = 1$), such that the matrix product of the Ms for a given index combination $(j_1, \ldots, j_L)$ yields a 1×1 matrix which we can identify as the coefficient $\psi_{j_1,\ldots,j_L}$.

a) As in Exercise 6.2, generate the ground state of the transverse field Ising model with open boundary conditions for $L = 14, g = 1.5, J \equiv 1$. Make sure it is normalized to $\langle\psi|\psi\rangle = 1$.

b) Write a function `compress(psi, L, chimax)`, which takes the state, the length of the chain and the maximal desired bond dimension `chimax` as input and compresses the state into MPS form using successive SVDs. It should return a list of L numpy arrays, namely the $M^{[n]}$, each with 3 indices $(\alpha_n, j_n, \alpha_{n+1})$.

Hint: Let us define the indices $R_n = (j_n, j_{n+1}, \ldots, j_L)$, such that $R_1 \equiv i$.

First, introduce the dummy index α_1 with a reshape of psi into shape $(1, 2^L)$ for the indices α_1, R_1 Then you can perform a loop over n which generates one $M^{[n]}$ in each iteration by splitting $\psi_{\alpha_n,R_n} = M^{[n]j_n}_{\alpha_n,\alpha_{n+1}} \psi_{\alpha_{n+1},R_{n+1}}$. The necessary steps for this iteration are:

- Reshape ψ_{α_n,R_n} into shape $(\chi_n \cdot 2, \dim(R_{n+1}))$. Note that $\dim(R_n) = 2^{L-(n-1)}$. This corresponds to a regrouping of the indices into $L_n \equiv (\alpha_n, j_n)$ and $R_{n+1} = (j_{n+1}, j_{n+2}, \ldots, j_L)$.
- Perform an SVD to split $\psi_{L_n,R_n} = \sum_{\alpha_{n+1}} M_{L_n,\alpha_{n+1}} \lambda_{\alpha_{n+1}} \tilde{\psi}_{\alpha_{n+1},R_{n+1}}$.
- If necessary, truncate to smaller dimension $\chi_{n+1} \leq \chi_{max}$. With numpy arrays, this can be done as follows:

```
keep = np.argsort(lambda_n)[::-1][:chimax]
M_n = M_n[:, keep]
lambda_ = lambda_n[keep]
psitilde = psitilde[keep, :]
```

- Reshape $M^{[n]}$ into shape $(\chi_n, 2, \chi_{n+1})$ to obtain the indices $(L_n, \alpha_{n+1}) \to (\alpha_n, j_n, \alpha_{n+1})$.

[1] for periodic boundary condition the MPS would be

$$|\psi\rangle = \sum_{j_1,\ldots,j_L} \sum_{\alpha_2=0}^{\chi_2-1} \cdots \sum_{\alpha_L=0}^{\chi_L-1} \mathrm{Tr}\left[M^{[1]j_1}_{\alpha_1\alpha_2} M^{[2]j_2}_{\alpha_2\alpha_3} \ldots M^{[L]j_L}_{\alpha_L\alpha_{L+1}}\right] |j_1, j_2, \ldots, j_L\rangle \,. \tag{2}$$

- Re-absorb the Λ_n into $\psi_{\alpha_{n+1},R_{n+1}} = \lambda_{\alpha_{n+1}}\tilde{\psi}_{\alpha_{n+1},R_{n+1}}$ using
  `psi = lambda[:, np.newaxis] * psitilde[:, :]`

The final $\psi_{\alpha_{L+1},R_{L+1}}$ is just a 1×1 matrix containing at most a phase (and overall norm of ψ, you can simply discard it.

c) What is the maximally necessary bond dimension for $L = 14$? Call `compress()` for the ground state with χ_{max} larger than that to get an *exact* MPS representation $\left|\psi_{ex}^{MPS}\right\rangle$.

d) Call `compress()` again with $\chi_{max} = 10$ to get a compressed MPS $\left|\psi_{compr}^{MPS}\right\rangle$. Compare the number of floats stored in both MPS.

Hint: The number of elements in a numpy array M are given by `M.size`.

e) Write a function to calculate the overlap between two MPS. Recall from class that there is an inefficient way (first contracting the bra and ket on top and bottom separately and finally contracting over the $j_1, \dots j_n$) and an efficient way (contracting from left to right); implement the efficient one! Check that the overlap $\left\langle\psi_{ex}^{MPS}\middle|\psi_{ex}^{MPS}\right\rangle$ is (close to) 1 and calculate the overlap $\left\langle\psi_{ex}^{MPS}\middle|\psi_{compr}^{MPS}\right\rangle$.

f) Write the state $|\uparrow\uparrow\cdots\uparrow\rangle$ as an MPS with bond dimension 1. Calculate the overlap of this state with the ground state (using MPS techniques, i.e. use the function you wrote in e)).

Exercise 7.2: The AKLT model

In this exercise we will consider the construction of a MPS of a non-trivial quantum state. Namely, the ground state of the *Affleck-Kennedy-Lieb-Tasaki* model introduced in 1987 [2]. The **spin-1** Hamiltonian is given by

$$\hat{H} = \sum_i \boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \frac{1}{3}\left(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}\right)^2. \tag{3}$$

This model has by construction a ground state in which all nearest neighboring spins share a valence bond, i.e. a spin-$\frac{1}{2}$ singlet

$$\frac{|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle}{\sqrt{2}}. \tag{4}$$

This means that each spin-1 can be thought to be broken up in two spin-$\frac{1}{2}$, and each of the spin-$\frac{1}{2}$ forms a singlet with a spin-$\frac{1}{2}$ on the adjacent site (see also Fig. 1 (d) and (e)).

a) First construct a dimerized **spin-$\frac{1}{2}$** chain of singlets, i.e. we consider a **product of singlets** $\left(\frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle\right) \otimes \cdots \otimes \left(\frac{1}{\sqrt{2}}|\uparrow\downarrow\rangle - \frac{1}{\sqrt{2}}|\downarrow\uparrow\rangle\right)$ on neighboring sites. Convince yourself that this state can be written in the MPS framework with 1×2 matrices on odd sites and 2×1 matrices on even sites given by

$$M^{[2n-1]\uparrow} = \begin{pmatrix}\frac{1}{\sqrt{2}} & 0\end{pmatrix}, \quad M^{[2n-1]\downarrow} = \begin{pmatrix}0 & \frac{-1}{\sqrt{2}}\end{pmatrix}, \quad M^{[2n]\uparrow} = \begin{pmatrix}0\\1\end{pmatrix}, \quad M^{[2n]\downarrow} = \begin{pmatrix}1\\0\end{pmatrix}. \tag{5}$$

[2] see Affleck, Kennedy, Lieb, Tasaki. "Rigorous results on valence-bond ground states in antiferromagnets". PRL 59 (7): 799–802, 1987.

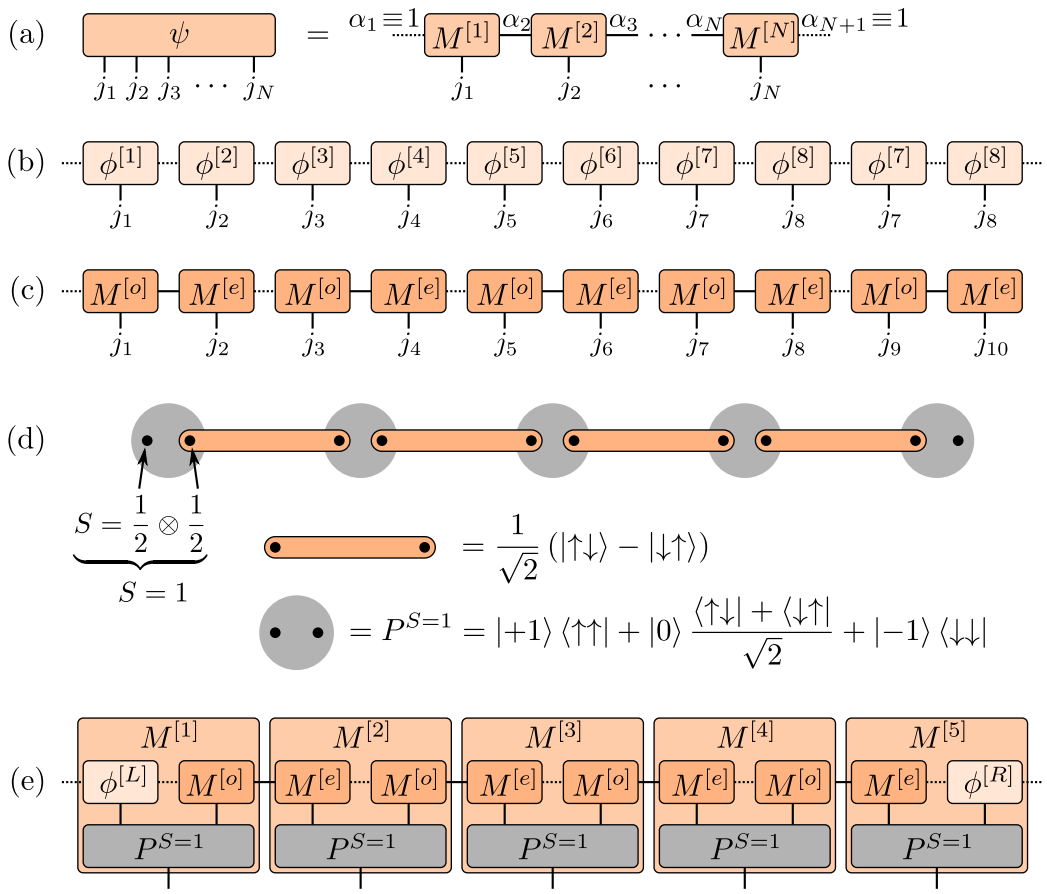

Figure 1: (a) In an MPS, the amplitude of the wave function is decomposed into a product of matrices $M^{[n]j_n}$. The indices α_1 and α_{N+1} are trivial, which we indicate by dashed lines. (b) A product state can be written as a trivial MPS with bond dimensions $\chi = 1$. (c) The MPS for a product of singlets on neighboring sites, with $M^{[1]}, M^{[2]}$ given in eq. (5). (d) Diagrammatic representation of the AKLT state. The $S = 1$ sites (grey circles) are decomposed into two $S = \frac{1}{2}$ that form singlets between neighboring sites. With open boundary conditions, the $S = \frac{1}{2}$ spins on the left and right are free edge modes leading to a four-fold degeneracy of the ground state. (e) The AKLT state can be represented by an MPS with bond dimension $\chi = 2$. - Figure from Johannes lecture notes, see `https://arxiv.org/abs/1805.00055`.

This is shown in Fig. 1 (c) in which the bold lines represent the singlet bonds with bond dimension 2. We will work with open boundary conditions, and we will put single spins-$\frac{1}{2}$ on the edges (to make the AKLT projection later on) but they do not matter. So you can just for instance choose them up.

b) Use the overlap function between two MPS that you wrote in the previous exercise to check the norm of this singlet MPS, and to compute the spin-correlation function $\langle \sigma_i^z \sigma_j^z \rangle$. You should observe that this gives always 0 for $|i - j| > 1$.

c) Construct the spin-1 projector and apply it to the singlet MPS as shown in Fig. 1 (d) and (e). This gives the MPS representation of the AKLT ground state.

d) Check the normalization of your AKLT MPS ground state (again using the overlap function), make sure it is normalized.

e) Calculate the correlation function $|\langle S_i^z S_j^z \rangle|$ (again using the overlap function), and plot it as a function of the distance $|i-j|$, what do you observe ?