UNIVERSITEIT VAN AMSTERDAM

Advanced Numerical Methods in Many-Body Physics - Homework 3

Tensor Networks

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Exercises

Exercise 1

For this first exercise we perform some operations on the Heisenberg model hamiltonian

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}_i^z \hat{S}_j^z + \frac{1}{2} \left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+ \right)$$

First of all, we construct the matrix form of the 2-site hamiltonian using Kronecker products the same way as in the exercise for exact diagonalization, and reshape it into the desired tensor form,

$$\left[H_{2\ \mathrm{s}}^z\right]_{j1j_2}^{i_1 i_2} = \left[S_1^z\right]_{j_1}^{i_1} \otimes \left[S_2^z\right]_{j_2}^{i_2} = \left[H_{2s}^z\right]_{\mathrm{j}}^{\mathrm{i}}$$

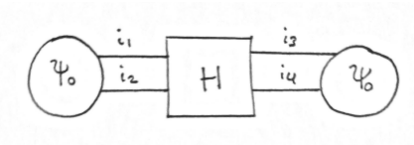
the result is a $(2, 2, 2, 2)$ tensor, and the elements of the $\hat{S}_1^z \hat{S}_2^z$ term are in positions $(1, 2, 2, 1)$ and $(2, 1, 1, 2)$ as we expected them to be. Then, we calculate the eigenvalues and eigenvectors of the hamiltonian in its matrix form. The ground state is given by the singlet term

$$|\psi\rangle = \frac{1}{\sqrt{2}} |+-\rangle - \frac{1}{\sqrt{2}} |-+\rangle$$

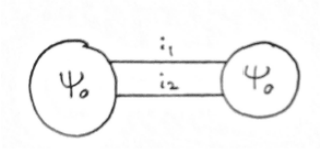
while its matrix form after reshaping it to a $(2, 2)$ matrix is:

$$|\psi_0\rangle_{i_1 i_2} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} & 0 \end{pmatrix}$$

The tensor network diagram corresponding to the computation $\langle \psi_0 | H | \psi_0 \rangle$ is given by



while for $\langle \psi_0 \mid \psi_0 \rangle$ is



using np.tensordot we obtain the values

$$\langle \psi_0 | H | \psi_0 \rangle = -0.75$$

$$\langle \psi_0 | \psi_0 \rangle = 1$$

Lastly we apply the function numpy.transpose. Applying it over the groundstate $|\psi_0\rangle_{i_1 i_2}$ and calculating the contraction $\langle\psi_0 \mid \psi_0\rangle$ we see how if we transpose only one of the matrices, the result changes it's parity while applying it over both matrices returns the same value

$$\langle \psi_0^T | \psi_0 \rangle = -1$$

$$\langle \psi_0^T | \psi_0^T \rangle = 1$$

this is due to the form of the ground state given above. On the other hand, we can see how the tensor form of the hamiltonian is hermitian by applying the transpose operation and comparing both forms. Using Python's comparison operator, we can check how all elements are equal for both the transposed and not transposed tensor forms.

Exercise 2

In this exercise we get familiar with some basic concepts of tensor network methods. First of all we compute the ground state of a $S = 1/2$ Heisenberg chain with open boundary conditions and $N = 16$ using the sparse matrix diagonalization code used for the previous hand-in. The result is a $2^{16} = 65536$ dimensional vector.

Then, we can split the ground state in the middle of the chain using SVD by reshaping it into a square matrix of size 256×256 in order to apply the partition in the middle of the chain and then applying the SVD command on Numpy. The resulting entanglement entropy is given by the formula

$$S_A = -\sum_k p_k \log p_k = 0.592$$

applied over the squared singular values $p_k = s_k^2$. We do the same but this time over a random state in Hilbert space. To generate this random state, we perform a sum over the first 50 eigenvectors of the hamiltonian with some random normalized amplitudes α_i. The resulting entanglement entropy is now

$$S_A = 1.304$$

We see how the random state has a higher entanglement entropy, as expected.

We can plot the eigenvalues for both the ground state and the random state to observe their behavior with respect to the position. In logarithmic scale, it is given by Figure 1. We observe how the first 100 eigenvalues of the random state contribute much more to the reduced density matrix than the first 100 eigenvalues of the random state. Thus, keeping only the first D Schmidt coefficients s_k when computing the truncation of the MPS will be a better approximation for the ground state than for an arbitrary random state.

To finish the exercise, we calculate the relative error of the energies between the exact solutions and the approximate solutions taking some value for the maximal bond D. To do this, we have to invert the SVD decomposition after truncation in order to build the approximated wave function. In logarithmic scale, it is given by Figure 2. We can observe how the relative difference between the exact and the approximated energies decreases much faster for the ground state, reaching machine precision at approximately $D \approx 60$, while for the random state it also decreases albeit much more slowly.

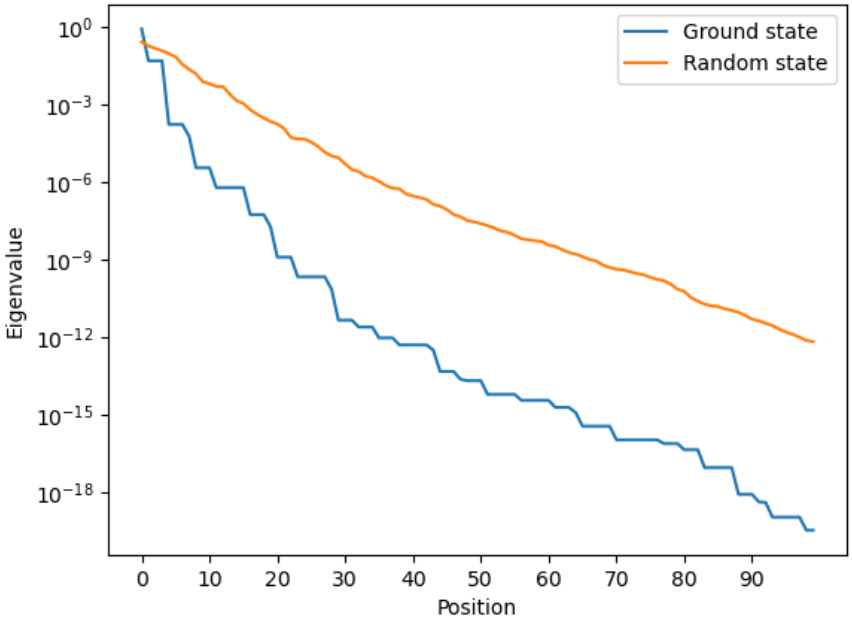


Figure 1: *Reduced density matrix eigenvalues for the ground state and the random state*

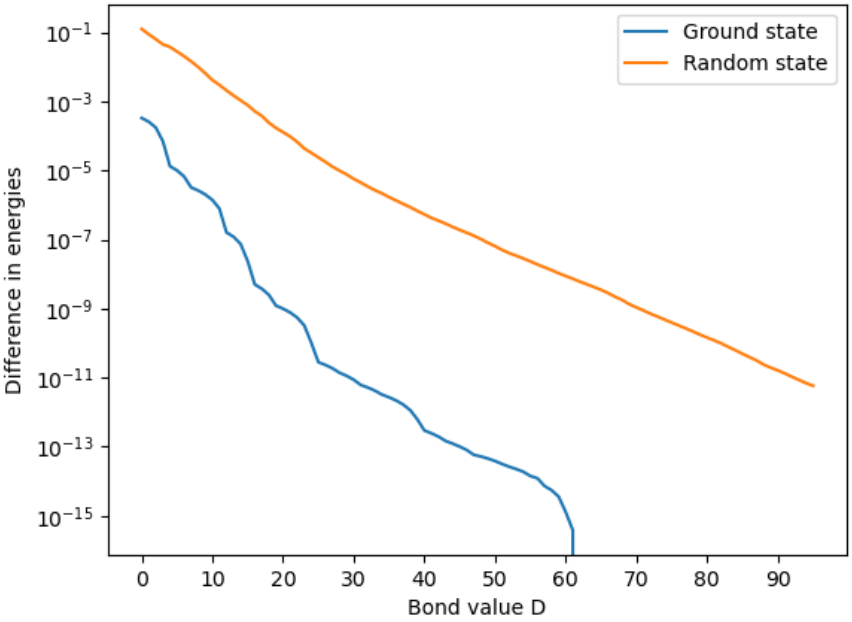


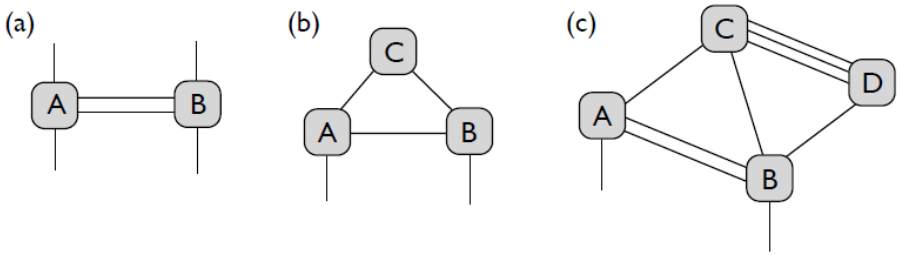
Figure 2: *Relative variation in energy for the ground state and random state*

Exercise 3

For this exercise, we do a full decomposition of a state into an MPS by using a sequence of SVDs. Unfortunately I've been incapable of programming a code that properly implements the MPS decomposition because I didn't know how to thread together the dimensions and number of elements of the distincts matrices of the SVD, so only an outline of the code which would've been used is provided.

Exercise 4

In this exercise we calculate the computational cost of the following tensor network contractions.



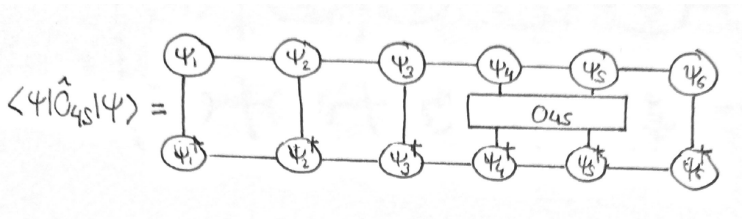
We know from the lecture notes that the computational cost can be determined by counting the number of involved legs in the diagram, each contributing with a bond dimension D. Therefore, the computational cost for a total contraction of the diagrams is

- $O(D^6)$ for diagram a)
- $O(D^5)$ for diagram b)
- $O(D^{10})$ for diagram c)

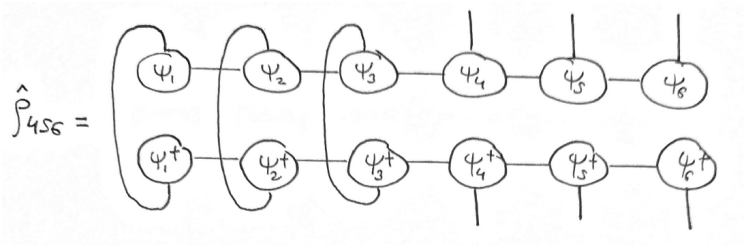
Exercise 5

In this exercise we represent the following formulas as a tensor network:

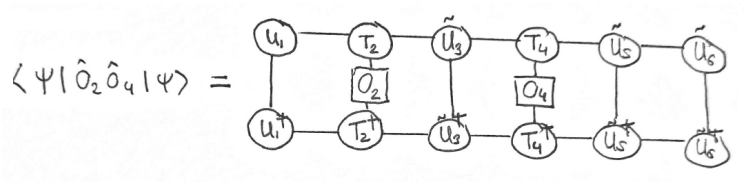
A. $\left\langle \Psi \middle| \hat{O}_{45} \middle| \Psi \right\rangle$, where $\hat{O}_{45}$ is a 2 -site operator acting on sites 4 and 5.



B. $\hat{\rho}_{456} = \mathrm{Tr}_{123}\,\hat{\rho}$, where Tr_{123} is the trace over sites $1, 2, 3$, and $\hat{\rho}_{456}$ is the reduced density matrix on sites $4, 5, 6$, and $\hat{\rho} = |\Psi\rangle\langle\Psi|$ the density operator (pure state).



C. $\left\langle \Psi \middle| \hat{O}_2 \hat{O}_4 \middle| \Psi \right\rangle$, assuming that the MPS is in a mixed canonical form. Draw how the network simplifies in this case. The operators $\hat{O}_2$ and $\hat{O}_4$ are one-site operators acting on sites 2 and 4 , respectively.



The network simplifies as