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Computational Quantum Physics
Exercise Sheet 4

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Exercise class in HCI J7 or via Zoom, Meeting ID: 6929 2810 031

Exercise 1. MPS representations

The goal of this exercise is to find Matrix Product State (MPS) and Matrix Product Operator (MPO) expressions of particular states and the Heisenberg Hamiltonian (analytically).

1. Find a set of MPS tensors encoding the state

$$|\Psi_1\rangle = \frac{1}{\sqrt{2}}(|01010...\rangle + |10101...\rangle) \tag{1}$$

   for N spins. Distinguish between even and odd number of spins.

   Hint: Modify the MPS representation of the GHZ state discussed in the lecture.

2. Find the MPS representation of the state

$$|\Psi_2\rangle = \frac{1}{\sqrt{2}^N}(|0\rangle + |1\rangle)^{\otimes N}, \tag{2}$$

   with N an arbitrary number of spins.

It has been discussed in the lecture that an MPS can be written in Vidal's canonical form:

$$|\Psi\rangle = \sum_{\sigma_1,\dots,\sigma_N} \Lambda^{[0]}\Gamma^{[1]\sigma_1}\Lambda^{[1]}\Gamma^{[2]\sigma_2}\Lambda^{[2]} \dots \Lambda^{[N-1]}\Gamma^{[N]\sigma_N}\Lambda^{[N]}, \tag{3}$$

where $\Lambda^{[i]}$ are diagonal matrices. For a system with open boundary conditions, $\Lambda^{[0]}$ and $\Lambda^{[N]}$ are scalars and determine the normalization. We can normalize the wavefunction by setting them to 1. Interestingly, the diagonal entries of the matrix $\Lambda^{[i]}$ correspond to the Schmidt values of a bipartion of the system between sites i and $i+1$.

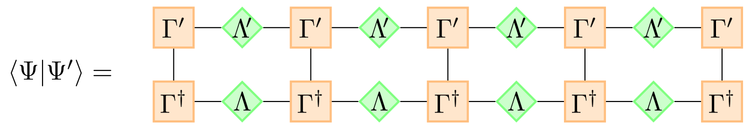
3. Find the canonical form of the MPS representation of the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$.

Exercise 2. Canonization and overlaps with MPS

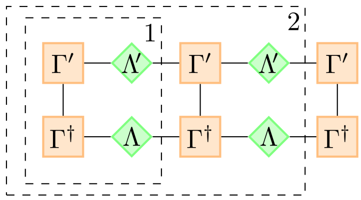
The goal of this exercise is to implement overlaps and expectation values using MPS and MPO. These calculations are much simpler when working in the Vidal canonical form (3), so we will first implement a canonization procedure. *Hint: you might find the following numpy functions useful: np.dot, np.tensordot, np.reshape, np.transpose, np.conj, np.linalg.svd.*

1. Given a general (non-canonical) MPS representation $M = [M^{[1]\sigma_1}, \dots, M^{[N]\sigma_N}]$ of a state $|\Psi\rangle$, write a function that constructs the Vidal canonical form and returns the matrices $[\Gamma^{[1]\sigma_1}, \dots, \Gamma^{[N]\sigma_N}]$ and $[\Lambda^{[1]}, \dots, \Lambda^{[N-1]}]$. Use the implemented function to determine the Vidal canonical form of the states $|\Psi_1\rangle$ and $|\Psi_2\rangle$ introduced in exercise 1 and compare to your result of exercise 1.3.

In the following, we assume that the MPS are in Vidal's canonical form. We start by evaluating the overlap between two states:



We efficiently evaluate the overlap by iteratively contracting the matrices, starting from the left and contracting one more site in each step. The first two steps of the iteration process are depicted in the following diagram:



Step 2 is repeated until the last site is reached (in the last step, only Γ matrices are included). Equivalently, one can start at the rightmost site and contract from the right to the left.

2. What would be the complexity (i.e. the number of terms) of the contraction operation, if we would first contract all matrix indices (horizontal legs in the diagram) and then all physical indices (vertical legs in the diagram)?

3. Given MPS representations of two states $|\Psi\rangle$ and $|\Psi'\rangle$ in Vidal's canonical form $[\Gamma^{[1]\sigma_1}, \dots, \Gamma^{[N]\sigma_N}]$, $[\Lambda^{[1]}, \dots, \Lambda^{[N-1]}]$ and $[\Gamma'^{[1]\sigma_1}, \dots, \Gamma'^{[N]\sigma_N}]$, $[\Lambda'^{[1]}, \dots, \Lambda'^{[N-1]}]$, write a function that evaluates their overlap $\langle\Psi|\Psi'\rangle$ as described above. Calculate the overlap between $|\Psi_1\rangle$ and $|\Psi_2\rangle$ for $N = 30$ spins. Verify the correct implementation of your function by calculating the normalization of an arbitrary MPS state in canonical form (should be equal to 1).