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Exercise class in HCI J7.

Exercise 1. Phase transition of transverse field Ising model

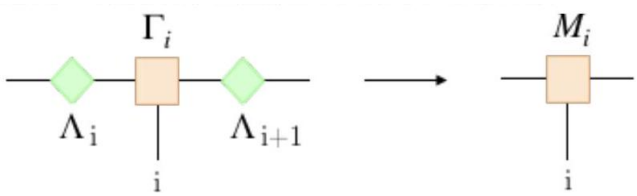
After implementing the necessary MPS/MPO routines and the DMRG algorithm in the last exercise sheets, we want to apply DMRG to the transverse field Ising model (TFIM). We have discussed the TFIM already in exercise sheet 4 on exact diagonalization (ED). The TFIM is described by the Hamiltonian

$$H = -J \sum_{i=1}^{L-1} S_z^i S_z^{i+1} + h \sum_{i=1}^{L} S_x^i \tag{1}$$

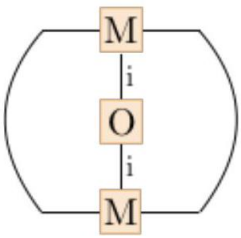
and undergoes a phase transition for $|h/J| = 1$. The goal of this exercise is to analyze this phase transition using DMRG, and thereby gain some intuition on the MPS representation of quantum states.

Part I: Preparations

1. We have seen the Vidal canonical form of an MPS in previous exercises. Implement a function that calculates the local matrices $M^{[i]}$ from the canonized Λ and Γ matrices.



2. One of the strengths of MPS is the calculation of local expectation values. If the MPS is in mixed canonical form, i.e. left-normalized up to site $i-1$ and right-normalized up to site $i+1$, calculating the expectation value of an operator $O^{[i]}$ at site i is very efficient. The contractions of the left- and right-normalized parts of the MPS reduce to identities, and we are left with a contraction involving only the local $M^{[i]}$ matrices and the operator. Implement a function that calculates the local expectation values of a single-site operator for all sites.



3. The phase transition of the TFIM can be observed at the antiferromagnetic order parameter

$$S_{\mathrm{AFM}} = \frac{1}{L}\sum_{i=1}^{L}(-1)^i S_z^i \tag{2}$$

Write a function that calculates $\langle\psi\,|S_{\mathrm{AFM}}|\,\psi\rangle$ for an MPS $|\psi\rangle$ in canonized form. Hint: use the local expectation values you implemented above.

4. Another strength of the canonized MPS form is that the local $\Lambda^{[i]}$ matrices contain the Schmidt values of the quantum state at each bond. As you have learned, we can obtain the entanglement entropy at bond i from these Schmidt values as

$$S_{\mathrm{ent}}(i) = -\sum_j \left(\Lambda_j^{[i]}\right)^2 \log\left(\Lambda_j^{[i]}\right)^2 \tag{3}$$

Implement a function to obtain the entanglement entropy from a Λ-matrix.

1. Use DMRG to calculate the ground state of the classical Ising model ($h = 0$). Use bond dimensions $\chi = 1$ and $\chi = 5$. Use the local expectation values implemented above to analyze the ground states and compare the results. What is the ground state and does it depend on the bond dimension?

2. Use DMRG to calculate the ground state with only the transverse field ($J = 0$). Again use bond dimensions $\chi = 1, 5$. What does the ground state look like now? Does it depend on the bond dimension?

3. For small system sizes, we can compare DMRG to exact diagonalization results. For $L = 8, J = -1$, different $h \in [-2, 2]$ and bond dimensions $\chi \in [1, 2, 4, 8, 16, 32, 64]$, compare the DMRG ground state energy to the exact result. For which values of h/J is the error the largest?

4. Use DMRG to find the ground state of the TFIM with $J = -1, h = 1$. Try different bond dimensions. If you plot the intermediate energies obtained from the local optimizations, you will see the convergence towards a final state. Does the final state depend on the bond dimension?

5. It is time to see the phase transition! Calculate $|\langle\psi\,|S_{\mathrm{AFM}}|\,\psi\rangle|$ for the DMRG ground states obtained for different $h \in [-2, 2]$ and a high enough bond dimension. Can you observe the phase transition?

6. Finally, we want to analyze the entanglement of the middle bond of our spin chain. For $L = 40, J = -1$, different $h \in [0.5, 1.5]$ and bond dimensions $\chi \in [1, 2, 4, 8, 16]$, calculate the entanglement entropy S_{ent} ($i = L/2$). What can you observe?

Exercise 2. TEBD and many-body localization*

This exercise is optional, but very cool!

In this exercise, we want to implement the time evolution of a many-body wavefunction, using time-evolving block decimation (TEBD) and study the many-body localization transition in the disordered Heisenberg model governed by

$$H = \sum_i \left(S_x^i S_x^{i+1} + S_y^i S_y^{i+1} + S_z^i S_z^{i+1} \right) + \sum_i h_i S_z^i \tag{4}$$

with $h_i \in [-W, W]$ chosen randomly.

Part I: Preparations

1. Write a function that generates a matrix product state in the canonical form for the antiferromagnetic state $|\uparrow\downarrow\uparrow\downarrow \ldots \uparrow\downarrow\rangle$ for a lattice of size L.

Part II: Implementation of TEBD

Time-evolving block decimation is a numerical method to evolve a matrix product state in time, which is particularly efficient in systems with limited entanglement.

1. First, implement the two-site Hamilton operator for the Heisenberg model with a random field h_i per site,

$$H_{i,i+1} = S_x^i S_x^{i+1} + S_y^i S_y^{i+1} + S_z^i S_z^{i+1} + \frac{1}{2}\left(h_i S_z^i + h_{i+1} S_z^{i+1} \right) \tag{5}$$

Note that the two-site operator looks slightly different for the first and second-last site.

2. We also need a function which computes the unitary time-evolution operator $U_{i,i+1} = \exp\left(-iH_{i,i+1}\Delta t\right)$ for each bond. The function scipy.linalg. expm might be helpful with this. Use this to create a list of all bond operators in the right order to iterate through.

3. Now we want to evolve the wavefunction by applying the operator U to our initial MPS. To this end, we first calculate the action on all even bonds, followed by all odd bonds. For each bond update we perform the following procedure:

a. Construct the two-site tensor at the sites $i, i+1$ by contracting the corresponding Λ and Γ matrices over their shared virtual bonds.

b. The resulting operator θ should be of rank 4, with two virtual and two physical indicies.

c. Apply the bond operator U.
d. To ensure that the wavefunction remains compressed with our chosen bond dimension $\chi_{\max}$,

we have to truncate it by performing a singular value decomposition on the tensor θ and keeping only the largest $\chi_{\max}$ singular values. The function scipy . linalg. svd might be helpful.

e. The SVD results in three new tensors, the new $\tilde{\Lambda}$ matrix of Schmidt values at bond $i+1$, and two tensors A, B left and right of it.

f. To bring the MPS back to canonical form, we multiply both tensors A, B with the inverse of Λ at the corresponding sites.

g. The final update of the MPS changes the Γ tensors at sites $i, i+1$ and updates the Λ values as obtained from the truncation.

This procedure is repeated for all bonds, first even then odd, and a given number of timesteps N. Throughout this procedure, you will need the function numpy.tensordot several times.

Part III: Disordered Heisenberg Model

The Heisenberg model in a random field can be used to study the transition between an ergodic and a localized phase. Starting from the antiferromagnetic state of Part I, a clean system is expected to evolve to zero antiferromagnetic order in thermal equilibrium. However, if the system is localized due to the presence of disorder, a finite antiferromagnetic order will remain. Additionally, an interesting property to study is the growth of the half-chain entropy. This quantity describes the entanglement between the two halves of the chain and changes significantly when entering the localized phase. If you are interested, check out https://arxiv.org/pdf/1202.5532.pdf to see the first numerical analysis of the effects of interactions on the many-body-localized phase (and compare it to your own results).

1. First, check convergence and bond truncation for several disorder strengths in a chain of length $L = 14$. How does the truncation error change with increasing disorder?

2. Reproduce the behaviour of the antiferromagnetic order parameter outlined above. To this end, plot the time evolution of the operator

$$S_{\mathrm{AFM}} = \frac{1}{L} \sum_i (-1)^i S_z^i \tag{6}$$

for various strengths W of the disorder potential.

3. Consider the entanglement-entropy growth of a cut in the middle of the chain $i = L/2$:

$$S_{\mathrm{ent}}\,(i) = -\sum_j \left(\Lambda_j^{[i]}\right)^2 \log\left(\Lambda_j^{[i]}\right)^2 \tag{7}$$

where $\Lambda_j^{[i]}$ are the Schmidt values at site i. Can you explain the behaviour for various disorder strengths W ?

Hint (optional): Average over several random fields in order to remove unwanted oscillations.