LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Fakultät für Physik im WS 2025/26
Advanced computational physics for many-body systems
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Sheet 6: Matrix Product State basics

In this exercise, we want to consider basic properties and operations to obtain and use matrix product states. We will make use of the simple spin-$1/2$ exact diagonalization code from Problem Sheet 2. If you have not written an exact diagonalization code at this point, you can use the very basic code provided in the moodle.

Problem 1 Getting your first matrix product state

We go back to the transverse field Ising model that we have considered before. You can use your basis and Hamiltonian representation from Problem Sheet 2, the basis should ideally use the binary representation.

a) We consider open boundary conditions and an even number of sites L. Calculate the ground state of the TFIM for your choice of parameter g/J. So far, this is the same as what you did e.g. for Problem Sheet 5.

b) We now want to follow the procedure discussed in the lecture in order to go from your 2^L dimensional vector representation of the ground state to a matrix product state representation. The following should be the content of a function that you define, which takes the maximum bond dimension you want your matrix product state to have as an input. The output of the function will be an array of matrices, representing your matrix product state. First, set up the function with its inputs and outputs.

c) Now, we start from the left and reshape the vector into a matrix. Then, perform an SVD to obtain matrices U, S, $V^\dagger$ (see lecture notes). At this point, if the dimensions are to big, the truncation occurs. This means that the lowest Schmidt values (contained in S) are discarded, and the dimensions of the matrices are adapted accordingly. U then has to be decomposed into the matrices A^{σ_1} of your matric product state.

d) The product of S and $V^\dagger$ is again a vector, which you in a next step reshape into a matrix again. From here on, the same steps are repeated, so you might want to have the operations in a loop in your code.

e) If you don't do any compression, with what bond dimension do you end up for a given system size (e.g. $L = 10$)?

Problem 2 Doing something with matrix product states

We now want to do some basic operations using matrix product states.

a) For this exercise, you need some matrix product state. Ideally, you do the first exercise first and thereby have a function that gives you a given quantum state as matrix product state. Alternatively, you can follow the lecture notes to represent a simple product state, or a state with singlets on nearest neighboring bonds as matrix product state. Write this function in a

general way, such that you can easily generate two different matrix product states, e.g. ground states of the TFIM at different values of g/J, or different product states, or states with singlets between even versus odd bonds.

b) Now we want to calculate the overlap between two MPS. Write a function that takes two MPS as input. In order to calculate the overlap, the matrices have to be multiplied. Follow the lecture where we discussed in which order to efficiently perform the necessary contractions. What is the overlap between the different states that you chose? As a consistency check, you can evalute the overlap of an MPS with itself.

c) Now we want to evaluate expectation values. Follow the lecture notes to write a new function that takes an MPS and an operator. If you want to calculate correlation functions like $\langle \S_i^z S_J^z \rangle$, what information do you need to pass to your function? This task is very similar to the overlap function you wrote before, but now you have to include an operator $\hat{O}$ (e.g. S^z) in your contractions. Calculate meaningful observables in the matrix product states you constructed and compare the outcome with your expectations.

d) Taking the compression from Exercise 1, you can now take the ground state of the TFIM and represent it as an MPS with a smaller bond dimension (i.e. some compression takes place, i.e. some Schmidt values are discarded). As a function of the maximum allowed bond dimension, how do energy and spin correlations in the corresponding MPS behave?