ETH
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Computational Quantum Physics
Exercise 3

FS 09
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Problem 3.1 Infinite DMRG

This week, we will implement the DMRG algorithm. As a short repetition, here are the steps of the algorithm:

1. Set up the Hamiltonian for block and environment consisting of very few spins, e.g. 2 each. You should use the code you wrote last week to perform this task. If you had **any** problems, **now** is the time to ask. Besides the Hamiltonian, you will need to keep some operators in order to be able to couple system and environment block to the new sites. What are these?

2. Construct the following Hamiltonians:

   - For system and environment, add one site and couple it to the old block. You also need to add all single-site terms on the new sites to this.
   - A term coupling the two new sites together.
   - The superblock Hamiltonian which puts everything together: system, two new sites, environment.

   It's probably a good idea to work out all terms on paper first, it's easy to forget something!

3. Diagonalize the superblock Hamiltonian and store the eigenvector with lowest energy. You can compare the energy you find here to your previous exact diagonalization results. As long as you don't truncate your basis, they should match exactly. **If they don't, do not proceed before you fix this!**

4. Calculate the reduced density matrix for a splitting of the superblock such that system and environment grow by one site each, tracing out the environment. Find the dominant M eigenvectors of this matrix; for the earliest iterations, it may well be that you do not have to truncate at all. The eigenvectors will give you the transformation matrix that you need to project into the new renormalized Hilbert space you're working in. You need to apply it

   - to the system-plus-one-site Hamiltonian that you found previously,
   - to all operators that you will need in the next iteration to couple that block to new sites; these are essentially the same that you kept in step 1,
   - to operators that you might want to measure later.

5. You can make use of the system's reflection symmetry to find the other block.

6. If the energy per site has not converged, go back to step 2.

Implement the above procedure and apply it to the Heisenberg model on a 1d chain that was previously examined with exact diagonalization.