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Computational Many-Body Physics

Assignment 7

Summer Term 2015

website: http://www.thp.uni-koeln.de/trebst/Lectures/2015-CompManyBody.shtml
due date: Bonus sheet – discuss with broecker [at] thp.uni-koeln.de

16. Hack away at the unessential

Introduction

The first method we learnt about to numerically study quantum lattice systems was exact diagonalization. It enabled us to study ground state and finite temperature properties of arbitrary models. Unfortunately, the exponentially large Hilbert space restricted us to putting these models on small lattices. On the previous sheet, you got to know stochastic series expansions as an unbiased way to learn about the finite temperature properties of a particular class of (sign-free) models on potentially large lattices. In this exercise, we will treat the third pillar of exact numerical methods which is the **Density Matrix Renormalization Group** (DMRG). Its significance can hardly be overemphasized, as it has basically solved the problem of calculating ground state properties of one dimensional quantum systems.

As background material, we would like to refer you to a number of relevant papers [1], [2], [3], [4], [5] tracing the development from the early days to modern formulations. This assignment follows the content of [3], expanding on some aspects if needed.

We reconsider the Heisenberg model and focus on determining the ground state energy of the *infinite* chain. Although working in the thermodynamic limit, it actually turns out to be the simpler algorithm to implement. Feel free though to also code the finite system algorithm discussed in detail in the lecture.

The algorithm

In this assignment, we will try to give a very detailed and hands-on description of how you should go about setting up the program. Because there will be quite a number of indices and parameters flying around, let us start by clearing up the notation. We are considering $SU(2)$ $s = 1/2$ spins on a chain lattice that interact via the Heisenberg Hamiltonian

$$H = -\sum_i S_i^z S_{i+1}^z + \frac{1}{2}(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+)\,. \tag{1}$$

The lattice consists of **sites** on which the degrees of freedom live. The degrees of freedom can appear in a number of states $|d_i\rangle$, where the i indexes the particular state out of D possible ones

and not the lattice site. In our case, each site carries the same $SU(2)$ representation and has states $|d_1\rangle = |\uparrow\rangle$, $|d_2\rangle = |\downarrow\rangle$. Multiple sites are grouped into **blocks** of length l. At the heart of DMRG is the truncation of the number of states describing these blocks, m. This number m is typically much smaller than the full Hilbert space dimension of the block and has to be adjusted throughout the simulation. In the literature, you will see this being referred to as the **bond dimension** or **number of states**. A block is denoted by $B(l,m)$ with the two parameters block (spatial) size l and block Hilbert space size m. Its Hamiltonian and states are then denoted by H_B and $\{|b_1\rangle, \ldots, |b_m\rangle\}$, respectively. Finally, we will enlarge a given block by adding another site. This enlarged block is described by states $\{|e_k\rangle\}$ that are a direct product of the block states $\{|b_1\rangle, \ldots, |b_m\rangle\}$ and the single site states $\{|d_1\rangle, \ldots, |d_D\rangle\}$:

$$|e_k\rangle = |b_i\rangle \otimes |d_j\rangle \,. \tag{2}$$

The index mapping from i, j to k can be done analogously to mapping the contents of a two dimensional array to a one dimensional one $k = (i-1) * D + j$.

Now that we have our notation straight, let us describe a single DMRG step in detail. Initially, we start with only a single site that is denoted as $B(1,2)$, meaning that the block is made up of 1 site that can be in 2 possible states, $|b_1\rangle = |\uparrow\rangle$ and $|b_2\rangle = |\downarrow\rangle$. Because no other sites are around, the Hamiltonian of this one site block H_B is 0. We now continue by adding an additional site to enlarge the current system with states $|d_1\rangle = |\uparrow\rangle$ and $|d_2\rangle = |\downarrow\rangle$. The combined basis is then

$$|e_{(1-1)D+1=1}\rangle = |b_1\rangle \otimes |d_1\rangle = |\uparrow\uparrow\rangle \,, \tag{3}$$
$$|e_{(1-1)D+2=2}\rangle = |b_1\rangle \otimes |d_2\rangle = |\uparrow\downarrow\rangle \,, \tag{4}$$
$$|e_{(2-1)D+1=3}\rangle = |b_2\rangle \otimes |d_1\rangle = |\downarrow\uparrow\rangle \,, \tag{5}$$
$$|e_{(2-1)D+2=4}\rangle = |b_2\rangle \otimes |d_2\rangle = |\downarrow\downarrow\rangle \,. \tag{6}$$

We also have to adjust the Hamiltonian, that is made up of the unmodified old Hamiltonian $H_B \otimes \mathbb{I}_D$ where the identity is added to account for the enlarged system. In addition, the rightmost site of the old block can interact with the new site via $S_b^+ \otimes S_d^-$, $S_b^- \otimes S_d^+$, and $S_b^z \otimes S_b^z$ resulting in the Hamiltonian for the enlarged block:

$$H_E = H_B \otimes \mathbb{I}_D + \frac{1}{2}\left(S_b^+ \otimes S_d^- + S_b^- \otimes S_d^+\right) + S_b^z \otimes S_d^z \tag{7}$$

After a few steps, the Hilbert space for this enlarged block Hamiltonian H_E will be larger than m (the desired number of states to be kept), which is why we have to truncate at some point.

Two enlarged blocks, one with an additional site on the right, the other one with an additional site on the left, have to be combined into a superblock. The operators on the left and right sites are index by l and r, respectively and given by $S_r^{z,+,-} = \mathbb{I}_b \otimes S_d^{z,+,-}$ and $S_r^{z,+,-} = S_d^{z,+,-} \otimes \mathbb{I}_b$, respectively. The superblock Hamiltonian H_S is made up of the Hamiltonian from the left enlarged block H_E, the right enlarged block H_E' and connecting operators:

$$H_S = H_E \otimes \mathbb{I}_{E'} + \mathbb{I}_E \otimes H_{E'} + \frac{1}{2}\left(S_E^+ \otimes S_{E'}^- + S_E^- \otimes S_{E'}^+\right) + S_E^z \otimes S_{E'}^z \,. \tag{8}$$

When representing this Hamiltonian in matrix form, we may restrict ourselves to the $S_z = 0$ sector to gain significant speed, but it is not necessary in a first version of the code. Using an Lanczos algorithm, we then find the ground state of this matrix. The ground state vector

encodes the contributions of the respective basis vectors in the product basis for the left and right enlarged block:

$$|\psi_0\rangle = \sum_{i=1}^{m\cdot D}\sum_{j=1}^{m'\cdot D} a_{ij}\,|e_i\rangle\,\left|e'_j\right\rangle\,. \tag{9}$$

We want to discard some of the weights and need to have a measure to do so. This is achieved by viewing the left enlarged block as the system and the right enlarged block as the environment. Forming the reduced density matrix is the first step to selecting the correct states.

$$\rho_{ii'} = \sum_{j=1}^{m'\cdot D} a_{ij}a^*_{i'j}\,. \tag{10}$$

Note that this reduced density matrix again has the same dimension as the enlarged block we set up previously. We quickly reiterate its most important properties: Given that the universe, i.e. the system and the environment together, is in state $|\psi_0\rangle$, the eigenvectors $|u_\alpha\rangle$ of the reduced density matrix are realized with probability w_α which are the eigenvalues of ρ. This contraction can be carried out without usage of the particular basis vectors because of the way we setup the combined basis using the product of the bases. The ground state vector we find from the diagonalization procedure will then be reshaped into a matrix with m rows and then multiplied from the right with its adjoint to give the reduced density matrix.

Only its m eigenvectors corresponding to the largest eigenvalues are kept and put into a matrix U that is subsequently used to perform a partial transformation on the enlarged Hamiltonian H_E resulting in the new block Hamiltonian $H_{B(l+1,m)}$:

$$H_{B(l+1,m)} = UH_EU^\dagger\,. \tag{11}$$

Finally, let us describe how to choose the environment in the infinite system algorithm: It is simply the mirror image of the enlarged block!

Summary

These are all the ingredients you need. Let us briefly recap the most important steps:

- Start with a single site and its (zero) Hamiltonian
- Enlarge this block by applying the appropriate outer products of block operators with single site operators
- Form a superblock Hamiltonian from two copies of the enlarged block operators and diagonalize it. Reshape the resulting ground state into a matrix of $\dim(H_E)$ rows.
- Form the reduced density matrix ρ and fully diagonalize it. From the largest eigenvectors, form a transformation matrix U. The new block operators are found by transforming the enlarged block operators using U: $O' = U^\dagger OU$.
- As a measure for how justified your approximation with just m eigenstates is, calculate the truncated weight by summing up those eigenvalues of the the eigenvectors you did not use to set up the transformation matrix U.

Here are some ideas for what you can do with the codes you have acquired over the course of the lecture:

- Write an exact diagonalization procedure and study the convergence of the ground state energy to the thermodynamic limit for as long a chain you are able to diagonalize.
- Study the convergence of the DMRG procedure as a function of the states kept in the truncation procedure.
- By calculating the entanglement entropy of all eigenstates of the Heisenberg chain, verify that the ground state of the Heisenberg chain is a state of low entanglement.
- Compare the energy obtained for the very same system from an SSE simulation with the DMRG result.