Computational Many-Body Physics
Exercise Sheet 07

Summer Term 2021

Due date: Tuesday, **20th July**, 2021, 10 am

Website: thp.uni-koeln.de/trebst/Lectures/2021-CompManyBody.shtml

In this week's exercise sheet, you will apply the **density matrix renormalization group** (DMRG) to quantum spin models in one spatial dimension. We start with the spin-1 AKLT model which was discussed analytically in the lecture. In doing so, we will introduce you to the open-source `ITensors` software library. Code examples for the tasks we want to perform here can be found on the official `ITensors` documentation page. In a second step, we will then turn to the transverse field Ising model (TFIM), investigate its ground state (GS) phase diagram and analyze its entanglement properties at the critical point.

Exercise 18: Spin-1 AKLT chain

We start by looking at the ground state of the one-dimensional AKLT model whose Hamiltonian is a combination of bilinear and biquadratic spin couplings

$$H = \sum_{j,\gamma} \hat{S}_j^\gamma \hat{S}_{j+1}^\gamma + \Gamma \left(\hat{S}_j^\gamma \hat{S}_{j+1}^\gamma \right)^2 \tag{1}$$

where the $\hat{S}_j^\gamma$ are spin-1 operators and, for now, $\Gamma = 1/3$. In the lecture videos you have learned that the exact ground state of this model is known analytically and can be expressed by an assembly of two spin-1/2 degrees of freedom per site, connected with their neighbors by singlet bonds (i.e. a valence bond solid of spin-1/2's).

We consider a setting with *open* boundary conditions, such that the two spin-1/2's on the chain edges cannot form a singlet state with their neighbors, giving rise to two "dangling spin-1/2" degrees of freedom at the chain ends, so-called *edge states*. We will probe the existence of such gapless edge states in a bulk-gapped state in this exercise.
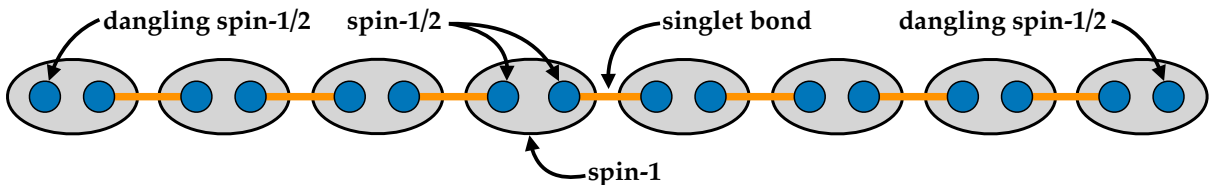

Figure 1: **The Affleck-Kennedy-Lieb-Tasaki (AKLT) state** is built from decomposing local spin-1 degrees of freedom as two spin-1/2 particles linked between neighboring sites by singlet bonds. At the chain boundaries, two "dangling" spin-1/2 degrees of freedom remain unpaired, giving rise to gapless edge states.

a) To set the stage, you will need to **install the `ITensors` package**. In Julia, this can easily be done via the package manager using

```
]add ITensors
```

b) To begin with, **implement the AKLT Hamiltonian** in `ITensors`. To accomplish this, you can extend the code snippet given below, which implements the DMRG algorithm for the antiferromagnetic spin-1 Heisenberg chain, i.e. the first bilinear coupling term in Eq. (1).

Listing 1: Example code for simulating the antiferromagnetic spin-1 chain with `ITensors`.

```julia
using ITensors

let
  # create 64 spin-1 degrees of freedom
  N     = 64
  sites = siteinds("S=1", N)

  # define Hamiltonian as sum of spin operators
  # and convert to matrix product operator (MPO)
  ampo = AutoMPO()

  for j = 1 : N-1
    ampo += 0.5, "S+", j, "S-", j+1
    ampo += 0.5, "S-", j, "S+", j+1
    ampo +=      "Sz", j, "Sz", j+1
  end

  H = MPO(ampo, sites)

  # configure parameters for DMRG simulation:
  # number of sweeps is 10
  # maximum bond dimension is 10
  # truncation treshhold for SVD is 1E-10
  sweeps = Sweeps(10)
  maxdim!(sweeps, 10)
  cutoff!(sweeps, 1E-10)

  # create random matrix product state (MPS)
  # with bond dimension 2 as initial state for DMRG
  psi0 = randomMPS(sites, 2)

  # run the DMRG algorithm
  # returning the GS energy and optimized MPS
  energy, psi = dmrg(H, psi0, sweeps)

  return
end
```

c) We now want to run the DMRG algorithm for this model system, playing with some of the fundamental DMRG parameters detailed here. As a first benchmark, we look at the **convergence of the ground state energy** with increasing bond dimension. Before running the DMRG calculation, try to formulate an expectation of what you would expect to see, based on your knowledge of the AKLT state. In a second step, plot the ground state energy per spin as a function of the maximum bond dimension for the optimized MPS returned by the DMRG algorithm and compare with your initial idea.

d) Following up on the results obtained in **c)**, compute the singular values and **entanglement entropy** S_1 for a bond in the middle of the chain. To this end, you will have to get yourself acquainted with the ITensors documentation. Compare your findings with the results presented in the lecture video.

e) As a next step, we want to probe the **dangling spin-1/2 degrees of freedom** at the edges of the chain by measuring the expectation value $\langle S_i^z \rangle$ for every site i along the chain. You can do this either by defining and passing an additional DMRGObserver object to the dmrg function or by applying the S_i^z operator to the optimized MPS wave function. Plot $\langle S_i^z \rangle$ along the chain. What do you observe?

f) As a final exercise, we want to vary the prefactor of the biquadratic term in Eq. (1). Consider, for example, the cases $\Gamma = 0$ (i.e. the pure spin-1 Heisenberg chain which is also referred to as the **Haldane chain**) and $\Gamma = 1$ (which is a **point of special interest** as you will see).

Repeat your DMRG simulations for these modified couplings and plot $\langle S_i^z \rangle$ along the chain. In both cases, plot the spectrum of singular values $\log(s_n)$ for a bond in the middle of the chain using a large maximum bond dimension for the DMRG. Discuss your results with respect to the appearance of edge states and the energetics, i.e. is the spectrum gapped or gapless?

Exercise 19: Revisiting the Transverse Field Ising Model with DMRG

In this exercise, we want to return to the one-dimensional transverse field Ising model (TFIM)

$$H = -\sum_j \hat{S}_j^z \hat{S}_{j+1}^z - h \hat{S}_j^x \hat{S}_{j+1}^x, \tag{2}$$

where S_i^μ are now spin-1/2 Pauli matrices and $h > 0$. Our focus lies on the critical point and its entanglement properties. More precisely, we want to use the DMRG algorithm to show that the system is gapless right at the critical field strength and that the entanglement entropy does *not* obey a one-dimensional boundary law (i.e. it is not constant).

a) To begin our analysis, you need to **implement the TFIM Hamiltonian** for a chain of length L using your results from the previous exercise. Augment your DMRG algorithm by measurements of $\langle S^z \rangle$ and $\langle S^x \rangle$, where $\langle S^\mu \rangle = \frac{1}{L} \sum_j \langle S_j^\mu \rangle$.

b) With the DMRG set up, you can now scan the **phase diagram** of the TFIM in the range $h \in [0, 2]$ and plot the expectation values $\langle S^z \rangle$ and $\langle S^x \rangle$ as a function of h. Determine the critical value h_c, where the system undergoes a phase transition between a disordered phase at high fields and an ordered, ferromagnetic phase at small values of h.

c) In the **thermodynamic limit** $L \to \infty$, the exact ground state energy of the TFIM is

$$\frac{E_0}{L} = -\frac{h}{\pi} \int_0^\pi \eta_q \, dq \,, \tag{3}$$

with the dispersion $\eta_q = \sqrt{1 + 1/h^2 + 2\cos(q)/h}$.

Compute the numerical value of E_0/L with DMRG at the critical point determined in **b)** for increasing system sizes $L \in \{32, 64, 128, 256, 512, 1024\}$ and plot E_0/L as a function of $1/L$ to perform a **finite-size scaling**. Choose an appropriate fitting function and extrapolate E_0/L to the thermodynamic limit $1/L \to 0$. Compute the exact ground state energy with an integration library of your choice and compare with the DMRG result.

d) We now want to analyze the critical point in more detail. Firstly, we want to extract the **excitation gap** Δ, defined as the difference in energy between ground (E_0) and first excited state (E_1), i.e. $\Delta = E_1 - E_0$. To this end, we need to perform DMRG simulations with an additional constraint on the overlap of the excited MPS with the ground state MPS. Given the wave function $|\psi_0\rangle$ for the ground state, we want to find that state $|\psi_1\rangle$ with the lowest energy that also minimizes the inner product $\langle \psi_1 | \psi_0 \rangle$. In `ITensors` we can simply do this, by adding an additional penalty state to the `dmrg` function. Implement the computation of the first excited state in your DMRG algorithm and determine the excitation gap for $h \in [1.0, 2.0]$. Compare your result with the exact values $\Delta = 2|h - 1|$. For more detail and helpful hints on how to choose DMRG parameters in this case, see the `ITensors` documentation.

e) As a last step, we want to look at the **Renyi entropy** $S_n(L)$ at the critical point. In the previous exercise you have already learned how to extract it from the DMRG-optimized MPS wave function. Here, we want to study the scaling of the entropy with system size. To this end, compute and plot the first few Renyi entropies $S_n(L)$ (e.g. for a set of values $n = 1, 2, 3, \ldots$) as a function of $\log(L)$ for large values of L (e.g. $L = 32, 64, 128, \ldots, 1024$), by considering a bipartition that cuts the chain in two equal parts of length $L/2$. Do so both for the critical point and deep in the ordered and disordered phase. Evaluate your results in light of the boundary law, which has been derived in the lecture. Another important property of the critical point is the corresponding conformal field theory (CFT), which can be identified via its central charge c. For open boundary conditions, the latter is connected to the entanglement entropy by

$$S_n(L) = \frac{c}{12} \left(1 + \frac{1}{n}\right) \log(L) + k_n \,, \tag{4}$$

for $L \gg 1$. Here, k_n is a constant. Compute the central charge by performing a linear regression for S_n as a function of $\log(L)$ and compare to the exact value $c = 1/2$.

Finally, shift the bond chosen for the bipartition of the system, i.e. start cutting the first, second, third bond and so forth and plot the entanglement entropies along the bonds in the chain in both phases and at the critical point.