FOR 1807 Winter School 2018 Marburg

Exact Diagonalization hands-on session

Exercise sheet

In the following exercises we will make use of the scripts `hamiltonian_tfi.py`, `hamiltonian_hb_staggered.py` and `hamiltonian_hb_xxz.py`. Internally, spin states are encoded in a binary representation, for example

$$|\uparrow\downarrow\uparrow\uparrow\rangle = (1011)_2 = 11. \tag{1}$$

The three files contain each contain a function `get_hamiltonian_sparse` which creates the Hamiltonian matrix in a sparse matrix format. The following Hamiltonians are given

- `hamiltonian_tfi.py`: The *Transverse Field Ising* model,

$$H = J \sum_{\langle i,j \rangle} S_i^z S_j^z + h_x \sum_i S^x, \tag{2}$$

  where S^z and S^x are the spin-1/2 spin operators, on a one-dimensional chain lattice (with periodic boundary conditions). This model does not conserve total S^z. Momentum conservation is not implemented.

- `hamiltonian_hb_staggered.py`: The *Heisenberg model in a staggered magnetic field* ,

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j + h_S \sum_i (-1)^i S^z, \tag{3}$$

  one-dimensional chain lattice (with periodic boundary conditions). This model does conserve total S^z. Momentum conservation is not implemented.

- `hamiltonian_hb_xxz.py`: The *Heisenberg model with Ising anisotropy* ,

$$H = J \sum_{\langle i,j \rangle} \left[S_i^z S_j^z + (1+\Delta) \left(S_i^x S_j^x + S_i^y S_j^y \right) \right] \tag{4}$$

  one-dimensional chain lattice (with periodic boundary conditions). This model does conserve total S^z. Momentum conservation is implemented.

An example how to use these functions for computations can be found in the file `example_groundstate_energy.py`

Exercise 1: Impementing a Hamiltonian, computing static correlations (basic)

1. Use the script `hamiltonian_tfi.py` to compute ground state energies for J and for a range of values h_x from 0 to 1.

2. Alter the script `hamiltonian_tfi.py` to create the Hamiltonian of the Heisenberg model in a staggered magnetic field, as given by Eq. 3. Cross check the ground state energy with the script `hamiltonian_hb_staggered.py` for total $S^z = 0$.

3. Compute the ground state spin correlations $\langle 0|S_0^z S_r^z|0\rangle$ and $\langle 0|\mathbf{S}_0 \cdot \mathbf{S}_r|0\rangle$ of the Heisenberg model in a staggered magnetic field. Check whether

$$\langle 0|\mathbf{S}_0 \cdot \mathbf{S}_r|0\rangle = 3\,\langle 0|S_0^z S_r^z|0\rangle$$

for $h_s = 0$.

Exercise 2: Computing dynamical correlations functions

In this exercise we compute the ground state Greeen's function,

$$G^{zz}(\mathbf{q}, z) = \langle 0|S^\dagger(\mathbf{q})\frac{1}{z-H}S(\mathbf{q})|0\rangle\,, \text{ where } z = \omega + i\eta, \tag{5}$$

and the corresponding dynamical spin structure factor

$$S^{zz}(\mathbf{q}, \omega) = -\frac{1}{\pi}\lim_{\eta\to 0}\mathrm{Im}G^{zz}(\mathbf{q}, \omega + i\eta), \tag{6}$$

where

$$S(\mathbf{q}) = \frac{1}{\sqrt{L}}\sum_{\mathbf{r}} e^{-i\mathbf{q}\mathbf{r}}.$$

We will compute these quantities for the isotropic Heisenberg chain, as in Eq. 3 with $h_s = 0$. L denotes the length of the chain whose discrete momenta are given by $\mathbf{q} = 2\pi/L \cdot 0, 2\pi/L \cdot 1, \ldots, 2\pi/L \cdot (L-1)$. The Hamiltonian H can be created using the script `hamiltonian_hb_staggered.py`.

1. (basic) Fix a small but finite η. Compute the Green's function Eq. 5 and the dynamical spin structure factor Eq. 6 by creating a dense matrix H of the Hamiltonian and inverting $(z - H)$ numerically for small system sizes.

2. (advanced) The Green's function can be evaluated without fully inverting the matrix $(z - H)$ using the *continuous fraction expansion*,

$$G^{zz}(\mathbf{q}, z) = \cfrac{\langle 0|S^\dagger(\mathbf{q})S(\mathbf{q})|0\rangle}{z - \alpha_0 - \cfrac{\beta_1^2}{z-\alpha_1 - \cfrac{\beta_2^2}{z-\cdots}}} \tag{7}$$

Here, α_n, β_n are given by the Lanczos recursion,

$$\begin{aligned} |v_{n+1}\rangle &= \beta_{n+1}^{-1}\left[(H-\alpha_n)\,|v_n\rangle - \beta_n\,|v_{n-1}\rangle\right] \\ \alpha_n &= \langle v_n|H|v_n\rangle \\ \beta_{n+1} &= \| \,(H-\alpha_n)\,|v_n\rangle - \beta_n\,|v_{n-1}\rangle\,\|, \end{aligned}$$

with starting vector $|v_0\rangle = S(\mathbf{q})\,|0\rangle$. A basic implementation of the Lanczos recursion creating the coefficients α_n and β_n can be found in the file `algorithm_lanczos.py`. Compare the results from continuous fraction expansion to the results from full inversion. For details on the continuous fraction expansion see e.g. Koch [2011].

Exercise 3: Hamiltonian symmetries

In this exercise we investigate the Heisenberg XXZ model Eq. 4. This model has a discrete translational symmetry $T : \mathbf{S}_i \mapsto \mathbf{S}_{i+1}$. Hence, a symmetrized basis with fixed momentum $2\pi\mathbf{k}$Ł can be chosen. The script `hamiltonian_hb_xxz.py` creates the Hamiltonian of the Heisenberg model with Ising anisotropy in the basis of momentum eigenstates. $\mathbf{k}$ can be specified.

1. (basic) Compute the low-lying eigenvalues of the Hamiltonian for each $\mathbf{k} = 0, \ldots, L-1$ and plot the energies as a function of momentum for the isotropic Heisenberg case. Cross-check the eigenvalues by also computing them in a non-symmetrized basis by using the script `hamiltonian_hb_staggered.py`.

2. (expert) The model has an additional C_2 reflectional symmetry, $P : \mathbf{S}_i \mapsto \mathbf{S}_{L-1-i}$, which has an even and an odd representation. Extend the script `hamiltonian_hb_xxz.py` to also work in a symmetrized basis of both parity and translational symmetry. Compute the eigenvalues of the Hamiltonian in this new symmetrized basis and compare them with the eigenvalues without parity symmetry. For details on the implementation of discrete symmetries see e.g. Weiße and Fehske [2007].

References

Erik Koch. The lanczos method. *The LDA+ DMFT approach to strongly correlated materials*, 2011. `https://www.cond-mat.de/events/correl11/manuscripts/koch.pdf`.

Alexander Weiße and Holger Fehske. Exact diagonalization techniques, lecture notes in physics. 2007. `http://citeseerx.ist.psu.edu/viewdoc/download?doi=10.1.1.627.8371&rep=rep1&type=pdf`.