Sheet 2: Exact diagonalization

In this exercise, we will study the ground states of one-dimensional spin-$1/2$ systems using exact diagonalization.

Problem 1 Ground states of spin-$1/2$ systems

We start by considering the transverse field Ising model in one dimension, given by the Hamiltonian

$$H = -J \sum_{j=0}^{L-1} \sigma_j^z \sigma_{j+1}^z - g \sum_{j=0}^{L+1} \sigma_j^x. \tag{1}$$

a) Construct the basis for a spin-$1/2$ without using any conservation laws.

b) As discussed in the lecture, construct the spin operators σ_j^x and σ_j^z for each site $j = 0, ..., L-1$ using your basis from a).

c) Write a function that constructs the Hamiltonian as a sparse matrix for given parameters J and g.

d) Benchmark your functions so far – do your matrices make sense? One possible check is to start with very small systems. You might want to convert your sparse matrix to a full matrix for easier comparison.

e) Could you have arrived at your Hamiltonian matrix without a)? How?

f) Use a built in routine to obtain the ground state. Check the documentation to figure out what is happening behind the scenes.

g) Calculate the ground state for a range of system sizes – what are reasonable system sizes? Evaluate meaningful observables while scanning the transverse field g. Plot your results in a meaningful way.

Problem 2 Using symmetries

We now want to take symmetries into account. For this, we consider the TFIM from above with periodic boundary conditions, i.e. $\sigma_0^\alpha = \sigma_L^\alpha$.

a) We start with $g = 0$, where we have a $U(1)$ symmetrie, i.e. conservation of the total magnetization. Construct the basis in the $\sigma^{z,tot} = 0$ sector. What else do you need for your operators?

b) Construct your spin operators. Use your Hamiltonian generating function from Problem 1 to construct the Hamiltonian.

c) Think about useful benchmarks for this case.

d) Repeat the construction for different $S^{z,tot}$ sectors – which one yields the lowest overall energy? Does this depend on the sign of J?

e) We now consider general g, which means that we loose the $U(1)$ symmetry. Due to the periodic boundary conditions, we still have translational symmetry, which we want to use now. Follow the prescription given in the lecture to construct the basis using representative states. You might want to write a function to find those representatives.

f) Next, we want to construct the Hamiltonian. By acting with the off-diagonal part of the Hamiltonian on a given basis state, we go to a new basis state. Remember to check if this is a corresponding representative and if not, how to correctly find the representative state.

g) Think again about useful benchmarks.

h) In the case of translational symmetry, we can now search for the ground state in different momentum sectors. This gives us $E(k)$. Plot this and compare the outcome for different g/J.

i) How does the computational effort change for different system sizes L? How do the relevant Hilbert space dimensions compare? What are the largest system sizes L that you can calculate (in reasonable time) on your computer with and without symmetries taken explicitely into account?