Sheet 2: Exact Diagonalization

Released: 05/05/23; Submit until: 05/19/23 (**20 Points**)

On this sheet we will set up a small exact diagonalization code to solve a fundamental problem of quantum mechanics: the one-dimensional transverse-field Ising model. Solving the exercises, we will try to follow the paradigm of *test-driven development*, which is a standard paradigm when developing complex code. There are many neat tools for various languages. If you are working in `Python`, you may find it helpful to have a closer look at the `Pytest` framework, which is already available on ASC cluster (after sourcing `init_modules.sh`). If your are working in `C++`, you can use the header file `catch.hpp` in the folder `exact_diagonalization` of the exercise-git to set up unit tests (as for instance explained here).

Problem 1 A tensor product Hilbert space (8 Points)

We are considering a chain of $L \in \mathbb{N}$ spins, each of which being described by a two-dimensional degree of freedom $|s_j\rangle \in \mathbb{C}^2$ where $j \in \{0, \ldots, L-1\}$ labels the lattice site. The transverse-field Ising model with periodic boundary conditions in one dimension is now defined by the Hamiltonian

$$\hat{H} = -\sum_{j=0}^{L-1} \hat{\sigma}_j^z \hat{\sigma}_{j+1}^z - h \sum_{j=0}^{L-1} \hat{\sigma}_j^x \,, \tag{1}$$

where $h \in \mathbb{R}$ is the transverse magnetic field. Here, the $\hat{\sigma}_j^\alpha$ are Pauli operators acting on the jth spin of the many-body Hilbert space $\mathcal{H} = \bigotimes_{j=0}^{L-1} \mathbb{C}^2$, fulfilling the commutation relations

$$\left[\hat{\sigma}_i^\alpha, \hat{\sigma}_j^\beta\right] = 2\delta_{ij}\epsilon^{\alpha\beta\gamma}\hat{\sigma}_j^\gamma \,, \tag{2}$$

where $\alpha, \beta, \gamma \in \{x, y, z\}$ and $\epsilon^{\alpha\beta\gamma}$ is the Levi-Civita symbol.

Implement a class that represents the Hilbert space $\mathcal{H}$ and operators acting on it, for a given number of lattice sites L. It should at least provide the following functionality:

- Generation of a random state, a ferromagnetic state along the z-direction and a ferromagnetic state along the x-direction, represented as vectors $\vec{x} \in \mathbb{C}^{2^L}$.
- Generation of operators $\hat{\sigma}_j^\alpha$ as well as the identity, acting on $\mathcal{H}$, represented as matrices $\mathbf{M} \in \mathbb{C}^{2^L \times 2^L}$.
- Action of an operator $\hat{O}$ on a state $|\psi\rangle \in \mathcal{H}$.
- Calculation of the standard scalar product $\langle\cdot|\cdot\rangle$ on $\mathcal{H}$.

For each functionality, write a proper testcase which reasonably validates your implementation.

Problem 2 Determining the ground-state phase diagram **(12 Points)**

Now that we have set the stage, we can start to study eq. (1), numerically.

(2.a) **(3P)** Implement a function which generates a matrix representation of $\hat{H}$ as a function of the transverse field. Write at least two testcases, which reasonably validate your implementation.

(2.b) **(3P)** Calculate the ground-state energy density $e(h) = \langle \hat{H} \rangle / L$ as a function of the transverse field h by determining the ground state energy of $\hat{H}$. Also, evaluate the average ground-state magnetization as a function of the transverse field

$$m(h) = \frac{1}{2L} \sum_{j=0}^{L-1} \langle \hat{\sigma}_j^z \rangle \ . \tag{3}$$

(2.c) **(4P)** Repeat your calculations for different number of lattice sites and determine the critical field $h_\mathrm{c}(L)$ at which the model undergoes a quantum phase transition. Perform a finite-size scaling of $h_\mathrm{c}(L)$ to estimate $h_\mathrm{c}(L \to \infty)$, i.e., the critical field in the thermodynamic limit. How does your result compare to the literature?

(2.d) **(2P)** Show numerically that in the limits $h \to 0$ and $h \to \infty$, the ground states $|\psi_0(h)\rangle$ of eq. (1) approach the mean-field solutions

$$|\psi_0(h)\rangle = \begin{cases} |{\uparrow}\rangle \otimes |{\uparrow}\rangle \cdots \text{ or } |{\downarrow}\rangle \otimes |{\downarrow}\rangle \cdots \ , & \text{if } h \to 0, \\ |{\rightarrow}\rangle \otimes |{\rightarrow}\rangle \cdots \ , & \text{if } h \to \infty. \end{cases} \tag{4}$$

Here, $|{\uparrow}\rangle, |{\downarrow}\rangle$ denote the eigenstates of $\hat{\sigma}_j^z$ at a given lattice site j, and $|{\rightarrow}\rangle, |{\leftarrow}\rangle$ the eigenstates of $\hat{\sigma}_j^x$.