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Exercise class in HCI J7.

Exercise 1. ***Transverse field Heisenberg model: exact diagonalisation***

Consider the transverse field Ising model given by the Hamiltonian

$$H = \sum_{i=0}^{N-1} \sigma_i^z \sigma_{i+1}^z + h \sum_i \sigma_i^x \tag{1}$$

In this exercise we impose periodic boundary conditions. You will need to perform the exact diagonalisation and plot the low-energy spectrum of the model as the function of h. To this end, you will construct the Hamiltonian matrix in the σ^z basis of the 2^N-dimensional Hilbert space.

Part A: Dense matrix approach

1. Consider a reasonably large system size N that your computer can still handle (e.g. pick $N = 8$). Construct the Hamiltonian in the σ^z basis using the *np*.kron function.

2. Consider 40 evenly distributed values of h in the interval $[-2, 2]$.

3. For every field h plot the lowest 10 energy levels.

4. To make the effect of phase transitions at $|h| = 1$ more visible, plot the difference between 10 lowest energy levels and the ground state energy.

Hint: In the .ipynb exercise file you will find the template for this pipeline, which you can use. The functions np.linalg.eigh, np.linspace and np.kron might be helpful.

Part B: Sparse matrix

Instead of constructing a dense matrix, you can also use the bitstring representation to implement the action of the Hamiltonian in terms of bitwise operations. This function can be used as a scipy linear operator scipy.sparse.linalg.LinearOperator in the Lanczos eigenvalue solver scipy.sparse.linalg.eigsh. This procedure is particularly useful for larger problems. Implement the action of the Hamiltonian as a bitwise operation (you might find it helpful to consider the diagonal and non-diagonal parts separately)

Reminder: To employ the bitstring representation, the basis element number k should be written in the binary representation to get the individual spin orientations. For instance, the basis element $k = 415 = 256 + 128 + 16 + 8 + 2 + 1$ with $N = 10$ spins would correspond to the bitstring $(0, 1, 1, 0, 0, 1, 1, 1, 1, 1)$, meaning, 0 -th, 3 -rd and 4 -th spins are down, others up.

Part C: Symmetry operators

The transverse field Ising Hamiltonian has many symmetries. Finding the symmetry essentially means finding another basis where the Hamiltonian takes the block-diagonal form, Among the possible symmetries, there are:

1. Flipping all spins with the operator $X = \otimes_i \sigma_i^x$,

2. Total magnetisation conservation with the operator $M = \sum_i \sigma_i^z$ (only at $h = 0$),

3. Translation symmetry $T : |s_1, s_2, \ldots, s_N\rangle \to |s_N, s_1, \ldots, s_{N-1}\rangle$ with a rather non-local operator form.

If the Hamiltonian has a symmetry $[H, A] = 0$, H and A can be diagonalized simultaneously. This means that the Hamiltonian does not mix the eigenstates from sectors with different eigenvalues of A (i.e. H has block-diagonal form in the eigenbasis of A). This fact allows one to search for H eigenstates in the sectors of A eigenvalues one-by-one, which might significantly reduce the ED-complexity.

At the end of the first exercise, please construct the operators for the symmetries (1) and (2) and explicitly check that $[H, A] = 0$ for both of them.

Exercise 2. ***Transverse field Heisenberg model: exact diagonalization with symmetries***

In this exercise we will work with the translational symmetry given by

$$T : |s_1, s_2, \ldots, s_N\rangle \to |s_N, s_1, \ldots, s_{N-1}\rangle$$

For any spin configuration, this operator shifts all spins one position forward (recall that we assume periodic boundary conditions). Since $T^N = \mathbb{1}$, the possible eigenvalues are

$$z_k = \exp\left(2\pi i \frac{k}{N}\right) \tag{2}$$

The Hamiltonian commutes with the (unitary) operator T. This can be utilized in order to decrease the Hilbert space size of the problem in the following way. For every state (bitstring) $|s\rangle$, define its orbit as $O(|s\rangle) = \{T^n|s\rangle\}_n$, e.g. the set of all possible different bitstrings that can be constructed out of $|s\rangle$ by applying T arbitrarily many times.

This defines an equivalence relation: all the bitstrings split into non-intersecting orbits (equivalence classes) $O_1, O_2, \ldots, O_m$. Since H and T can be diagonalized simultaneously, let us fix some specific eigenvalue z_k of T and for each orbit O_α construct one T eigenstate as

$$|\chi_k^\alpha\rangle = \frac{1}{\sqrt{|O_\alpha|}} \sum_{i=0}^{|O_\alpha|-1} z_k^{-i} T^i |\phi^\alpha\rangle \tag{3}$$

Here $|\phi^\alpha\rangle$ is the orbit representative - any priorly chosen state of the O_α orbit. It can be shown that the states $|\chi_k^\alpha\rangle$ united over all eigenvalues z_k and orbits α form a new basis in the Hilbert space.

Finally, in this basis it can be shown that $\left\langle \chi^{\alpha}_{k_1} | H | \chi^{\beta}_{k_2} \right\rangle \propto \delta_{k_1 k_2}$: the Hamiltonian takes the block-diagonal form, different T eigenvalues do not mix and the problem can be solved for every z_k independently.

Note that each orbit can have only specific eigenvalues, namely, we require that

$$z_k^{|O_\alpha|} = 1 \tag{1}$$

which is quite obvious: if one shifted the state so many times that it comes into itself (length of the orbit O_α), the amplitude should be the same.

Now we are ready to rewrite the Hamiltonian in the new basis of $|\chi^{\alpha}_{k}\rangle$. Since the Hamiltonian has the blockdiagonal form in the χ-basis, we will write a routine that will construct the block of a given eigenvalue z_k. The algorithm for this might be as follows:

1. Loop over all orbits O_α and find those that satisfy the $z_k^{|O_\alpha|} = 1$ property. Write down the list of representatives. The length of this list is the block dimension.

2. Express the Hamiltonian in the χ-basis. Luckily, we know the exact formula for every $|\chi^{\alpha}_{k}\rangle$ as the decomposition into bitstring basis states (see above). Let us consider explicitly the action of the two components

(a) The action of H_J on the bitstring is trivial (diagonal). It leaves all bitstrings in their orbits, which means that H_J does not mix different orbits and is diagonal in the χ-basis:

$$\left\langle \chi^{\alpha}_{k} | H_J | \chi^{\beta}_{k} \right\rangle = \delta_{\alpha\beta} \frac{1}{|O_\alpha|} \sum_{j=0}^{|O_\alpha|-1} \left\langle T^j \phi^\alpha | H_J | T^j \phi^\alpha \right\rangle = \delta_{\alpha\beta} \left\langle \phi^\alpha | H_J | \phi^\alpha \right\rangle \tag{4}$$

where we used $|z_k| = 1$ and the translational invariance of H_J.

(b) The $H_h = h \sum_i \sigma^x_i$ field term flips spins and kicks bitstring to another orbit. To write down its matrix elements, let us fix some specific spin σ^x_s. Then spins of the orbit O_α are mapped to some other orbit. This can be written as, $\sigma^x_s T^j |\phi^\alpha\rangle = T^{\zeta(j)} \left|\phi^{\gamma(j)}\right\rangle$ for some functions $\gamma(j)$ and $\zeta(j)$. So, for every j one has to define the resulting orbit index $\gamma(j)$ and the shift from the representative $\zeta(j)$. Then the matrix element reads

$$\left\langle \chi^{\beta}_{k} | \sigma^x_s | \chi^{\alpha}_{k} \right\rangle = \frac{1}{\sqrt{|O_\alpha| \, |O_\beta|}} \sum_{j=0}^{|O_\alpha|-1} z_k^{\zeta(j)-j} \delta_{\beta\gamma(j)} \tag{5}$$

Note that for any selected s there will be projections onto orbitals that are not compatible with z_k. This is no surprise though: the Hamiltonian becomes translationally symmetric only after taking the sum over s. So, when constructing H_h we can neglect such contributions (but keep in mind that they vanish only if the sum over s is performed).

TO-DO FOR STUDENTS

1. Implement the action of the operator T on a state (given as a bitstring). It is convenient to define T^n as an operator for an arbitrary power n.

2. Now we need to define the lookup table: it assigns to every bitstring the bitstring of its representative in the orbit. We will also need the list of unique representatives for each orbit. There is no obvious way to systematically define each orbit representative. So, a possible approach would be to pick the bitstring with lowest value (as an integer) for the representative. You may reuse your solution from the previous sheet.

3. Start with the listing of orbits O_α that are compatible with a specific eigenvalue z_k, i.e. the orbits that satisfy $z_k^{|O_\alpha|} = 1$. Store them as a list of representatives for z_k. You may again reuse your solution from the previous sheet.

4. Write a routine to calculate the diagonal part of H^χ and the non-diagonal part (set $h = 1$) given the above formulae. You will need to define the shift function $\zeta(j)$ and the orbit function $\gamma(j)$. To check your implementation, compare your resulting H-matrix for the case of $N = 4, k = 0, 1$ with your analytic results from Exercise 2, Question 2.

5. Plot the ground state energy in each z_k-segment.

6. Measure the performance gain: how much faster is it to diagonalise two blocks independently than the initial Hamiltonian as a whole?

7. Verify that the energy spectrum agrees with the one obtained in Exercise 1.

Hint: The functions np.linalg.eigh, np.kron, np. unique, np. where, np.any might be useful.