UNIVERSITEIT VAN AMSTERDAM

Advanced Numerical Methods in Many-Body Physics - Homework 2

Exact Diagonalization of Heisenberg Spin Chain

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Exercises

Exercise 7.1

Part a

For this first exercise we compute the matrix elements of the 2-site $S = \frac{1}{2}$ Heisenberg model,

$$\hat{H} = J \sum_{\langle i,j \rangle} \hat{S}_i^z \hat{S}_j^z + \frac{1}{2}\left(\hat{S}_i^+ \hat{S}_j^- + \hat{S}_i^- \hat{S}_j^+\right) \tag{1}$$

by hand and using the Kronecker product implemented in numpy.
By hand, taking tensor products of the ladder operators,

$$S^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad S^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

and of the z Pauli matrix,

$$S^z = \frac{1}{2}\sigma_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

we arrive at the expression

$$\hat{H} = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Using the Kronecker product np.kron we arrive at the same matrix. Using np.linalg.eigh to compute the eigenvalues and eigenvectors we get

$$\lambda_i = \{-\frac{3}{4}, \frac{1}{4}, \frac{1}{4}, \frac{1}{4}\}$$

$$V = \begin{pmatrix} 0 & 1 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

which corresponds to the ground state $V_0 = (0, \frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}, 0)$ with energy $E_0 = -\frac{3}{4}$ and the three triplet states.

Part b

For this exercise we repeat the same as before but for a spin $S = 1$ system, which is characterized by having three basis states per site, $|s^z = 1\rangle, |s^z = 0\rangle, |s^z = -1\rangle$. For this case, the ladder operators take the form

$$S_+ = \sqrt{2}\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad S_- = \sqrt{2}\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

while the z spin operator is

$$S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Doing the computation by hand we arrive at the matrix

$$\hat{H} = \frac{1}{4}\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

on the other hand, doing the computation using Python we arrive at the same matrix. The eigenvectors and eigenvalues are given by

$$\lambda_i = \{-2, -1, -1, -1, 1, 1, 1, 1, 1\}$$

$$V = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -0.707107 & 0 & 0 & 0 & 0 & 0 & -0.707107 & 0 \\ 0.57735 & 0 & 0 & 0.707107 & 0 & 0 & 0 & 0 & -0.408248 \\ 0 & 0.707107 & 0 & 0 & 0 & 0 & 0 & -0.707107 & 0 \\ -0.57735 & 0 & 0 & -1.54065 \cdot 10^{-17} & 0 & 0 & 0 & 0 & -0.816497 \\ 0 & 0 & 0.707107 & 0 & 0 & 0 & 0.707107 & 0 & 0 \\ 0.57735 & 0 & 0 & -0.707107 & 0 & 0 & 0 & 0 & -0.408248 \\ 0 & 0 & -0.707107 & 0 & 0 & 0 & 0.707107 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \end{bmatrix}$$

where now it's harder to convert the numerical values obtained to their closed form. Observe the spurious $-1.54065 \cdot 10^{-17}$ term obtained by using np.linalg.eigh, which is probably given by a roundoff error.

Exercise 7.2

In this exercise we perform the exact diagonalization of the Heisenberg model for $S = \frac{1}{2}$ as well as $S = 1$ and for different lattice sizes. For this, we have coded a script `diagonalization.py` that implements exact diagonalization in Python which receives as an input the spin S, the number of lattice sites n, the type of boundary conditions and whether or not the matrices are sparse or dense, and outputs the constructed hamiltonian H, an array with its eigenvalues and an array with its eigenvectors (for a sparse matrix the first k eigenvalues and eigenvectors).

Part 1

Using this script we compute the ground energy for a $S = \frac{1}{2}$ Heisenberg spin chain with open boundary conditions and four lattice sites. The result is

$$E_0 = -1.6160254037844386$$

which coincides with what should be obtained.

Part 2

In this section we do the same but in this case supposing H to be a sparse matrix instead of dense, and also supposing periodic boundary conditions. To do this, we need to use the commands provided in the exercise such as `sp.csr_matrix(H)` to define the sparse matrices, as well as implement the boundary term for the hamiltonian by acting on the first and last lattice sites with the Heisenberg hamiltonian (1).

The resulting ground energy is

$$E_0 = -2.0000000000000004$$

which coincides with what should be obtained, with the exception of some roundoff errors that alter its value slightly.

Part 3

In this section we compare the memory usage of dense and sparse matrices by storing the number of bits used by the arrays for the dense hamiltonian H and the sparse hamiltonian H_{sparse} using the commands `Hdense.nbytes` and `Hsparse.data.nbytes` respectively. In particular, we compare the sizes of the arrays for $S = \frac{1}{2}$ and 10 lattice sites. The results are:

$$S_{dense} = 8388608 \text{ bytes}$$

$$S_{sparse} = 45056 \text{ bytes}$$

Thus, the memory usage of the sparse matrix is 99.46% smaller than that of the dense matrix.

Part 4

In this section we plot the ground energies E_0 of the spin $S = \frac{1}{2}$ Heisenberg spin chains with periodic boundary conditions and sparse hamiltonian for different lattice sites. Using the `diagonalization.py` script and plotting for $N = [2, 3, \ldots, 14]$ we obtain:

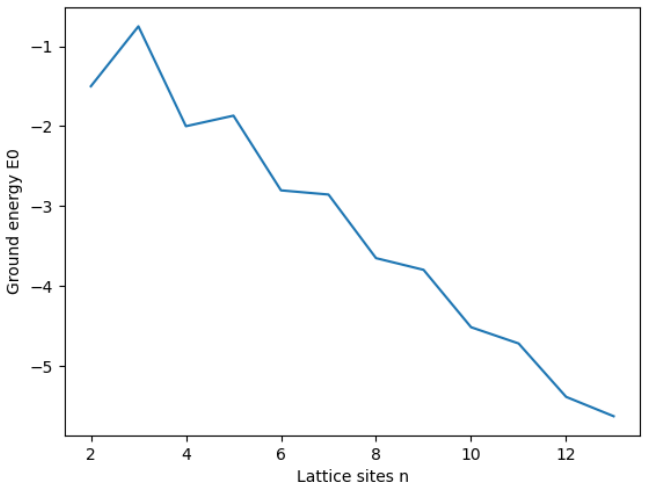

Figure 1: *Ground energies for periodic boundary conditions*

We observe how the ground energy oscillates for different values of n. In particular, the energies seem to decrease faster for even multiples of n and to decrease less or even increase for odd multiples of n. The reason for this oscillation might be related to the periodic boundary conditions, because we can observe how for open boundary conditions this behavior is softened.

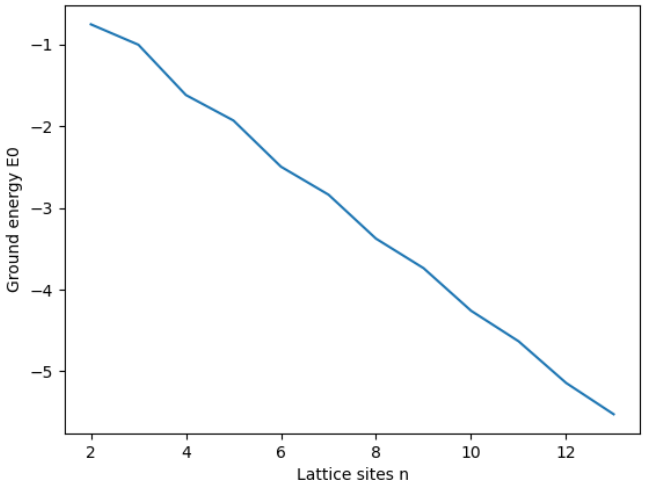

Figure 2: *Ground energies for open boundary conditions*

Part 5

In this section we plot the energy gap between the first excited state and the ground state,

$$\Delta E = E_1 - E_0$$

for different even values of n against $\frac{1}{n}$. Then, we perform a linear extrapolation to 0 using the last 3 values of ΔE in order to see the criticality of the spin chain for $S = \frac{1}{2}$.

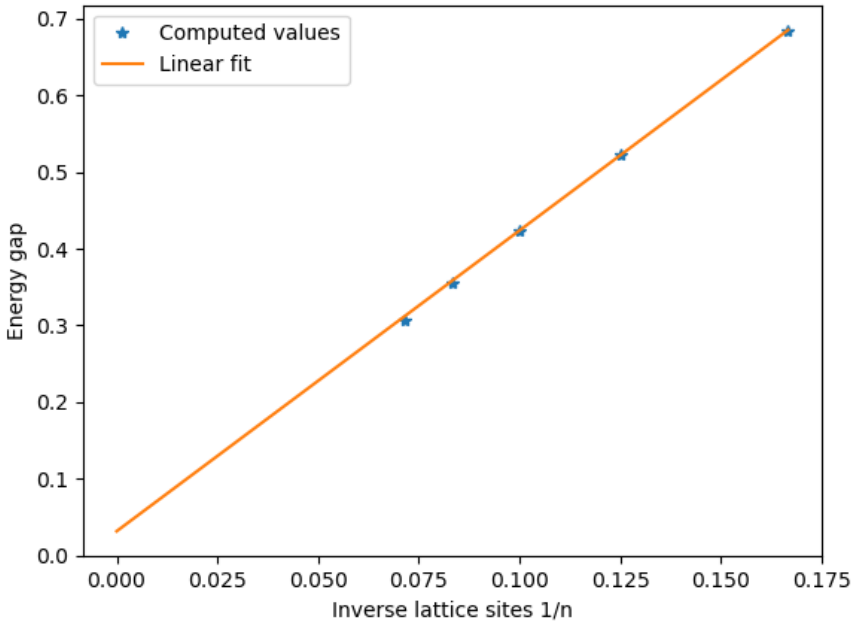

Figure 3: *Fitted ground energies for different lattice sizes*

We see how the linear fit converges to 0 at $\frac{1}{n} \to 0$, that is, at the thermodynamic limit $n \to \infty$. However, more precisely for this many lattice sizes the linear fit converges to the value

$$\Delta E_0 = 0.03188094591246846$$

This means that the ground state at the thermodynamic limit of the $S = \frac{1}{2}$ spin chain is critical, and there is no gap between the ground state and the first excited state.

Part 6

In this section, we do the same as in the previous one but in this case considering a $S = 1$ spin chain. At first sight, it seems that its behavior should resemble that of the $S = \frac{1}{2}$ chain but Haldane proved that this system is gapped.

Considering even lattice sizes between 6 and 10, and performing a fit with a second-order polynomial we get the following chart

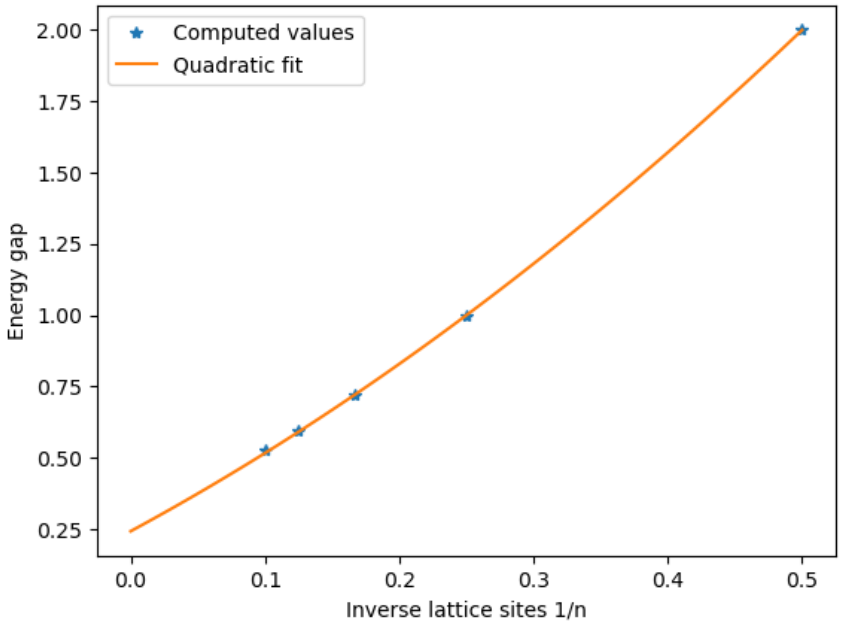

Figure 4: *Fitted ground energies for different lattice sizes*

Where the fitted value of the gap is now given by

$$\Delta E_0 = 0.24282313180735282$$

however the exact value of the Haldane gap is 0.410.

This means that the $S = 1$ Heisenberg model is gapped at the thermodynamic limit, which has profound implications in its physical properties and makes it considerably different to the $S = \frac{1}{2}$ gapless model.