# Computational Tools for Quantum Many-Body Physics (WS 24/25)
# Exercise Sheet 4

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Consider the one-dimensional XXZ chain, as described by the Hamiltonian

$$H = -J \sum_j \left( S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \right) + \Delta \sum_j S_j^z S_{j+1}^z \tag{1}$$

where $S_j^\mu = \frac{1}{2}\sigma_j^\mu$ ($\mu = x, y, z$) is the $\mu$-component of the spin-1/2 operator acting on lattice site $j$, the parameter $J > 0$ denotes the strength of the exchange interaction, and $\Delta$ is the strength of the Ising interaction between neighboring spins. The aim is to study this model with exact diagonalization (ED), implementing symmetries such as total $S_z$ conservation and translation invariance, for investigating the quantum phase transitions that occur as a function of $\Delta$.

*Remark*: With an elaborate analytical technique known as the *Bethe Ansatz*, the XXZ model above may be solved exactly (see [1] and references therein).

1. **Analytical warm-up: Mapping to spinless fermions and qualitative phase diagram**
   By applying Jordan-Wigner transformation, map the XXZ Hamiltonian (1) to a Hamiltonian of spinless fermions $H_{\mathrm{JW}}$. Check that the resulting Hamiltonian commutes with the total number of particles $N = \sum_j c_j^\dagger c_j$, and check that this corresponds to the total $S_z$ conservation in (1), that is, $[H, S_z] = 0$ with $S_z = \sum_j S_j^z$.

   On a qualitative level, study the limits $\Delta \to -\infty$, $\Delta \to 0$ and $\Delta \to \infty$. What would be the ground-state of the system in these limiting cases?

   *Hint*: Through JW transformation you should arrive at the following Hamiltonian

$$H_{\mathrm{JW}} = -\frac{J}{2} \sum_{j=1}^{L-1} \left( c_j^\dagger c_{j+1} + \mathrm{h.c.} \right) + \Delta \sum_{j=1}^{L-1} \left( c_j^\dagger c_j - \frac{1}{2} \right) \left( c_{j+1}^\dagger c_{j+1} - \frac{1}{2} \right) \tag{2}$$

   where $L$ is the number of sites of the chain, and with the addition of the following term if periodic boundary conditions are assumed

$$H_{\mathrm{JW,PBC}} = \frac{J}{2} (-1)^{\sum_j c_j^\dagger c_j} \left( c_L^\dagger c_1 + c_1^\dagger c_L \right) . \tag{3}$$

2. **Exact diagonalization with total $S_z$ conservation**
   Write an ED code for computing the ground-state energy of (1) both with open and periodic boundary conditions. Make use of the total $S_z$ conservation for reducing the dimension of the Hamiltonian matrix to be diagonalized. Compute the ground-state energy of (1) with $J = 1$ and $L = 14, \ldots, 20$ fixed for the cases $\Delta = \pm 2$ and $\Delta = \pm 0.5$. In these cases, which total $S_z$ sector does the ground-state correspond to?

   You can benchmark your code with the case $\Delta = 0$, where (1) maps to free fermions through JW transformation. However, in the case of PBC be aware of the boundary term when comparing the energies obtained from ED and from free spinless fermions. For further comparison of your results, the following table shows the ground-state energies obtained for $L = 16$.

| $\Delta$ | PBC | OBC | $S_z$ |
|---|---|---|---|
| $-2$ | $-8$ | $-7.5$ | $\pm L/2$ |
| $-0.5$ | $-4.413613$ | $-4.190956$ | 0 |
| 0.5 | $-6.042763$ | $-5.835389$ | 0 |
| 2 | $-9.906586$ | $-9.510953$ | 0 |

3. **Detecting phase transitions in the XXZ chain from energy levels**
Fix $J = 1$ and $L = 14, \ldots, 20$ with PBC, and plot the ground-state energy of (1) as a function of $\Delta \in [-2, 2]$. What happens as $\Delta = -1$? The phase transition occurring as $\Delta = 1$ is less immediate to detect from the spectrum. Define

$$\Delta E(S_z = 0) \equiv E_1(S_z = 0) - E_0(S_z = 0) \tag{4}$$

as the excitation gap in the $S_z = 0$ magnetization sector, i.e. the difference between the first excited state energy $E_1(S_z = 0)$ and the lowest energy $E_0(S_z = 0)$ for the $S_z = 0$ sector, and

$$\Delta E_{1\mathrm{p}} \equiv E_0(S_z = \pm 1/2) - E_0(S_z = 0) \tag{5}$$

the *one-particle* gap, i.e. the difference between the first ground-state energies in the $S_z = 1/2$ (or $-1/2$) and $S_z = 0$ sectors. Plot $\Delta E(S_z = 0)$ and $\Delta E_{1\mathrm{p}}$ as a function of $\Delta \in [0, 2]$. What can you observe as $\Delta = 1$?

*Hint*: If you want to use the simple Lanczos algorithm of the previous exercise sheet to compute the energy of the first excited states, you need to be careful to the possible appearance of *ghost eigenvalues* (see e.g. [2, 3]). Alternatively, pre-defined sparse matrix diagonalization routines (e.g. in Python or Matlab) can be used, where this problem is already taken care of.

4. **(Bonus) Exact diagonalization with translation invariance: $k$ resolved spectrum**
For the XXZ model (1) with PBC and total $S_z$ conservation, implement translation invariance and plot the first 6 eigenvalues as a function of the total momentum $k$ (the $k$-resolved spectrum) for $L = 14, \ldots, 20$, the $S_z = 0$ magnetization sector, and the following values of $\Delta$: $\pm 10$, $\pm 2$, $\pm 1$, $\pm 0.5$ and 0.

*Hint*: For implementing translation invariance, use the fact that the (normalized) eigenstates $|\boldsymbol{\sigma}_{\mathrm{R}}, k\rangle$ of the translation operator $T$ that satisfy $T|\boldsymbol{\sigma}_{\mathrm{R}}, k\rangle = e^{ik}|\boldsymbol{\sigma}_{\mathrm{R}}, k\rangle$, can be written as

$$|\boldsymbol{\sigma}_{\mathrm{R}}, k\rangle = \frac{\sqrt{Q_{\boldsymbol{\sigma}}}}{L} \sum_{\ell=0}^{L-1} e^{-ik\ell}\, T^{\ell} |\boldsymbol{\sigma}_{\mathrm{R}}\rangle \tag{6}$$

where $\boldsymbol{\sigma}_{\mathrm{R}}$, is the representative (i.e. the lowest in lexicographic order) spin configuration within a translation orbit generated by $T$ with period $Q_{\boldsymbol{\sigma}}$ (i.e. $T^{Q_{\boldsymbol{\sigma}}}|\boldsymbol{\sigma}_{\mathrm{R}}\rangle = |\boldsymbol{\sigma}_{\mathrm{R}}\rangle$), and where the quasi-momentum $k = n_k \frac{2\pi}{L}$ ($n_k = 0, ..., L-1$) must satisfy the compatibility condition with the periodicity $Q_{\boldsymbol{\sigma}}$

$$\mathrm{mod}\ (Q_{\boldsymbol{\sigma}} n_k, L) = 0\ . \tag{7}$$

Thus, given two translation eigenstates $|\boldsymbol{\sigma}_{\mathrm{R}}, k\rangle$, $|\boldsymbol{\zeta}_{\mathrm{R}}, k\rangle$ generated by representatives $|\boldsymbol{\sigma}_{\mathrm{R}}\rangle$, $|\boldsymbol{\zeta}_{\mathrm{R}}\rangle$ whose periodicities $Q_{\boldsymbol{\sigma}}$, $Q_{\boldsymbol{\zeta}}$ are compatible with the quasi-momentum $k$, the matrix elements of the Hamiltonian block associated with a fixed $k$ are given by

$$\langle \boldsymbol{\zeta}_{\mathrm{R}}, k|H|\boldsymbol{\sigma}_{\mathrm{R}}, k\rangle = \sqrt{\frac{Q_{\boldsymbol{\sigma}}}{Q_{\boldsymbol{\zeta}}}} \sum_{\ell=0}^{Q_{\boldsymbol{\zeta}}-1} e^{-ik\ell}\, \langle T^{-\ell}\boldsymbol{\zeta}_{\mathrm{R}}|H|\boldsymbol{\sigma}_{\mathrm{R}}\rangle\ . \tag{8}$$

Your code should first generate the basis state for a fixed $k = n_k \frac{2\pi}{L}$, that is, find all the representative spin configurations $|\boldsymbol{\sigma}_{\mathrm{R}}\rangle$ among all the states with fixed $S_z = 0$, whose periodicity $Q_{\boldsymbol{\sigma}}$ is compatible with the chosen value of $n_k$. Check that summing up the numbers of representatives for all values of $n_k = 0, ..., L-1$ gives back the dimension of the Hilbert space with fixed $S_z = 0$. Once this is done, one has to generate the Hamiltonian with elements (8), and find its lowest eigenvalues. As a benchmark, check that your results for the energy match with what you computed in the previous exercises.

Once again, for the diagonalization of the Hamiltonian it is advised to use existing sparse matrix diagonalization routines (such as `eigs` in Python or Matlab).

# References


[1] J. Lamers, *A pedagogical introduction to quantum integrability, with a view towards theoretical high-energy physics*, arXiv:1501.06805v2 (2015).

[2] A. Weiße, H. Fehske, *Exact Diagonalization Techniques*, in Lecture Notes in Physics **739**, *Computational Many-Particle Physics*, Springer (2007).

[3] E. Koch, *The Lanczos Method*, in *The LDA+DMFT approach to strongly correlated materials*, Forschungszentrum Jülich, Zentralbibliothek, Verlag (2011).