

Sheet 4: Exact diagonalization Part 3: Fermions

In this exercise, we will implement exact diagonalization for the Fermi-Hubbard model.

Problem 1 Setting up spinful fermions

We consider the paradigmatic Fermi-Hubbard model in one dimension, given by the Hamiltonian

$$\hat{\mathcal{H}} = -t \sum_{\langle \mathbf{i}, \mathbf{j} \rangle, \sigma} \left(\hat{c}_{\mathbf{i}, \sigma}^\dagger \hat{c}_{\mathbf{j}, \sigma} + \text{H.c.} \right) + U \sum_{\mathbf{i}} \hat{n}_{\mathbf{i}, \uparrow} \hat{n}_{\mathbf{i}, \downarrow}, \quad (1)$$

where $\hat{c}_{\mathbf{i}, \sigma}^{(\dagger)}$ annihilates (creates) a fermion with spin $\sigma = \uparrow, \downarrow$ on site \mathbf{i} , and $\langle \mathbf{i}, \mathbf{j} \rangle$ denotes nearest-neighbor pairs on a lattice.

You can use your basis and Hamiltonian representation from Problem Sheet 2 (either with or without symmetries, as you prefer). Our goal is now to implement the Lanczos algorithm to find the ground state.

- First, we need to generate the basis for our Hilbert space. For this, we can combine separate bases for the up and down fermions, each constructed as for a simple spin-1/2 system. Due to the large local Hilbert space dimension, it is advisable to use the spin-1/2 basis with $U(1)$ symmetry enforced, i.e. fixing the total number of up and down fermions.
- Now, we need to construct operators. For this, you can re-use the spin operators you constructed on previous problem sheets and use a direct product to obtain (bosonic) operators acting on the full Hilbert space (i.e. up and down fermions combined).
- The bosonic operators can be made fermionic through the Jordan-Wigner transformation. Construct fermionic creation and annihilation operators, or directly the Fermi-Hubbard Hamiltonian. Think about (and implement) ways to benchmark that your operators are correct.
- Use built-in routines (or your own Lanczos code from previous exercises!) to find the ground state. How can you benchmark your implementations? Think about limits where you know what to expect (or can easily find the correct solution).
- What are meaningful observables to evaluate in the ground state?