Example on how to build up a numerical project

We will use a simple examle to illustrate how we can build up a many-body project using different methods. Before we present the physics case, it is worth considering some simple guidelines. A structured approach to solving problems could involve

- How to structure a code in terms of functions
- How to make a module
- How to read input data flexibly from the command line
- How to create graphical/web user interfaces
- How to write unit tests (test functions or doctests)
- How to refactor code in terms of classes (instead of functions only)
- How to conduct and automate large-scale numerical experiments
- How to write scientific reports in various formats (LaTeX, HTML)

The conventions and techniques outlined here will save you a lot of time when you incrementally extend software over time from simpler to more complicated problems. In particular, you will benefit from many good habits:

- New code is added in a modular fashion to a library (modules)
- Programs are run through convenient user interfaces
- It takes one quick command to let all your code undergo heavy testing
- Tedious manual work with running programs is automated,
- Your scientific investigations are reproducible, scientific reports with top quality typesetting are produced both for paper and electronic devices.
- And you should always use version control (git is recommended).

We present a simplified Hamiltonian consisting of an unperturbed Hamiltonian and a so-called pairing interaction term. It is a model which to a large extent mimicks some central features of atomic nuclei, certain atoms and systems which exhibit superfluiditity or superconductivity. To study this system, we will use a mix of many-body perturbation theory (MBPT), Hartree-Fock (HF) theory, coupled-cluster theory (CC) and full configuration interaction (FCI) theory. The latter will also provide us with the exact answer. When setting up the Hamiltonian matrix you will need to solve an eigenvalue problem.

We define first the Hamiltonian, with a definition of the model space and the single-particle basis. Thereafter, we present the various exercises.

The Hamiltonian acting in the complete Hilbert space (usually infinite dimensional) consists of an unperturbed one-body part, $\hat{H}_0$, and a perturbation $\hat{V}$.

We limit ourselves to at most two-body interactions, our Hamiltonian is then represented by the following operators

$$\hat{H} = \sum_{\alpha\beta} \langle \alpha | h_0 | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | V | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma,$$

where $a_\alpha^\dagger$ and a_α etc. are standard fermion creation and annihilation operators, respectively, and $\alpha\beta\gamma\delta$ represent all possible single-particle quantum numbers. The full single-particle space is defined by the completeness relation $\hat{\mathbf{1}} = \sum_{\alpha=1}^{\infty} |\alpha\rangle\langle\alpha|$. In our calculations we will let the single-particle states $|\alpha\rangle$ be eigenfunctions of the one-particle operator $\hat{h}_0$. Note that the two-body part of the Hamiltonian contains anti-symmetrized matrix elements.

The above Hamiltonian acts in turn on various many-body Slater determinants constructed from the single-basis defined by the one-body operator $\hat{h}_0$. As an example, the two-particle model space $\mathcal{P}$ is defined by an operator

$$\hat{P} = \sum_{\alpha\beta=1}^{m} |\alpha\beta\rangle\langle\alpha\beta|,$$

where we assume that $m = \dim(\mathcal{P})$ and the full space is defined by

$$\hat{P} + \hat{Q} = \hat{\mathbf{1}},$$

with the projection operator

$$\hat{Q} = \sum_{\alpha\beta=m+1}^{\infty} |\alpha\beta\rangle\langle\alpha\beta|,$$

being the complement of $\hat{P}$.

Our specific model consists of N doubly-degenerate and equally spaced single-particle levels labelled by $p = 1, 2, \ldots$ and spin $\sigma = \pm 1$. These states are schematically portrayed in Fig. 1. The first two single-particle levels define a possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$.

We write the Hamiltonian as

$$\hat{H} = \hat{H}_0 + \hat{V},$$

where

$$\hat{H}_0 = \xi \sum_{p\sigma} (p-1) a^\dagger_{p\sigma} a_{p\sigma}$$

and

$$\hat{V} = -\frac{1}{2} g \sum_{pq} a^\dagger_{p+} a^\dagger_{p-} a_{q-} a_{q+}.$$

Here, H_0 is the unperturbed Hamiltonian with a spacing between successive single-particle states given by ξ, which we will set to a constant value $\xi = 1$ without loss of generality. The two-body operator $\hat{V}$ has one term only. It represents the pairing contribution and carries a constant strength g.

The indices $\sigma = \pm$ represent the two possible spin values. The interaction can only couple pairs and excites therefore only two particles at the time, as indicated by the rightmost four-particle state in Fig. 1. There one of the pairs is excited to the state with $p = 9$ and the other to the state $p = 7$. The two middle possibilities are not possible with the present model. We label single-particle states within the model space as hole-states. The single-particle states outside the model space are then particle states.

In our model we have kept both the interaction strength and the single-particle level as constants. In a realistic system like an atom or the atomic nucleus this is not the case.

Exercises

1. Show that the unperturbed Hamiltonian $\hat{H}_0$ and $\hat{V}$ commute with both the spin projection $\hat{S}_z$ and the total spin $\hat{S}^2$, given by

   $$\hat{S}_z := \frac{1}{2} \sum_{p\sigma} \sigma a^\dagger_{p\sigma} a_{p\sigma}$$

   and

   $$\hat{S}^2 := \hat{S}_z^2 + \frac{1}{2}(\hat{S}_+ \hat{S}_- + \hat{S}_- \hat{S}_+),$$

   where

   $$\hat{S}_\pm := \sum_p a^\dagger_{p\pm} a_{p\mp}.$$

   This is an important feature of our system that allows us to block-diagonalize the full Hamiltonian. We will focus on total spin $S = 0$. In this case, it is convenient to define the so-called pair creation and pair annihilation operators

   $$\hat{P}^+_p = a^\dagger_{p+} a^\dagger_{p-},$$

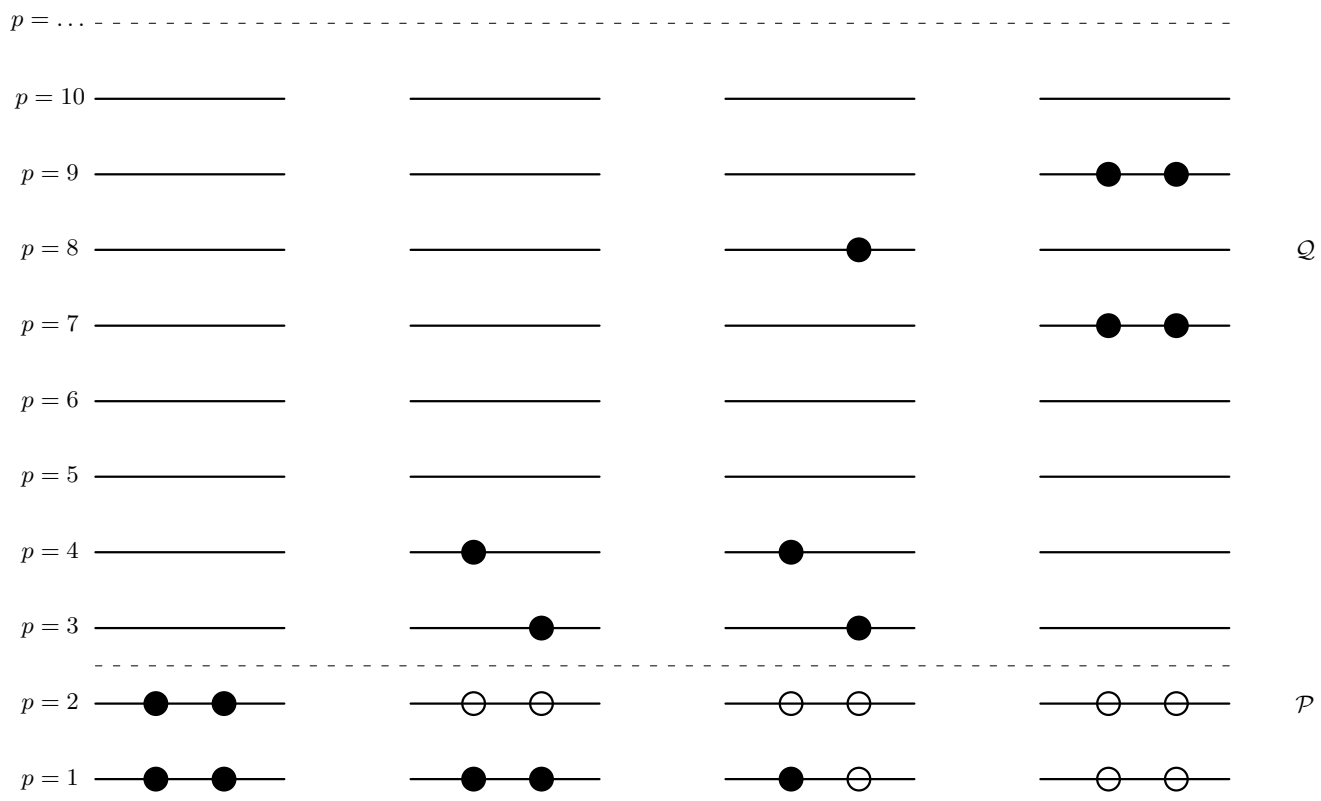

FIG. 1: Schematic plot of the possible single-particle levels with double degeneracy. The filled circles indicate occupied particle states while the empty circles represent vacant particle(hole) states. The spacing between each level p is constant in this picture. The first two single-particle levels define our possible model space, indicated by the label $\mathcal{P}$. The remaining states span the excluded space $\mathcal{Q}$. The first state to the left represents a possible ground state representation for a four-fermion system. In the second state to the left, one pair is broken. This possibility is however not included in our interaction.

and

$$\hat{P}_p^- = a_{p-}a_{p+},$$

respectively.

Show that you can rewrite the Hamiltonian (with $\xi = 1$) as

$$\hat{H} = \sum_{p\sigma}(p-1)a_{p\sigma}^\dagger a_{p\sigma} - \frac{1}{2}g\sum_{pq}\hat{P}_p^+\hat{P}_q^-.$$

Show also that Hamiltonian commutes with the product of the pair creation and annihilation operators. This model corresponds to a system with no broken pairs. This means that the Hamiltonian can only link two-particle states in so-called spin-reversed states.

2. Construct thereafter the Hamiltonian matrix for a system with no broken pairs and total spin $S = 0$ for the case of the four lowest single-particle levels indicated in the Fig. 1. Our system consists of four particles only. Our single-particle space consists of only the four lowest levels $p = 1, 2, 3, 4$. You need to set up all possible Slater determinants. Find all eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for values of $g \in [-1, 1]$. We refer to this as the exact calculation. Comment the behavior of the ground state as function of g.

3. Instead of setting up all possible Slater determinants, construct only an approximation to the ground state (where we assume that the four particles are in the two lowest single-particle orbits only) which includes at most two-particle-two-hole excitations. Diagonalize this matrix and compare with the exact calculation and comment your results. Can you set up which diagrams this approximation corresponds to?

4. We switch now to approximative methods, in our case Hartree-Fock theory and many-body perturbation theory. Hereafter we will define our model space to consist of the single-particle levels $p = 1, 2$. The remaining levels $p = 3, 4$ define our excluded space. This means that our ground state Slater determinant consists of four particles which can be placed in the doubly degenerate orbits $p = 1$ and $p = 2$. Our first step is to perform a Hartree-Fock calculation with the pairing Hamiltonian. Write first the normal-ordered Hamiltonian with respect to the above reference state given by four spin 1/2 fermions in the single-particle levels $p = 1, 2$. Define what is meant by a canonical Hartree-Fock case, a non-canonical case and a general case. For all three cases, write down the normal-ordered Hamiltonian and draw the diagrammatic form of the Hamiltonian for all three cases.

5. We will now set up the Hartree-Fock equations by varying the coefficients of the single-particle functions. The single-particle basis functions are defined as

$$\psi_p = \sum_{\lambda} C_{p\lambda} \psi_{\lambda}.$$

where in our case $p = 1, 2, 3, 4$ and $\lambda = 1, 2, 3, 4$, that is the first four lowest single-particle orbits of Fig. 1. Set up the Hartree-Fock equations for this system by varying the coefficients $C_{p\lambda}$ and solve them for values of $g \in [-1, 1]$. Comment your results and compare with the exact solution. Discuss also which diagrams in Fig. 2 that can be affected by a Hartree-Fock basis. Compute the total binding energy using a Hartree-Fock basis and comment your results.

We will now study the system using non-degenerate Rayleigh-Schrödinger perturbation theory to third order in the interaction. If we exclude the first order contribution, all possible diagrams (so-called anti-symmetric Goldstone diagrams) are shown in Fig. 2.

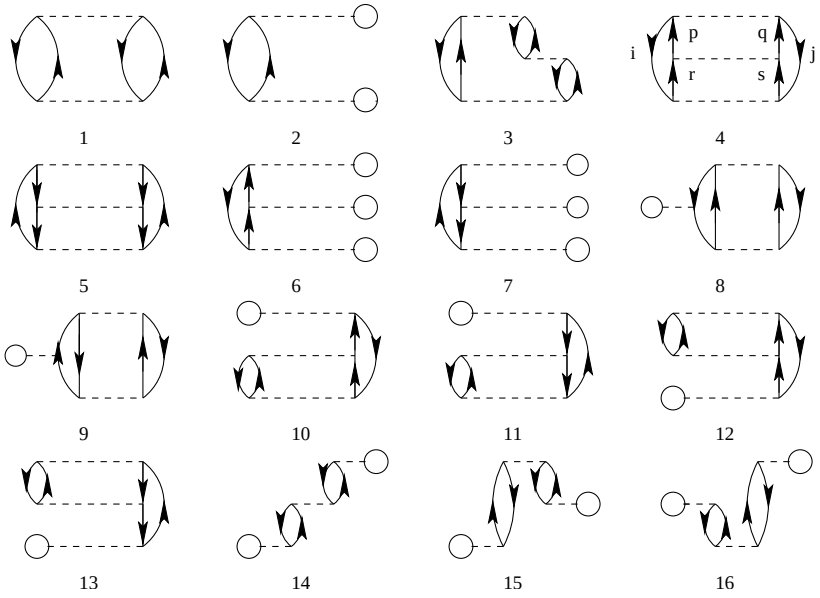

FIG. 2: Diagrams to third order in the interaction, including also non-canonical Hartree-Fock diagrams. The first order term is excluded. All interaction vertices represent anti-symmetrized matrix elements.

Based on the form of the interaction, which diagrams contribute to the binding energy of the ground state? Write down the expressions for the diagrams that contribute and find the contribution to the ground state energy as function $g \in [-1, 1]$. Comment your results. Compare these results with those you obtained in 2) and 3). Discuss your results for a canonical Hartree-Fock basis and a non-canonical Hartree-Fock basis.

6. Diagram 1 in Fig. 2 represents a second-order contribution to the energy and a so-called $2p-2h$ contribution to the intermediate states. Write down the expression for the wave operator in this case and compare the possible contributions with the configuration interaction calculations of exercise 3). Comment your results for various values of $g \in [-1, 1]$.

7. We limit now the discussion to the canonical Hartree-Fock case only. To fourth order in perturbation theory we can produce diagrams with $1p-1h$ intermediate excitations as shown in Fig. 3, $2p-2h$ excitations, see Fig. 4, $3p-3h$ excitations as shown in Fig. 5 and finally so-called diagrams with intermediate four-particle-four-hole excitations, see Fig. 6. Define first linked and unlinked diagrams and explain briefly Goldstone's

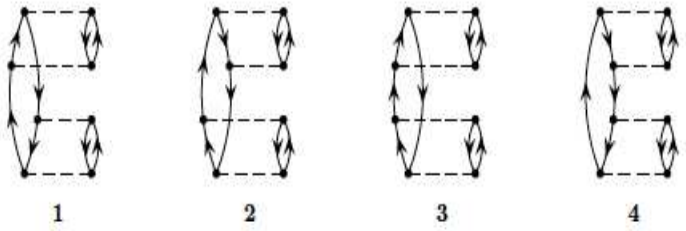

FIG. 3: One-particle-one-hole excitations to fourth order.

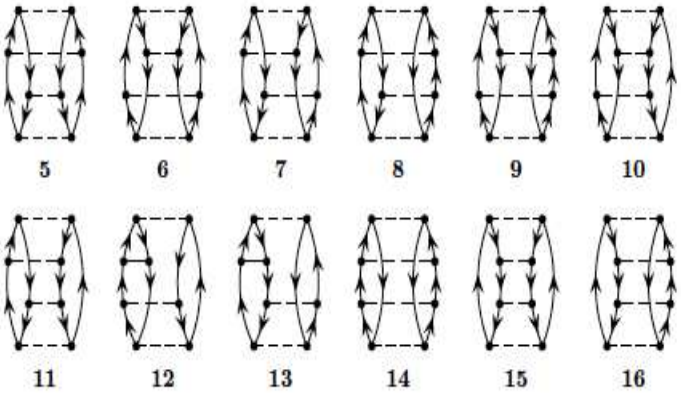

FIG. 4: Two-particle-two-hole excitations to fourth order.

linked diagram theorem. Based on the linked diagram theorem and the form of the pairing Hamiltonian, which diagrams will contribute to fourth order?

Calculate the energy to fourth order with a canonical Hartree-Fock basis for $g \in [-1, 1]$ and compare with the full diagonalization case in exercise 2). Discuss the results.

8. Finally, we will implement the coupled-cluster method by including only singles and doubles excitations. Explain why all singles excitation need not be included and find the diagrams that contribute to the doubles equations. Discuss the link with many-body perturbation theory and set up a code which solves the CCD equations.

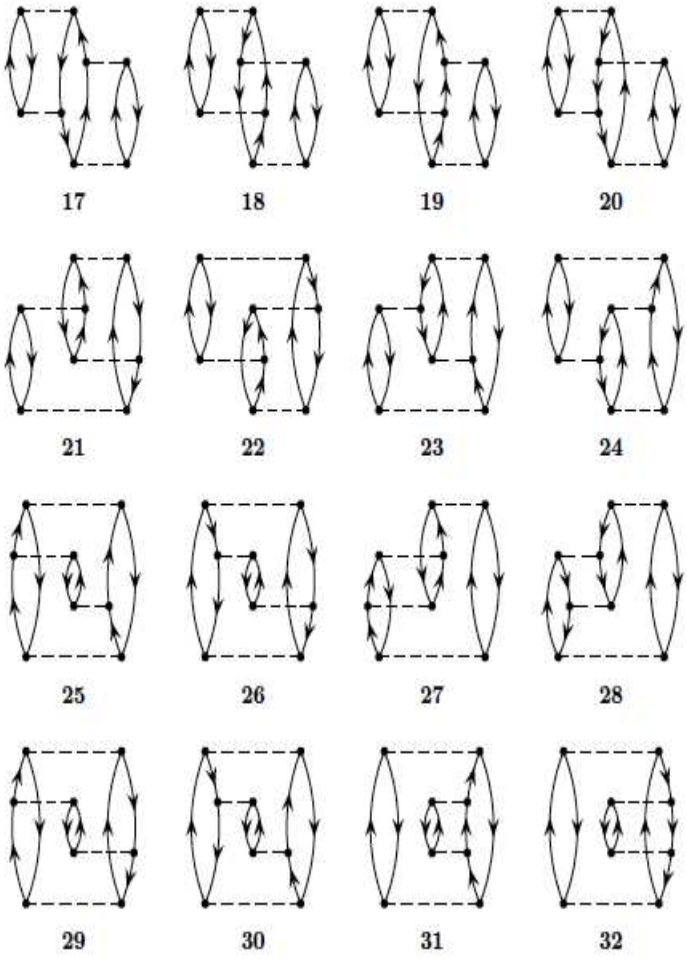

FIG. 5: Three-particle-three-hole excitations to fourth order.

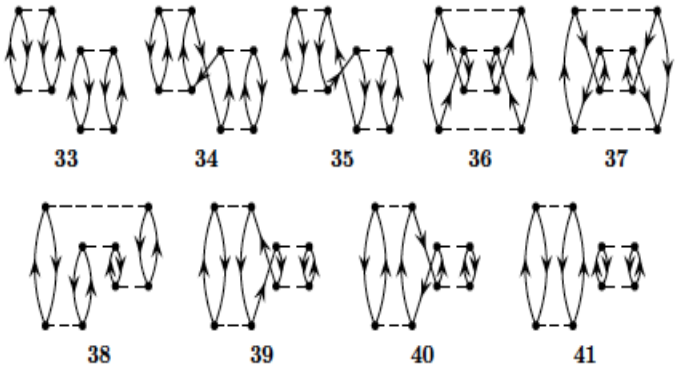

FIG. 6: Four-particle-four-hole excitations to fourth order.