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Introduction

An essential element of the Talent courses is to develop a large project(s) which allows you to study and understand theoretical concepts in nuclear physics. These concepts will in turn allow you to interpret results from experiments and understand the pertinent physics in terms of the underlying forces and laws of motion.

Together with the regular lectures in the morning, the hope is that during these three weeks you will be able to write and run a program which implements at least one of the methods discussed during the lectures. The lectures will also cover additional material which aims at giving you a broader view on what can be achieved with the methods to be discussed. Combined with the 'hands-on' afternoon sessions, the hope is that the lectures and the computational projects will together allow you to achieve these goals.

The project is divided in three main parts. The first part deals with a simple pairing model and the development of a shell-model program related to this model. This program can then serve as a benchmark program for the Coupled Cluster theory and in-medium SRG codes to be developed. The latter form the other two parts of the project.

We expect you to form working groups consisting of typically three (or more) participants. Every group should establish its own Github or Gitlab repository for the project.

Part 1, pairing problem

In the first part of the project we will thus work with a simplified Hamiltonian consisting of a one-body operator 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. Pairing plays a central role in nuclear physics, in particular, for identical particles it makes up large fractions of the correlations among particles. The partial wave ${}^1S_0$ of the nucleon-nucleon force plays a central role in setting up pairing correlations in nuclei. Without this particular partial wave, the $J = 0$ ground state spin assignment for many nuclei with even numbers of particles would not be possible.

We define first the Hamiltonian, with a definition of the model space and the single-particle basis. Thereafter, we present the various steps which are needed to develop a shell-model program for studying the pairing problem.

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

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

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{pq} \langle p|h_0|q\rangle a_p^\dagger a_q + \frac{1}{4}\sum_{pqrs} \langle pq|V|rs\rangle a_p^\dagger a_q^\dagger a_s a_r, \tag{1}$$

where $a_p^\dagger$ and a_q etc are standard fermion creation and annihilation operators, respectively, and $pqrs$ represent all possible single-particle quantum numbers. The full single-particle space is defined by the completeness relation $\hat{1} = \sum_{p=1}^{\infty} |p\rangle\langle p|$. In our calculations we will let the single-particle states $|p\rangle$ be eigenfunctions of the one-particle operator $\hat{h}_0$.

The above Hamiltonian acts in turn on various many-body Slater determinants constructed from the single-basis defined by the one-body operator $\hat{h}_0$.

Our specific model consists of only 2 doubly-degenerate and equally spaced single-particle levels labeled by $p = 1, 2, \dots$ and spin $\sigma = \pm 1$. In Eq. (1) the labels $pqrs$ could also include spin σ. From now and for the rest of this project, labels like $pqrs$ represent the states without spin. The spin quantum numbers need to be accounted for explicitely.

We write the Hamiltonian as

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

where

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

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 and is given by

$$\langle q+q-|V|s+s-\rangle = -g$$

where g is a constant. The above labeling means that for a general matrix elements $\langle pq|V|rs\rangle$ we require that the states p and q (and r and s) have the same number quantum number q but opposite spins. The two spins values are $\sigma = \pm 1$. When setting up the Hamiltonian matrix you need to figure out how to make the two-body interaction antisymmetric. The variables $\sigma = \pm$ represent the two possible spin values. The interaction can only couple pairs and excites therefore only two particles at the time.

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

The unperturbed Hamiltonian $\hat{H}_0$ and $\hat{V}$ commute with the spin projection $\hat{S}_z$ and the total spin $\hat{S}^2$. This is an important feature of our system that allows us to block-diagonalize the full Hamiltonian. In this project we will focus only on total spin $S=0$, this case is normally called the no-broken pair case.

Part 1a: Paper and pencil gym while we wait for the more serious stuff. 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

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

and

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

respectively.

The Hamiltonian (with $\xi = 1$) we will use can be written as

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

Show 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.

Part 1b: Simpler case. Assume now that the effective Hilbert space consists only of the two lowest single-particle states and that we have two particles only. Set up the possible two-particle configurations when we have only two single-particle states, that is $p = 1$ and $p = 2$. Construct thereafter the Hamiltonian matrix using second quantization and for example Wick's theorem for a system with no broken pairs and spin $S = 0$ (with projection $S_z = 0$) for the case of the two lowest single-particle levels and two particles only. This gives you a 2×2 matrix to be diagonalized.

Find the eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for selected values of $g \in [-1, 1]$ and comment your results.

Part 1c: Setting up the Hamiltonian matrix. Construct thereafter the Hamiltonian matrix for a system with no broken pairs and spin $S = 0$ for the case of the four lowest single-particle levels. 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 and the Hamiltonian matrix using second quantization and find all eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for values of $g \in [-1, 1]$. Your Hamiltonian matrix is a 6×6 matrix. These results will serve as a benchmark for the construction of our shell-model program. We refer to this as the exact results. Comment the behavior of the ground state as function of g.

Part 1d: Diagonalizing the Hamiltonian matrix. Our next step is to develop a code which sets up the above Hamiltonian matrices for two and four particles in 2 and 4 single-particles states (the same as what you did in exercises b) and c) and obtain the eigenvalues. To achieve this you should

- Decide whether you want to read from file the single-particle data and the matrix elements in m-scheme, or set them up internally in your code. The latter is the simplest possibility for the pairing model, whereas the first option gives you a more general code which can be extended to the more realistic cases discussed in the second part.

- Based on the single-particle basis, write a function which sets up all possible Slater determinants which have total $M = 0$. Test that this function reproduces the cases in b) and c). If you make this function more general, it can then be reused for say a shell-model calculation of sd-shell nuclei in the second part.

- Use the Slater determinant basis from the previous step to set up the Hamiltonian matrix.

- With the Hamiltonian matrix, you can finally diagonalize the matrix and obtain the final eigenvalues and test against the results of b) and c).

Codes to diagonalize in C++ or Fortran can be provided. For Python, numpy contains eigenvalue solvers based on for example Householder's and Givens' algorithms. These are topics which can we discuss separately. The lecture slides contain a rather detailed recipe on how to construct a Slater determinant basis and how to set up the Hamiltonian matrix to diagonalize.

Part 1e: Further benchmarks and optional part. In developing the code it also useful to test against cases which have closed-form solutions. One obvious case is that of removing the two-body interaction. Then we have only the single-particle energies. For the case of degenerate single-particle orbits, that is one value of total single-particle angular momentum only j, with degeneracy $\Omega = 2j+1$, one can show that the ground state energy E_0 is with n particles

$$E_0 = -\frac{g}{4} n \left(\Omega - n + 2\right).$$

Challenge: Enlarge now your system to six and eight fermions and to $p = 6$ and $p = 8$ single-particle states, respectively. Run your program for a degenerate single-particle state with degeneracy Ω and test against the exact result for the ground state. Introduce thereafter a finite single-particle spacing and study the results as you vary g, as done in b) and c). Comment your results.

Part 2, building your CC code the pairing case and extending it to infinite matter

Part 3, building your IMSRG code the pairing case and extending it to infinite matter