Building a Shell Model Code: The Pairing Model and the sd-Shell (and comparing results with NuShellX)

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Abstract

We have first implemented the pairing model which have a analytical solution (to benchmark the code). Then implemented the sd shell —> more general shell-model program that allows you to study general nuclear structure problems.

developing our own shell-model code that can perform shell-model studies of the oxygen isotopes using standard effective interactions (provided by us) using as example the 1s0d shell as model space.

We have also used the NushellX code in order to perform more advanced shell-model studies and compare the results obtained with your own shell-model code to those of NushellX

and found that.....results...

I. Introduction

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II. The pairing problem

The starting point is a pairing model: the system consists of fermions combined together in pairs of two, one with spin up and one with spin down. The assumption is that the 'breaking of pairs' is not allowed, i.e. the pairs of particles always will be coupled together, forming states with J=0. Of consequences the excited states are obtained from the excitation of two particles at the same time.

The physics of this system can be described by an Hamiltonian $\hat{H}$ consisting of an unperturbed one-body operator $\hat{H}_0$ and a two-body pertubation $\hat{V}$ defined as 'pairing potential': $\hat{H} = \hat{H}_0 + \hat{V}$. In second quantization we can write:

$$\hat{H}_0 = \sum_{p,\sigma} (\epsilon_p - 1) \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma}, \tag{1}$$

$$\hat{V} = -\frac{1}{2} g \sum_{p,q} \hat{a}_{p+}^\dagger \hat{a}_{p-}^\dagger \hat{a}_{q-} \hat{a}_{q+}, \tag{2}$$

where the fermion creation and annihilation operators are given by $\hat{a}_p^\dagger$ and $\hat{a}_q$ respectively and $pqrs$ represent all possible single-particle quantum numbers.

The single-particle states $|p\rangle$ are chosen as eigenfunctions of the one-particle operator $\hat{h}_0$, then the Hamiltonian H acts in turn on various many-body Slater determinants constructed from the single-basis defined by the one-body operator $\hat{h}_0$.

The two-body pairing operator $\hat{V}$ is:

$$\langle q_+ q_- | \hat{V} | s_+ s_- \rangle = -g \tag{3}$$

where it is explicitly shown that for a given matrix element $\langle pq | \hat{V} | rs \rangle$ the states p and q (or r and s) must have opposite spin ($\sigma = \pm 1$). g is the (constant) strenght of the pairing interaction.

Using the formalism of second-quantization, the rules of anticommutation for fermions and the products of commuting and anticommuting operators can be shown that $\hat{H}_0$ and $\hat{V}$ commute with the spin projection $\hat{J}_z$ and the total spin $\hat{J}^2$. This means that H can be diagonalized in separated blocks. And due to the 'no-broken pair' assumption, only $J = 0$ are allowed.

Constructing the Hamiltonian matrix We are now interested to consider a system consisting of only four particles to calculate its exact analytic solution as benchmark for our shell-model code. The single-particle space is constructed by the four lowest levels with single-particle level energies $\epsilon_p = 1, 2, 3, 4$. Every level ϵ_p contains two particles, one with spin up $|p+\rangle$ and one with spin down $|p-\rangle$.

The possible Slater determinants that we can build are 6:

$$|\Phi_0\rangle = \hat{a}_{2+}^\dagger \hat{a}_{2-}^\dagger \hat{a}_{1+}^\dagger \hat{a}_{1-}^\dagger |0\rangle$$
$$|\Phi_1\rangle = \hat{a}_{3+}^\dagger \hat{a}_{3-}^\dagger \hat{a}_{1+}^\dagger \hat{a}_{1-}^\dagger |0\rangle$$
$$|\Phi_2\rangle = \hat{a}_{4+}^\dagger \hat{a}_{4-}^\dagger \hat{a}_{1+}^\dagger \hat{a}_{1-}^\dagger |0\rangle$$
$$|\Phi_3\rangle = \hat{a}_{3+}^\dagger \hat{a}_{3-}^\dagger \hat{a}_{2+}^\dagger \hat{a}_{2-}^\dagger |0\rangle$$
$$|\Phi_4\rangle = \hat{a}_{4+}^\dagger \hat{a}_{4-}^\dagger \hat{a}_{2+}^\dagger \hat{a}_{2-}^\dagger |0\rangle$$
$$|\Phi_5\rangle = \hat{a}_{4+}^\dagger \hat{a}_{4-}^\dagger \hat{a}_{3+}^\dagger \hat{a}_{3-}^\dagger |0\rangle,$$

from which we can construct the basis for the Hamiltonian matrix:

$$|\Phi_0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |\Phi_1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \cdots \quad |\Phi_5\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

The matrix elements $H_{ij} = \langle \Phi_i | \hat{H} | \Phi_j \rangle$ [1] are obtained using the Hamiltonian of Eq. (1), the Slater determinants and the Wick-theorem. $\hat{H}_0$ acts only on the diagonal and results in terms proportional with $(\epsilon_p - 1)$. The interaction will excite or deexcite a pair of particles from level q to level p.

Using the Wick-theorem, we notice that only the Slater determinants that differ for maximum a pair can interact among them through the pairing potential:

$$\begin{aligned}
\langle \Phi_i | \hat{V} | \Phi_j \rangle &= \langle 0 | \hat{a}_{i_1-} \hat{a}_{i_1+} \hat{a}_{i_2-} \hat{a}_{i_2+} \left[-\frac{1}{2} g \sum_{p,q} \hat{a}_{p+}^\dagger \hat{a}_{p-}^\dagger \hat{a}_{q-} \hat{a}_{q+} \right] \hat{a}_{j_2+}^\dagger \hat{a}_{j_2-}^\dagger \hat{a}_{j_1+}^\dagger \hat{a}_{j_1-}^\dagger | 0 \rangle \\
&= -\frac{1}{2} g \left(\delta_{p,i_2} \delta_{q,j_2} \delta_{i_1,j_1} + \delta_{p,i_2} \delta_{q,j_1} \delta_{i_1,j_2} + \delta_{p,i_1} \delta_{q,j_2} \delta_{i_2,j_1} + \delta_{p,i_1} \delta_{q,j_1} \delta_{i_2,j_2} \right)
\end{aligned} \tag{4}$$

and Eq.(4) is not null only if at least one of $\delta_{i_1,j_1}, \delta_{i_1,j_2}, \delta_{i_2,j_1}$ or δ_{i_2,j_2} among bra and ket states is not zero.

For example the first term in Eq.(4) is obtained from the contractions

$$\langle 0 | \hat{a}_{i_1-} \hat{a}_{i_1+} \hat{a}_{i_2-} \hat{a}_{i_2+} \hat{a}_{p+}^\dagger \hat{a}_{p-}^\dagger \hat{a}_{q-} \hat{a}_{q+} \hat{a}_{j_2+}^\dagger \hat{a}_{j_2-}^\dagger \hat{a}_{j_1+}^\dagger \hat{a}_{j_1-}^\dagger | 0 \rangle = \delta_{p,i_2} \delta_{q,j_2} \delta_{i_1,j_1}.$$

Explicitly, the matrix element H_{00} is

$$\begin{aligned}
\langle \Phi_0 | \hat{H} | \Phi_0 \rangle &= \langle 0 | \hat{a}_{1-} \hat{a}_{1+} \hat{a}_{2-} \hat{a}_{2+} \left[\sum_{p,\sigma} (\epsilon_p - 1) \hat{a}_{p\sigma}^\dagger \hat{a}_{p\sigma} \right] \hat{a}_{2+}^\dagger \hat{a}_{2-}^\dagger \hat{a}_{1+}^\dagger \hat{a}_{1-}^\dagger | 0 \rangle \\
&+ \langle 0 | \hat{a}_{1-} \hat{a}_{1+} \hat{a}_{2-} \hat{a}_{2+} \left[-\frac{1}{2} g \sum_{p,q} \hat{a}_{p+}^\dagger \hat{a}_{p-}^\dagger \hat{a}_{q-} \hat{a}_{q+} \right] \hat{a}_{2+}^\dagger \hat{a}_{2-}^\dagger \hat{a}_{1+}^\dagger \hat{a}_{1-}^\dagger | 0 \rangle \\
&= 2 \cdot 0 + 2 \cdot (2 - 1) + 2 \cdot \left(-\frac{1}{2} g \right) = 2 - g.
\end{aligned} \tag{5}$$

The Hamiltonian matrix becomes

$$\hat{H} = \begin{pmatrix}
2-g & -g/2 & -g/2 & -g/2 & -g/2 & 0 \\
-g/2 & 4-g & -g/2 & -g/2 & 0 & -g/2 \\
-g/2 & -g/2 & 6-g & 0 & -g/2 & -g/2 \\
-g/2 & -g/2 & 0 & 6-g & -g/2 & -g/2 \\
-g/2 & 0 & -g/2 & -g/2 & 8-g & -g/2 \\
0 & -g/2 & -g/2 & -g/2 & -g/2 & 10-g
\end{pmatrix}. \tag{6}$$

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[1] We use the label 0 to indicate the Slater determinants with the 4 particles in the lowest states, then the first row first column matrix element is H_{00}....
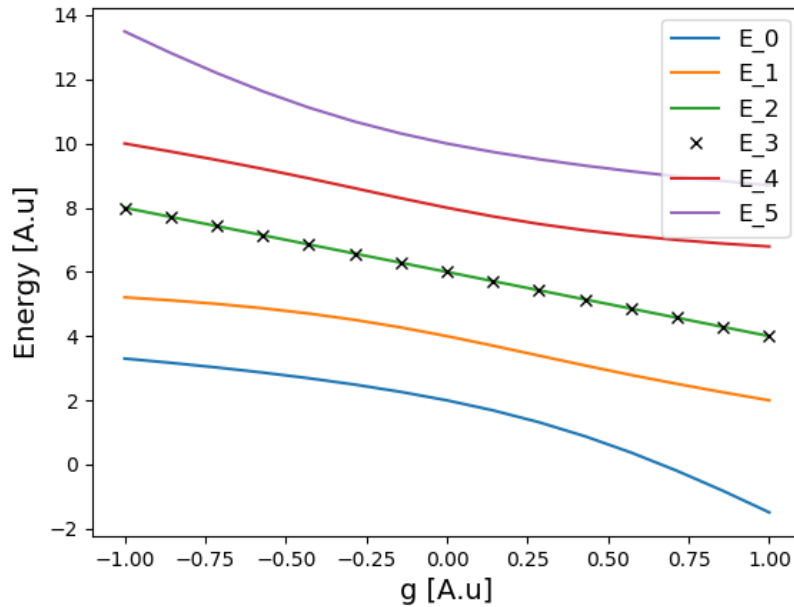
Figure 1: *The energy levels as a function of the strength g for the analytic case of the pairing model.*

In Figure 1 we see the eigenvalues of the Hamiltonian matrix (6) for the pairing model as a function of the strength $g \in [-1, 1]$. [2].

We can observe that the pairing potential increases the gap among the energy levels E_i, eigenvalues of Eq.(6). The case $g = 1$, corresponding to a strong attractive pairing, produces the more stable system (lowest energy levels).

III. Building the shell model code

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.

What did we choose?

- 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).

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[2]The diagonalization was done with numpy

Include some of this? Or too much? :
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.

i.   first step....

ii.   Unit tests and benchmarks

(have not done this?)

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

$$E_0 = -\frac{g}{4}n(\Omega - n + 2) \tag{7}$$

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.

(describe the unit test that we have implemented and how)

IV.   NuShellX

(describe what is, then put results in results section?)

V.   Results

VI.   Discussion

VII.   Conclusions

Structure of report (crude first idea):

1. Title

2. Abstract

3. Introduction

   - Why useful
   - Where useful (nuc. chart)
   - (Look at the TALENT proposal)
   - comparing different tools

4. The Pairing problem

   - theory
   - analytic / exact results

5. Building a shell-model code

- Describe the different parts/blocks of the code (basis, SD, states, int, hamiltonian...)
- Unit tests / benchmarks (analytic/exact results)
- Psedo code?
- Accuracy of our code
- Where our code fails, why and proposing solutions

6. NuShellX

- describe why useful / 'powerful tool' and what may be calculated
- compare with our own code
- Possible 'future calculations'

7. Conclusions / Summary

References

[Github of the TALENT School] MHJ and Alex Brown *link goes here*,