Building a Shell Model Code: The Pairing Model and the sd-Shell

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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.

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

I. Introduction

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II. Theory

i. The Pairing Model

The pairing model is one of a few systems that has a simple analytic solution. It is therefore very useful to use this model to check that the numerical solution matches the analytic solution while developing the code.

The pairing problem consists of a system where the fermions combines together in pairs of two, one with spin up and one with spin down. This model does not allow so-called 'breaking of pairs' meaning that the pairs of particles always will be coupled together. An excitation must excite two particles at the same time.

Mathematically the pairing model can be described by a simplified Hamiltonian consisting of a unperturbed one-body operator H^0 and a pertubation so-called 'pairing interaction term' H^I. We will limit ourselves to at most two-body interactions so that we can write the operators as:

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

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

so that the full Hamiltonian is given by the sum of the unperturbed term and the interacting part $\hat{H} = \hat{H}_0 + \hat{V}$. The fermion creation and annihilation operators are given by $\hat{a}^{\dagger}_p$ and $\hat{a}_q$ respectively and $pqrs$ represent all possible single-particle quantum numbers. To simplify the expressions we set the spacing between successive single-particle states given by $\xi = 1$.

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 $\hat{h}_0$.

The two-body operator $\hat{V}$ consists of one term:

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

representing the pairing contribution with (for simplicity) constant strength g. The labeling requires 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 ($\sigma = \pm 1$)

It can be shown that 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 allows us to block-diagonalize the full Hamiltonian. For the pairing case we have assumed that $S = 0$ giving the so-called 'no-broken pair' case.

Constructing the Hamiltonian matrix As an analytic solution we chose a system consisting of only four particles with a single-particle space consisting of only the four lowest levels $p = 1,2,3,4$. In our system every level p contains two particles, one with spin up and one with spin down. The goal is to set up all possible Slater determinants and the Hamiltonian matrix using second quantization and find all eigenvalues by diagonalizing the Hamiltonian matrix.

We construct the basis:

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

where

$$
\begin{aligned}
|\Phi_0\rangle &= \hat{a}^\dagger_{2+}\hat{a}^\dagger_{2-}\hat{a}^\dagger_{1+}\hat{a}^\dagger_{1-}|0\rangle = \hat{P}^+_2\hat{P}^+_1|0\rangle,\\
|\Phi_1\rangle &= \hat{P}^+_3\hat{P}^+_1|0\rangle,\\
|\Phi_2\rangle &= \hat{P}^+_4\hat{P}^+_1|0\rangle,\\
|\Phi_3\rangle &= \hat{P}^+_3\hat{P}^+_2|0\rangle,\\
|\Phi_4\rangle &= \hat{P}^+_4\hat{P}^+_2|0\rangle,\\
|\Phi_5\rangle &= \hat{P}^+_4\hat{P}^+_3|0\rangle.
\end{aligned}
$$

Given the above Slater determinants we can now compute the matrix elements $\langle\Phi_i|\hat{H}|\Phi_j\rangle$ using the Hamiltonian of Eq. (1). The one-body operator acts only on the diagonal and results in terms proportional with $(p1)$. The interaction will excite or deexcite a pair of particles from level q to level p. Using this it is easy to see that the Hamilotnian matrix becomes: (REWRITE THIS PARAGRAPH, ALL COPY)

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

For a given g this matrix can be used as the analytic result to compare with the output in the shell model code for the pairing case.

Table 1: *Example table*

Name		
First name	Last Name	Grade
John	Doe	7.5
Richard	Miles	2

We are only including two lowest single-particle levels and totally two particles. We want to construct the Hamiltonian matrix using second quantization and WickâĂŹs theorem for a system with no broken pairs and $S = 0$, $S_z = 0$

In this model we can only excite two particles at the same time, so we can define the ground state and the excited state which are the only two possible states:

(also include a figure with the states drawn?)

(for P=2) Find the eigenvalues by diagonalizing the Hamiltonian matrix. Vary your results for selected values of g âĹĹ [âĹŠ1, 1] and comment your results.

III. Methods

Text requiring further explanation[1].

IV. Results

V. Discussion

References

[Figueredo and Wolf, 2009] Figueredo, A. J. and Wolf, P. S. A. (2009). Assortative pairing and life history strategy - a cross-cultural study. *Human Nature*, 20:317–330.

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

[1]Example footnote