Nuclear Shell Model

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Slater determinants as basis states, Repetition

The simplest possible choice for many-body wavefunctions are **product** wavefunctions. That is

$$\Psi(x_1, x_2, x_3, \dots, x_A) \approx \phi_1(x_1)\phi_2(x_2)\phi_3(x_3)\dots$$

because we are really only good at thinking about one particle at a time. Such product wavefunctions, without correlations, are easy to work with; for example, if the single-particle states $\phi_i(x)$ are orthonormal, then the product wavefunctions are easy to orthonormalize.

Similarly, computing matrix elements of operators are relatively easy, because the integrals factorize.

The price we pay is the lack of correlations, which we must build up by using many, many product wavefunctions. (Thus we have a trade-off: compact representation of correlations but difficult integrals versus easy integrals but many states required.)

Because we have fermions, we are required to have antisymmetric wavefunctions, e.g.

$$\Psi(x_1, x_2, x_3, \dots, x_A) = -\Psi(x_2, x_1, x_3, \dots, x_A)$$

etc. This is accomplished formally by using the determinantal formalism

$$\Psi(x_1, x_2, \dots, x_A) = \frac{1}{\sqrt{A!}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \dots & \phi_1(x_A) \\ \phi_2(x_1) & \phi_2(x_2) & \dots & \phi_2(x_A) \\ \vdots & & & \\ \phi_A(x_1) & \phi_A(x_2) & \dots & \phi_A(x_A) \end{vmatrix}$$

Product wavefunction + antisymmetry = Slater determinant.

$$\Psi(x_1, x_2, \ldots, x_A) = \frac{1}{\sqrt{N!}} \det \begin{vmatrix} \phi_1(x_1) & \phi_1(x_2) & \ldots & \phi_1(x_A) \\ \phi_2(x_1) & \phi_2(x_2) & \ldots & \phi_2(x_A) \\ \vdots & & & \\ \phi_A(x_1) & \phi_A(x_2) & \ldots & \phi_A(x_A) \end{vmatrix}$$

Properties of the determinant (interchange of any two rows or any two columns yields a change in sign; thus no two rows and no two columns can be the same) lead to the Pauli principle:

- No two particles can be at the same place (two columns the same); and
- No two particles can be in the same state (two rows the same).

As a practical matter, however, Slater determinants beyond $N = 4$ quickly become unwieldy. Thus we turn to the **occupation representation** or **second quantization** to simplify calculations.

The occupation representation, using fermion **creation** and **annihilation** operators, is compact and efficient. It is also abstract and, at first encounter, not easy to internalize. It is inspired by other operator formalism, such as the ladder operators for the harmonic oscillator or for angular momentum, but unlike those cases, the operators **do not have coordinate space representations**.

Instead, one can think of fermion creation/annihilation operators as a game of symbols that compactly reproduces what one would do, albeit clumsily, with full coordinate-space Slater determinants.

We start with a set of orthonormal single-particle states $\{\phi_i(x)\}$. (Note: this requirement, and others, can be relaxed, but leads to a more involved formalism.) **Any** orthonormal set will do.

To each single-particle state $\phi_i(x)$ we associate a creation operator $\hat{a}_i^\dagger$ and an annihilation operator $\hat{a}_i$.

When acting on the vacuum state $|0\rangle$, the creation operator $\hat{a}_i^\dagger$ causes a particle to occupy the single-particle state $\phi_i(x)$:

$$\phi_i(x) \rightarrow \hat{a}_i^\dagger |0\rangle$$

But with multiple creation operators we can occupy multiple states:

$$\phi_i(x)\phi_j(x')\phi_k(x'') \rightarrow \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger |0\rangle.$$

Now we impose antisymmetry, by having the fermion operators satisfy **anti-commutation relations**:

$$\hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i^\dagger = [\hat{a}_i^\dagger, \hat{a}_j^\dagger]_+ = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0$$

so that

$$\hat{a}_i^\dagger \hat{a}_j^\dagger = -\hat{a}_j^\dagger \hat{a}_i^\dagger$$

Because of this property, automatically $\hat{a}_i^\dagger \hat{a}_i^\dagger = 0$, enforcing the Pauli exclusion principle. Thus when writing a Slater determinant using creation operators,

$$\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \dots |0\rangle$$

each index $i, j, k, \dots$ must be unique.

Full Configuration Interaction Theory

We have defined the ansatz for the ground state as

$$|\Phi_0\rangle = \left(\prod_{i \leq F} \hat{a}_i^\dagger \right) |0\rangle,$$

where the index i defines different single-particle states up to the Fermi level. We have assumed that we have N fermions. A given one-particle-one-hole ($1p1h$) state can be written as

$$|\Phi_i^a\rangle = \hat{a}_a^\dagger \hat{a}_i |\Phi_0\rangle,$$

while a $2p2h$ state can be written as

$$|\Phi_{ij}^{ab}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i |\Phi_0\rangle,$$

and a general $NpNh$ state as

$$|\Phi_{ijk\dots}^{abc\cdots}\rangle = \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \dots \hat{a}_k \hat{a}_j \hat{a}_i |\Phi_0\rangle.$$

We can then expand our exact state function for the ground state as

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{abij} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \cdots = (C_0 + \hat{C})|\Phi_0\rangle,$$

where we have introduced the so-called correlation operator

$$\hat{C} = \sum_{ai} C_i^a \hat{a}_a^\dagger \hat{a}_i + \sum_{abij} C_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i + \dots$$

Since the normalization of Ψ_0 is at our disposal and since C_0 is by hypothesis non-zero, we may arbitrarily set $C_0 = 1$ with corresponding proportional changes in all other coefficients. Using this so-called intermediate normalization we have

$$\langle \Psi_0 | \Phi_0 \rangle = \langle \Phi_0 | \Phi_0 \rangle = 1,$$

resulting in

$$|\Psi_0\rangle = (1 + \hat{C})|\Phi_0\rangle.$$

We rewrite

$$|\Psi_0\rangle = C_0|\Phi_0\rangle + \sum_{ai} C_i^a |\Phi_i^a\rangle + \sum_{abij} C_{ij}^{ab} |\Phi_{ij}^{ab}\rangle + \dots,$$

in a more compact form as

$$|\Psi_0\rangle = \sum_{PH} C_H^P \Phi_H^P = \left(\sum_{PH} C_H^P \hat{A}_H^P \right) |\Phi_0\rangle,$$

where H stands for $0, 1, \ldots, n$ hole states and P for $0, 1, \ldots, n$ particle states. Our requirement of unit normalization gives

$$\langle \Psi_0 | \Phi_0 \rangle = \sum_{PH} |C_H^P|^2 = 1,$$

and the energy can be written as

$$E = \langle \Psi_0 | \hat{H} | \Phi_0 \rangle = \sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'}.$$

Normally

$$E = \langle \Psi_0 | \hat{H} | \Phi_0 \rangle = \sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'},$$

is solved by diagonalization setting up the Hamiltonian matrix defined by the basis of all possible Slater determinants. A diagonalization is equivalent to finding the variational minimum of

$$\langle \Psi_0 | \hat{H} | \Phi_0 \rangle - \lambda \langle \Psi_0 | \Phi_0 \rangle,$$

where λ is a variational multiplier to be identified with the energy of the system. The minimization process results in

$$\delta \left[\langle \Psi_0 | \hat{H} | \Phi_0 \rangle - \lambda \langle \Psi_0 | \Phi_0 \rangle \right] =$$

$$\sum_{P'H'} \left\{ \delta[C_H^{*P}] \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} + C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle \delta[C_{H'}^{P'}] - \lambda (\delta[C_H^{*P}] C_{H'}^{P'} + C_H^{*P} \delta[C_{H'}^{P'}] \right\} = 0.$$

Since the coefficients $\delta[C_H^{*P}]$ and $\delta[C_{H'}^{P'}]$ are complex conjugates it is necessary and sufficient to require the quantities that multiply with $\delta[C_H^{*P}]$ to vanish.

This leads to

$$\sum_{P'H'} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} - \lambda C_H^P = 0,$$

for all sets of P and H.

If we then multiply by the corresponding C_H^{*P} and sum over PH we obtain

$$\sum_{PP'HH'} C_H^{*P} \langle \Phi_H^P | \hat{H} | \Phi_{H'}^{P'} \rangle C_{H'}^{P'} - \lambda \sum_{PH} |C_H^P|^2 = 0,$$

leading to the identification $\lambda = E$. This means that we have for all PH sets

$$\sum_{P'H'} \langle \Phi_H^P | \hat{H} - E | \Phi_{H'}^{P'} \rangle = 0. \tag{1}$$

An alternative way to derive the last equation is to start from

$$(\hat{H}-E)|\Psi_0\rangle = (\hat{H}-E)\sum_{P'H'} C_{H'}^{P'}|\Phi_{H'}^{P'}\rangle = 0,$$

and if this equation is successively projected against all Φ_H^P in the expansion of Ψ, then the last equation on the previous slide results. As stated previously, one solves this equation normally by diagonalization. If we are able to solve this equation exactly (that is numerically exactly) in a large Hilbert space (it will be truncated in terms of the number of single-particle states included in the definition of Slater determinants), it can then serve as a benchmark for other many-body methods which approximate the correlation operator $\hat{C}$.

For reasons to come (links with Coupled-Cluster theory and Many-Body perturbation theory), we will rewrite Eq. (**??**) as a set of coupled non-linear equations in terms of the unknown coefficients C_H^P. To obtain the eigenstates and eigenvalues in terms of non-linear equations is not a very practical approach. However, it serves the scope of linking FCI theory with approximative solutions to the many-body problem.

To see this, we look at the contributions arising from

$$\langle\Phi_H^P| = \langle\Phi_0|$$

in Eq. (**??**), that is we multiply with $\langle\Phi_0|$ from the left in

$$(\hat{H}-E)\sum_{P'H'} C_{H'}^{P'}|\Phi_{H'}^{P'}\rangle = 0.$$

If we assume that we have a two-body operator at most, Slater's rule gives then an equation for the correlation energy in terms of C_i^a and C_{ij}^{ab} only. We get then

$$\langle\Phi_0|\hat{H}-E|\Phi_0\rangle + \sum_{ai}\langle\Phi_0|\hat{H}-E|\Phi_i^a\rangle C_i^a + \sum_{abij}\langle\Phi_0|\hat{H}-E|\Phi_{ij}^{ab}\rangle C_{ij}^{ab} = 0,$$

or

$$E-E_0 = \Delta E = \sum_{ai}\langle\Phi_0|\hat{H}|\Phi_i^a\rangle C_i^a + \sum_{abij}\langle\Phi_0|\hat{H}|\Phi_{ij}^{ab}\rangle C_{ij}^{ab},$$

where the energy E_0 is the reference energy and ΔE defines the so-called correlation energy. The single-particle basis functions could be the results of a Hartree-Fock calculation or just the eigenstates of the non-interacting part of the Hamiltonian.

In our chapter on Hartree-Fock calculations, we have already computed the matrix $\langle\Phi_0|\hat{H}|\Phi_i^a\rangle$ and $\langle\Phi_0|\hat{H}|\Phi_{ij}^{ab}\rangle$. If we are using a Hartree-Fock basis, then the matrix elements $\langle\Phi_0|\hat{H}|\Phi_i^a\rangle$ and we are left with a correlation energy given by

$$E-E_0 = \Delta E^{HF} = \sum_{abij}\langle\Phi_0|\hat{H}|\Phi_{ij}^{ab}\rangle C_{ij}^{ab}.$$

Inserting the various matrix elements we can rewrite the previous equation as

$$\Delta E = \sum_{ai}\langle i|\hat{f}|a\rangle C_i^a + \sum_{abij}\langle ij|\hat{v}|ab\rangle C_{ij}^{ab}.$$

This equation determines the correlation energy but not the coefficients C. We need more equations. Our next step is to set up

$$\langle\Phi_i^a|\hat{H}-E|\Phi_0\rangle+\sum_{bj}\langle\Phi_i^a|\hat{H}-E|\Phi_j^b\rangle C_j^b+\sum_{bcjk}\langle\Phi_i^a|\hat{H}-E|\Phi_{jk}^{bc}\rangle C_{jk}^{bc}+\sum_{bcdjkl}\langle\Phi_i^a|\hat{H}-E|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd}=0,$$

as this equation will allow us to find an expression for the coefficents C_i^a since we can rewrite this equation as

$$\langle i|\hat{f}|a\rangle+\langle\Phi_i^a|\hat{H}|\Phi_i^a\rangle C_i^a+\sum_{bj\neq ai}\langle\Phi_i^a|\hat{H}|\Phi_j^b\rangle C_j^b+\sum_{bcjk}\langle\Phi_i^a|\hat{H}|\Phi_{jk}^{bc}\rangle C_{jk}^{bc}+\sum_{bcdjkl}\langle\Phi_i^a|\hat{H}|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd}=0.$$

We rewrite this equation as

$$C_i^a = -(\langle\Phi_i^a|\hat{H}|\Phi_i^a\rangle)^{-1}$$

$$\times\left(\langle i|\hat{f}|a\rangle+\sum_{bj\neq ai}\langle\Phi_i^a|\hat{H}|\Phi_j^b\rangle C_j^b+\sum_{bcjk}\langle\Phi_i^a|\hat{H}|\Phi_{jk}^{bc}\rangle C_{jk}^{bc}+\sum_{bcdjkl}\langle\Phi_i^a|\hat{H}|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd}\right).$$

Since these equations are solved iteratively (that is we can start with a guess for the coefficients C_i^a), it is common to start the iteration by setting

$$C_i^a = -\frac{\langle i|\hat{f}|a\rangle}{\langle\Phi_i^a|\hat{H}|\Phi_i^a\rangle},$$

and the denominator can be written as

$$C_i^a = \frac{\langle i|\hat{f}|a\rangle}{\langle i|\hat{f}|i\rangle-\langle a|\hat{f}|a\rangle+\langle ai|\hat{v}|ai\rangle}.$$

The observant reader will however see that we need an equation for C_{jk}^{bc} and C_{jkl}^{bcd} as well. To find equations for these coefficients we need then to continue our multiplications from the left with the various Φ_H^P terms.

For C_{jk}^{bc} we need then

$$\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_0\rangle+\sum_{kc}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_k^c\rangle C_k^c+$$

$$\sum_{cdkl}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{kl}^{cd}\rangle C_{kl}^{cd}+\sum_{cdeklm}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klm}^{cde}\rangle C_{klm}^{cde}+\sum_{cdefklmn}\langle\Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klmn}^{cdef}\rangle C_{klmn}^{cdef}=0,$$

and we can isolate the coefficients C_{kl}^{cd} in a similar way as we did for the coefficients C_i^a. At the end we can rewrite our solution of the Schrödinger

equation in terms of n coupled equations for the coefficients C_H^P. This is a very cumbersome way of solving the equation. However, by using this iterative scheme we can illustrate how we can compute the various terms in the wave operator or correlation operator $\hat{C}$. We will later identify the calculation of the various terms C_H^P as parts of different many-body approximations to full CI. In particular, ww can relate this non-linear scheme with Coupled Cluster theory and many-body perturbation theory. .

If we use a Hartree-Fock basis, we simplify this equation

$$\Delta E = \sum_{ai} \langle i|\hat{f}|a\rangle C_i^a + \sum_{abij} \langle ij|\hat{v}|ab\rangle C_{ij}^{ab}.$$

What about

$$\langle \Phi_i^a|\hat{H}-E|\Phi_0\rangle + \sum_{bj} \langle \Phi_i^a|\hat{H}-E|\Phi_j^b\rangle C_j^b + \sum_{bcjk} \langle \Phi_i^a|\hat{H}-E|\Phi_{jk}^{bc}\rangle C_{jk}^{bc} + \sum_{bcdjkl} \langle \Phi_i^a|\hat{H}-E|\Phi_{jkl}^{bcd}\rangle C_{jkl}^{bcd} = 0,$$

and

$$\langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_0\rangle + \sum_{kc} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_k^c\rangle C_k^c + \sum_{cdkl} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_{kl}^{cd}\rangle C_{kl}^{cd} +$$

$$\sum_{cdeklm} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klm}^{cde}\rangle C_{klm}^{cde} + \sum_{cdefklmn} \langle \Phi_{ij}^{ab}|\hat{H}-E|\Phi_{klmn}^{cdef}\rangle C_{klmn}^{cdef} = 0?$$

- TO DO: finish this discussion and discuss truncations like CISD, prepare the ground for MBPT and CC theories

Building a many-body basis

- TO DO: make figures of various approaches to the basis:
  1. Standard shell-model basis in one or two major shells
  2. Full CI in a given basis and no truncations
  3. CISD and CISDT (prepare for link to CC theory)
  4. No-core shell model and truncation in excitation energy

Let us now sketch how construct a working code that constructs the many-body Hamiltonian matrix in a basis of Slater determinants and allows us to find the low-lying eigenenergies. This is referred to as the configuration-interaction method or shell-model diagonalization (or the interacting shell model).

The first step in such codes is to construct the many-body basis.

While the formalism is independent of the choice of basis, the **effectiveness** of a calculation will certainly be basis dependent.

Furthermore there are common conventions useful to know.

First, the single-particle basis has angular momentum as a good quantum number. You can imagine the single-particle wavefunctions being generated

by a one-body Hamiltonian, for example a harmonic oscillator. Modifications include harmonic oscillator plus spin-orbit splitting, or self-consistent mean-field potentials, or the Woods-Saxon potential which mocks up the self-consistent mean-field.

For nuclei, the harmonic oscillator, modified by spin-orbit splitting, provides a useful language for describing single-particle states.

Each single-particle state is labeled by the following quantum numbers:

- Orbital angular momentum l
- Intrinsic spin $s = 1/2$ for protons and neutrons
- Angular momentum $j = l \pm 1/2$
- z-component j_z (or m)
- Some labeling of the radial wavefunction, typically n the number of nodes in the radial wavefunction, but in the case of harmonic oscillator one can also use the principal quantum number N, where the harmonic oscillator energy is $(N + 3/2)\hbar\omega$.

In this format one labels states by $n(l)_j$, with (l) replaced by a letter: s for $l = 0$, p for $l = 1$, d for $l = 2$, f for $l = 3$, and thenceforth alphabetical.

In practice the single-particle space has to be severely truncated. This truncation is typically based upon the single-particle energies, which is the effective energy from a mean-field potential.

Sometimes we freeze the core and only consider a valence space. For example, one may assume a frozen ^{4}He core, with two protons and two neutrons in the $0s_{1/2}$ shell, and then only allow active particles in the $0p_{1/2}$ and $0p_{3/2}$ orbits.

Another example is a frozen ^{16}O core, with eight protons and eight neutrons filling the $0s_{1/2}$, $0p_{1/2}$ and $0p_{3/2}$ orbits, with valence particles in the $0d_{5/2}, 1s_{1/2}$ and $0d_{3/2}$ orbits.

Sometimes we refer to nuclei by the valence space where their last nucleons go. So, for example, we call ^{12}C a p-shell nucleus, while ^{26}Al is an sd-shell nucleus and ^{56}Fe is a pf-shell nucleus.

There are different kinds of truncations.

- For example, one can start with 'filled' orbits (almost always the lowest), and then allow one, two, three... particles excited out of those filled orbits. These are called 1p-1h, 2p-2h, 3p-3h excitations.
- Alternately, one can state a maximal orbit and allow all possible configurations with particles occupying states up to that maximum. This is called *full configuration*.
- Finally, for particular use in nuclear physics, there is the *energy* truncation, also called the $N\hbar\Omega$ or N_{max} truncation.

Here one works in a harmonic oscillator basis, with each major oscillator shell assigned a principal quantum number $N = 0, 1, 2, 3, ...$

The $N\hbar\Omega$ or N_{max} truncation: Any configuration is given an noninteracting energy, which is the sum of the single-particle harmonic oscillator energies. (Thus this ignores spin-orbit splitting.)

Excited state are labeled relative to the lowest configuration by the number of harmonic oscillator quanta.

This truncation is useful because: if one includes *all* configuration up to some N_{max}, and has a translationally invariant interaction, then the intrinsic motion and the center-of-mass motion factor. In other words, we can know exactly the center-of-mass wavefunction.

In almost all cases, the many-body Hamiltonian is rotationally invariant. This means it commutes with the operators $\hat{J}^2, \hat{J}_z$ and so eigenstates will have good J, M. Furthermore, the eigenenergies do not depend upon the orientation M.

Therefore we can choose to construct a many-body basis which has fixed M; this is called an M-scheme basis.

Alternately, one can construct a many-body basis which has fixed J, or a J-scheme basis.

The Hamiltonian matrix will have smaller dimensions (a factor of 10 or more) in the J-scheme than in the M-scheme. On the other hand, as we'll show in the next slide, the M-scheme is very easy to construct with Slater determinants, while the J-scheme basis states, and thus the matrix elements, are more complicated, almost always being linear combinations of M-scheme states. J-scheme bases are important and useful, but we'll focus on the simpler M-scheme.

The quantum number m is additive (because the underlying group is Abelian): if a Slater determinant $\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k^\dagger \ldots |0\rangle$ is built from single-particle states all with good m, then the total

$$M = m_i + m_j + m_k + \ldots$$

This is *not* true of J, because the angular momentum group SU(2) is not Abelian.

The upshot is that

- It is easy to construct a Slater determinant with good total M;
- It is trivial to calculate M for each Slater determinant;
- So it is easy to construct an M-scheme basis with fixed total M.

Note that the individual M-scheme basis states will *not*, in general, have good total J. Because the Hamiltonian is rotationally invariant, however, the eigenstates will have good J. (The situation is muddied when one has states of different J that are nonetheless degenerate.)

Example: two $j = 1/2$ orbits

Index	n	l	j	m_j
1	0	0	1/2	-1/2
2	0	0	1/2	1/2
3	1	0	1/2	-1/2
4	1	0	1/2	1/2

Note: the order is arbitrary. There are $\begin{pmatrix} 4 \\ 2 \end{pmatrix} = 6$ two-particle states, which we list with the total M:

Occupied	M
1,2	0
1,3	-1
1,4	0
2,3	0
2,4	1
3,4	0

and 1 each with $M = \pm 1$.

Example: consider using only single particle states from the $0d_{5/2}$ space. They have the following quantum numbers

Index	n	l	j	m_j
1	0	2	5/2	-5/2
2	0	2	5/2	-3/2
3	0	2	5/2	-1/2
4	0	2	5/2	1/2
5	0	2	5/2	3/2
6	0	2	5/2	5/2

There are $\begin{pmatrix} 6 \\ 2 \end{pmatrix} = 15$ two-particle states, which we list with the total M:

Occupied	M	Occupied	M	Occupied	M
1,2	-4	2,3	-2	3,5	1
1,3	-3	2,4	-1	3,6	2
1,4	-2	2,5	0	4,5	2
1,5	-1	2,6	1	4,6	3
1,6	0	3,4	0	5,6	4

Example case: pairing Hamiltonian, the warm-up project

We consider a space with 2Ω single-particle states, with each state labeled by $k = 1, 2, 3, \Omega$ and $m = \pm 1/2$. The convention is that the state with $k > 0$ has $m = +1/2$ while $-k$ has $m = -1/2$.

The Hamiltonian we consider is

$$\hat{H} = -G\hat{P}_+\hat{P}_-,$$

where

$$\hat{P}_+ = \sum_{k>0} \hat{a}_k^\dagger \hat{a}_{-k}^\dagger.$$

and $\hat{P}_- = (\hat{P}_+)^\dagger$.

This problem can be solved using what is called the quasi-spin formalism to obtain the exact results. Thereafter we will try again using the explicit Slater determinant formalism.

One can show (and this is part of the project) that

$$\left[\hat{P}_+, \hat{P}_-\right] = \sum_{k>0} \left(\hat{a}_k^\dagger \hat{a}_k + \hat{a}_{-k}^\dagger \hat{a}_{-k} - 1\right) = \hat{N} - \Omega.$$

Now define

$$\hat{P}_z = \frac{1}{2}(\hat{N} - \Omega).$$

Finally you can show

$$\left[\hat{P}_z, \hat{P}_\pm\right] = \pm\hat{P}_\pm.$$

This means the operators $\hat{P}_\pm, \hat{P}_z$ form a so-called $SU(2)$ algebra, and we can use all our insights about angular momentum, even though there is no actual angular momentum involved

So we rewrite the Hamiltonian to make this explicit:

$$\hat{H} = -G\hat{P}_+\hat{P}_- = -G\left(\hat{P}^2 - \hat{P}_z^2 + \hat{P}_z\right)$$

Because of the SU(2) algebra, we know that the eigenvalues of $\hat{P}^2$ must be of the form $p(p+1)$, with p either integer or half-integer, and the eigenvalues of $\hat{P}_z$ are m_p with $p \geq |m_p|$, with m_p also integer or half-integer.

But because $\hat{P}_z = (1/2)(\hat{N} - \Omega)$, we know that for N particles the value $m_p = (N - \Omega)/2$. Furthermore, the values of m_p range from $-\Omega/2$ (for $N = 0$) to $+\Omega/2$ (for $N = 2\Omega$, with all states filled).

We deduce the maximal $p = \Omega/2$ and for a given n the values range of p range from $|N - \Omega|/2$ to $\Omega/2$ in steps of 1 (for an even number of particles)

Following Racah we introduce the notation $p = (\Omega - v)/2$ where $v = 0, 2, 4, ..., \Omega - |N - \Omega|$ With this it is easy to deduce that the eigenvalues of the pairing Hamiltonian are

$$-G(N - v)(2\Omega + 2 - N - v)/4$$

This also works for N odd, with $v = 1, 3, 5, \ldots$.

Let's take a specific example: $\Omega = 3$ so there are 6 single-particle states, and $N = 3$, with $v = 1, 3$. Therefore there are two distinct eigenvalues,

$$E = -2G, 0$$

Now let's work this out explicitly. The single particle degrees of freedom are defined as

Index	k	m
1	1	-1/2
2	-1	1/2
3	2	-1/2
4	-2	1/2
5	3	-1/2
6	-3	1/2

There are $\begin{pmatrix} 6 \\ 3 \end{pmatrix} = 20$ three-particle states, but there are 9 states with $M = +1/2$, namely $|1,2,3\rangle, |1,2,5\rangle, |1,4,6\rangle, |2,3,4\rangle, |2,3,6\rangle, |2,4,5\rangle, |2,5,6\rangle, |3,4,6\rangle, |4,5,6\rangle$.

In this basis, the operator

$$\hat{P}_+ = \hat{a}_1^\dagger \hat{a}_2^\dagger + \hat{a}_3^\dagger \hat{a}_4^\dagger + \hat{a}_5^\dagger \hat{a}_6^\dagger$$

From this we can determine that

$$\hat{P}_-|1,4,6\rangle = \hat{P}_-|2,3,6\rangle = \hat{P}_-|2,4,5\rangle = 0$$

so those states all have eigenvalue 0.

Now for further example,

$$\hat{P}_-|1,2,3\rangle = |3\rangle$$

so

$$\hat{P}_+\hat{P}_-|1,2,3\rangle = |1,2,3\rangle + |3,4,3\rangle + |5,6,3\rangle$$

The second term vanishes because state 3 is occupied twice, and reordering the last term we get

$$\hat{P}_+\hat{P}_-|1,2,3\rangle = |1,2,3\rangle + |3,5,6\rangle$$

without picking up a phase.

Continuing in this fashion, with the previous ordering of the many-body states ($|1,2,3\rangle, |1,2,5\rangle, |1,4,6\rangle, |2,3,4\rangle, |2,3,6\rangle, |2,4,5\rangle, |2,5,6\rangle, |3,4,6\rangle, |4,5,6\rangle$) the Hamiltonian matrix of this system is

$$H = -G \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

This is useful for our project. One can by hand confirm that there are 3 eigenvalues $-2G$ and 6 with value zero.

Another example Using the $(1/2)^4$ single-particle space, resulting in eight single-particle states

Index	n	l	s	m_s
1	0	0	1/2	-1/2
2	0	0	1/2	1/2
3	1	0	1/2	-1/2
4	1	0	1/2	1/2
5	2	0	1/2	-1/2
6	2	0	1/2	1/2
7	3	0	1/2	-1/2
8	3	0	1/2	1/2

and then taking only 4-particle, $M = 0$ states that have no 'broken pairs', there are six basis Slater determinants:

- $|1, 2, 3, 4\rangle$,
- $|1, 2, 5, 6\rangle$,
- $|1, 2, 7, 8\rangle$,
- $|3, 4, 5, 6\rangle$,
- $|3, 4, 7, 8\rangle$,
- $|5, 6, 7, 8\rangle$

Now we take the following Hamiltonian

$$\hat{H} = \sum_n n\delta \hat{N}_n - G\hat{P}^\dagger \hat{P}$$

where

$$\hat{N}_n = \hat{a}^\dagger_{n,m=+1/2}\hat{a}_{n,m=+1/2} + \hat{a}^\dagger_{n,m=-1/2}\hat{a}_{n,m=-1/2}$$

and

$$\hat{P}^\dagger = \sum_n \hat{a}^\dagger_{n,m=+1/2}\hat{a}^\dagger_{n,m=-1/2}$$

We can write down the 6×6 Hamiltonian in the basis from the prior slide:

$$H = \begin{pmatrix} 2\delta - 2G & -G & -G & -G & -G & 0 \\ -G & 4\delta - 2G & -G & -G & -0 & -G \\ -G & -G & 6\delta - 2G & 0 & -G & -G \\ -G & -G & 0 & 6\delta - 2G & -G & -G \\ -G & 0 & -G & -G & 8\delta - 2G & -G \\ 0 & -G & -G & -G & -G & 10\delta - 2G \end{pmatrix}$$

(You should check by hand that this is correct.)

For $\delta = 0$ we have the closed form solution of the g.s. energy given by $-6G$.