

Nuclear Shell Model

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Slater determinants as basis states

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.

Because we have fermions, we are required to have antisymmetric wavefunctions, that is

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

etc. This is accomplished formally by using the determinantal formalism

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

Product wavefunction + antisymmetry (Pauli principle) = Slater determinant.

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

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 following consequence of 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

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

We use letters $ijkl\dots$ for states below the Fermi level and $abcd\dots$ for states above the Fermi level. A general single-particle state is given by letters $pqrs\dots$

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

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

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 $0, 1, \dots, n$ hole states and P for $0, 1, \dots, n$ 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

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

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 notes 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 coefficients 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, we 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

$$\begin{aligned} & \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_0 \rangle + \sum_{kc} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_k^c \rangle C_k^c + \sum_{cdkl} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{kl}^{cd} \rangle C_{kl}^{cd} + \\ & \sum_{cdeklm} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klm}^{cde} \rangle C_{klm}^{cde} + \sum_{cdefklmn} \langle \Phi_{ij}^{ab} | \hat{H} - E | \Phi_{klmn}^{cdef} \rangle C_{klmn}^{cdef} = 0? \end{aligned}$$

Suppose, as an example, that we have six fermions below the Fermi level. This means that we can make at most $6p - 6h$ excitations. If we have an infinity of single particle states above the Fermi level, we will obviously have an infinity of say $2p - 2h$ excitations. Each such way to configure the particles is called a **configuration**. We will always have to truncate in the basis of single-particle states. This gives us a finite number of possible Slater determinants. Our Hamiltonian matrix would then look like (where each block can have a large dimensionalities):

	0p-0h	1p-1h	2p-2h	3p-3h	4p-4h	5p-5h	6p-6h
0p-0h	x	x	x	0	0	0	0
1p-1h	x	x	x	x	0	0	0
2p-2h	x	x	x	x	x	0	0
3p-3h	0	x	x	x	x	x	0
4p-4h	0	0	x	x	x	x	x
5p-5h	0	0	0	x	x	x	x
6p-6h	0	0	0	0	x	x	x

with a two-body force. Why are there non-zero blocks of elements? If we use a Hartree-Fock basis, this corresponds to a particular unitary transformation where matrix elements of the type $\langle 0p-0h|\hat{H}|1p-1h\rangle = 0$ and our Hamiltonian matrix becomes

	0p-0h	1p-1h	2p-2h	3p-3h	4p-4h	5p-5h	6p-6h
0p-0h	\tilde{x}	0	\tilde{x}	0	0	0	0
1p-1h	0	\tilde{x}	\tilde{x}	\tilde{x}	0	0	0
2p-2h	\tilde{x}	\tilde{x}	\tilde{x}	\tilde{x}	\tilde{x}	0	0
3p-3h	0	\tilde{x}	\tilde{x}	\tilde{x}	\tilde{x}	\tilde{x}	0
4p-4h	0	0	\tilde{x}	\tilde{x}	\tilde{x}	\tilde{x}	\tilde{x}
5p-5h	0	0	0	\tilde{x}	\tilde{x}	\tilde{x}	\tilde{x}
6p-6h	0	0	0	0	\tilde{x}	\tilde{x}	\tilde{x}

What happens if we have a three-body interaction and a Hartree-Fock basis?