Definitions and notations

Our Hamiltonian is invariant under the permutation (interchange) of two particles. Since we deal with fermions however, the total wave function is antisymmetric. Let \( \hat{P} \) be an operator which interchanges two particles. Due to the symmetries we have ascribed to our Hamiltonian, this operator commutes with the total Hamiltonian, 
\[
[\hat{H}, \hat{P}] = 0,
\]
meaning that \( \psi_{1}(x_{1}, x_{2}, . . . , x_{A}) \) is an eigenfunction of \( \hat{P} \) as well, that is
\[
\hat{P}\psi_{1}(x_{1}, x_{2}, . . . , x_{A}) = -\beta\psi_{1}(x_{1}, x_{2}, . . . , x_{A}),
\]
where \( \beta \) is the eigenvalue of \( \hat{P} \). We have introduced the suffix \( ij \) in order to indicate that we permute particles \( i \) and \( j \). The Pauli principle tells us that the total wave function for a system of fermions has to be antisymmetric, resulting in the eigenvalue \( \beta = -1 \).

Definitions and notations

Before we proceed we need some definitions. We will assume that the interacting part of the Hamiltonian can be approximated by a two-body interaction. This means that our Hamiltonian is written as the sum of some one-body part and a two-body part
\[
\hat{H} = \hat{H}_{0} + \hat{H}_{\text{int}} = \sum_{i=1}^{A} \hat{h}_{0}(x_{i}) + \sum_{i<j}^{A} \hat{V}_{ij},
\]
with
\[
\hat{h}_{0} = \sum_{i=1}^{A} \hat{h}_{0}(x_{i}).
\]

The one-body part \( \hat{h}_{0}(x_{i}) \) is normally approximated by a harmonic oscillator or Woods-Saxon potential or for electronic systems the Coulomb interaction an electron feels from the nucleus. However, other potentials are fully possible, such as one derived from the self-consistent solution of the Hartree-Fock equations to be discussed here.

Definitions and notations

In our case we assume that we can approximate the exact eigenfunction with a Slater determinant
\[
\Phi(x_{1}, x_{2}, . . . , x_{A}, \alpha, \beta, . . . , \gamma) = \frac{1}{\sqrt{A!}} \prod_{i=1}^{A} \psi_{\alpha_{i}}(x_{i}) \psi_{\beta_{i}}(x_{i}) \ldots \psi_{\gamma_{i}}(x_{i}),
\]
where \( x_{i} \) stand for the coordinates and spin values of a particle \( i \) and \( \alpha, \beta, . . . , \gamma \) are quantum numbers needed to describe remaining quantum numbers.
Definitions and notations

The single-particle function $\psi_\alpha(x_i)$ are eigenfunctions of the one-body Hamiltonian $h_i$, that is

$$h_i(x) = \hat{A}(x) + \hat{V}(x).$$

with eigenvalues

$$h_i(\psi_\alpha(x_i)) = \{h_i(x_i) + \hat{V}(x_i)\} \psi_\alpha(x_i) = \epsilon_\alpha \psi_\alpha(x_i).$$

The energies $\epsilon_\alpha$ are the so-called non-interacting single-particle energies, or unperturbed energies. The total energy is in this case the sum over all single-particle energies, if no two-body or more complicated many-body interactions are present.

Brief reminder on some linear algebra properties

Before we proceed with a more compact representation of a Slater determinant, we would like to repeat some linear algebra properties which will be useful for our derivations of the energy as function of a Slater determinant, Hartree-Fock theory and later the nuclear shell model.

The inverse of a matrix is defined by

$$A^{-1} \cdot A = I.$$

A unitary matrix $A$ is one whose inverse is its adjoint

$$A^{-1} = A^\dagger.$$

A real unitary matrix is called orthogonal and its inverse is equal to its transpose. A hermitian matrix is its own self-adjoint, that is

$$A = A^\dagger.$$

Definitions and notations

Let us denote the ground state energy by $E_0$. According to the variational principle we have

$$E_0 \leq \langle \Phi | \hat{H} | \Phi \rangle = \int \Phi^* \hat{H} \Phi \, d\tau,$$

where $\Phi$ is a trial function which we assume to be normalized

$$\int \Phi^* \Phi \, d\tau = 1,$$

where we have used the shorthand $d\tau = dx_1 dr_2 \ldots dr_A$.

Basic Matrix Features

Since we will deal with Fermions (identical and indistinguishable particles) we will form an ansatz for a given state in terms of so-called Slater determinants determined by a chosen basis of single-particle functions.

For a given $n \times n$ matrix $A$ we can write its determinant

$$\det(A) = |A| = \begin{vmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{vmatrix},$$

in a more compact form as

$$|A| = \sum_{\Pi} (-1)^{\Pi} \hat{P}_{\Pi} a_{12} a_{22} \cdots a_{nn},$$

where $\hat{P}_{\Pi}$ is a permutation operator which permutes the column indices 1, 2, $\ldots$, $n$ and the sum runs over all permutations $\Pi$.

Basic Matrix Features, simple $2 \times 2$ determinant

A simple $2 \times 2$ determinant illustrates this. We have

$$\det(A) = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = (-1)^2 a_{11} a_{22} + (-1)^1 a_{12} a_{21},$$

where in the last term we have interchanged the column indices 1 and 2. The natural ordering we have chosen is $a_{11}, a_{22}$.
Definitions and notations

With the above we can rewrite our Slater determinant in a more compact form. In the Hartree-Fock method the trial function is the Slater determinant of Eq. (3) which can be rewritten as

\[ \Phi(x_1, x_2, \ldots, x_A, \alpha, \beta, \ldots, \nu) = \frac{1}{\sqrt{A!}} \sum_p (-)^p \hat{P} \psi_\alpha(x_1) \psi_\beta(x_2) \cdots \psi_\nu(x_A) \]

where we have introduced the antisymmetrization operator \( \hat{A} \) defined by the summation over all possible permutations of two particles.

It is defined as

\[ \hat{A} = \frac{1}{2^A A!} \sum_p (-)^p \hat{P}, \quad (4) \]

with \( p \) standing for the number of permutations. We have introduced for later use the so-called Hartree-function, defined by the simple product of all possible single-particle functions

\[ \Phi_0(x_1, x_2, \ldots, x_A, \alpha, \beta, \ldots, \nu) = \psi_\alpha(x_1) \psi_\beta(x_2) \cdots \psi_\nu(x_A). \]

Both \( \hat{H}_0 \) and \( \hat{H}_1 \) are invariant under all possible permutations of any two particles and hence commute with \( \hat{A} \)

\[ [\hat{H}_0, \hat{A}] = [\hat{H}_1, \hat{A}] = 0. \quad (5) \]

Furthermore, \( \hat{A} \) satisfies

\[ \hat{A}^2 = \hat{A}, \quad (6) \]

since every permutation of the Slater determinant reproduces it.

The expectation value of \( \hat{H}_0 \)

\[ \int \Phi^* \hat{H}_0 \Phi d\tau = A! \int \Phi^* \hat{A} \hat{H}_0 \hat{A} \Phi d\tau, \]

is readily reduced to

\[ \int \Phi^* \hat{H}_0 \Phi d\tau = A! \int \Phi^* \hat{H}_0 \hat{A} \hat{H}_0 \hat{A} \Phi d\tau, \]

where we have used Eqs. (5) and (6). The next step is to replace the antisymmetrization operator by its definition and to replace \( \hat{H}_0 \) with the sum of one-body operators

\[ \int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{i=1}^{A} \sum_p (-)^p \int \Phi^*_i \hat{H}_0 \Phi_i d\tau. \]

The integral vanishes if two or more particles are permuted in only one of the Hartree-functions \( \Phi_i \), because the individual single-particle wave functions are orthogonal. We obtain then

\[ \int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{i=1}^{A} \int \phi_i^* \hat{H}_0 \phi_i d\tau. \]

Orthogonality of the single-particle functions allows us to further simplify the integral, and we arrive at the following expression for the expectation values of the sum of one-body Hamiltonians

\[ \int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{i=1}^{A} \int \phi_i^* \hat{H}_0 \phi_i d\tau = \sum_{i=1}^{A} \int \psi_i^* \hat{h}_0 \psi_i d\tau. \quad (7) \]

We introduce the following shorthand for the above integral

\[ \langle \mu | \hat{h}_0 | \mu \rangle = \int \psi_i^* \hat{h}_0 \psi_i(x) dx. \]

and rewrite Eq. (7) as

\[ \int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{\mu=1}^{A} \langle \mu | \hat{h}_0 | \mu \rangle. \quad (8) \]
The expectation value of the two-body part of the Hamiltonian is obtained in a similar manner. We have
\[
\int \Phi^\dagger \hat{H} \Phi d\tau = A! \int \Phi^\dagger_0 \hat{H} \Phi_0 d\tau,
\]
which reduces to
\[
\int \Phi^\dagger \hat{H} \Phi d\tau = \sum_{\mu \nu} \sum_{i < j} (-1)^p \int \Phi^\dagger_\mu |v_{ij}| \Phi_\nu d\tau,
\]
by following the same arguments as for the one-body Hamiltonian.

Because of the dependence on the inter-particle distance \( r_{ij} \), permutations of any two particles no longer vanish, and we get
\[
\int \Phi^\dagger \hat{H} \Phi d\tau = \sum_{i < j} \int \Phi^\dagger_\mu |v_{ij}| (1 - P_{ij}) \Phi_\nu d\tau.
\]
where \( P_{ij} \) is the permutation operator that interchanges particle \( i \) and particle \( j \). Again we use the assumption that the single-particle wave functions are orthogonal.

We introduce the following shorthands for the above two integrals
\[
\langle \mu \nu | v_{ij} | \mu \nu \rangle = \int \psi_{\mu}(x_i) \psi_{\nu}(x_j) v_{ij} \psi_{\mu}(x_i) \psi_{\nu}(x_j) dx_i dx_j,
\]
and
\[
\langle \mu \nu | v_{ij} | \nu \mu \rangle = \int \psi_{\nu}(x_i) \psi_{\mu}(x_j) v_{ij} \psi_{\nu}(x_i) \psi_{\mu}(x_j) dx_i dx_j.
\]

The last equation allows us to introduce some further definitions. The single-particle wave functions \( \psi_\mu(x) \), defined by the quantum numbers \( \mu \) and \( x \) are defined as the overlap
\[
\psi_\mu(x) = \langle x | \mu \rangle.
\]

Our functional can then be written in a compact version as
\[
E[\Phi] = \sum_{\mu} \langle \mu | \hat{h}_0 | \mu \rangle + \frac{1}{2} \sum_{\mu \nu} \left[ \langle \mu \nu | v_{ij} | \mu \nu \rangle - \langle \nu \mu | v_{ij} | \mu \nu \rangle \right].
\]
Properties of the interaction elements

Since the interaction is invariant under the interchange of two particles it means for example that we have
\[ \langle \mu \nu | \hat{v} | \mu \nu \rangle = \langle \nu \mu | \hat{v} | \nu \mu \rangle, \]
or in the more general case
\[ \langle \mu \nu | \hat{v} | \sigma \tau \rangle = \langle \nu \mu | \hat{v} | \tau \sigma \rangle. \]

Redefining the matrix elements

The direct and exchange matrix elements can be brought together if we define the antisymmetrized matrix element
\[ \langle \mu \nu | \hat{v} | \mu \nu \rangle_{\text{AS}} = \langle \mu \nu | \hat{v} | \mu \nu \rangle - \langle \mu \nu | \hat{v} | \nu \mu \rangle, \]
or for a general matrix element
\[ \langle \mu | \hat{v} | \sigma \rangle_{\text{AS}} = \langle \mu | \hat{v} | \sigma \rangle - \langle \mu | \hat{v} | \sigma \rangle. \]
It has the symmetry property
\[ \langle \mu | \hat{v} | \sigma \rangle_{\text{AS}} = -\langle \nu | \hat{v} | \sigma \rangle_{\text{AS}} = -\langle \mu | \hat{v} | \sigma \rangle_{\text{AS}}. \]
The antisymmetric matrix element is also hermitian, implying
\[ \langle \mu | \hat{v} | \sigma \rangle_{\text{AS}} = \langle \sigma | \hat{v} | \mu \rangle_{\text{AS}}. \]

Rewriting the energy functional

With these notations we rewrite the energy functional as
\[ \int \Phi^* \hat{H} \Phi d\tau = \ldots \]
In our coordinate space derivations below we will spell out the Hartree-Fock equations in terms of their integrals.

Variational Calculus and Lagrangian Multipliers, simple example

Let us specialize to the expectation value of the energy for one particle in three-dimensions. This expectation value reads
\[ E = \int dydz \psi^*(x,y,z) \hat{H} \psi(x,y,z), \]
with the constraint
\[ \int dydz \psi^*(x,y,z) \psi(x,y,z) = 1, \]
and a Hamiltonian
\[ \hat{H} = -\frac{1}{2} \nabla^2 + V(x,y,z). \]
We will, for the sake of notational convenience, skip the variables \(x,y,z\) below, and write for example \( V(x,y,z) = V \).

Manipulating terms

The integral involving the kinetic energy can be written as, with the function \( \psi \) vanishing strongly for large values of \( x,y,z \) (given here by the limits \( a \) and \( b \)),
\[ \int_a^b \int dydz \psi^*(x,y,z) \left(-\frac{1}{2} \nabla^2 \psi + \psi \nabla^2 \psi + \frac{1}{2} \nabla \psi \nabla \psi + V \psi \right) \]
We will drop the limits \( a \) and \( b \) in the remaining discussion. Inserting this expression into the expectation value for the energy and taking the variational minimum we obtain
\[ \delta E = \delta \left\{ \int dydz \left( \frac{1}{2} \nabla \psi \nabla \psi + V \psi \right) \right\} - 0. \]
Adding the Lagrangian multiplier

The constraint appears in integral form as

$$\int \text{d}x \text{d}y \text{d}z |\psi|^2 = \text{constant},$$

and multiplying with a Lagrangian multiplier \( \lambda \) and taking the variational
minimal we obtain the final variational equation

$$\delta \left\{ \int \text{d}x \text{d}y \text{d}z \left( \frac{1}{2} \nabla |\psi|^2 + V |\psi|^2 - \lambda |\psi|^2 \right) \right\} = 0.$$  

We introduce the function \( f \)

$$f = \frac{1}{2} \nabla |\psi|^2 + V |\psi|^2 - \lambda |\psi|^2 - \frac{1}{2} \left( \psi_1^2 + \psi_2^2 + \psi_3^2 \right) + V |\psi|^2 - \lambda |\psi|^2,$$

where we have skipped the dependence on \( x, y, z \) and introduced
the shorthand \( \psi_x, \psi_y, \) and \( \psi_z \) for the various derivatives.

And with the Euler-Lagrange equations we get

$$\frac{\partial f}{\partial \psi^*} - \frac{\partial f}{\partial \psi} x = 0,$$

which results in

$$-\frac{1}{2} \left( \psi_{xx} + \psi_{yy} + \psi_{zz} \right) + V \psi = \lambda \psi.$$

We can then identify the Lagrangian multiplier as the energy of the
system. The last equation is nothing but the standard Schrödinger
equation and the variational approach discussed here provides a
powerful method for obtaining approximate solutions of the wave
function.

Hartree-Fock by varying the coefficients of a wave function
expansion

In deriving the Hartree-Fock equations, we will expand the
single-particle functions in a known basis and vary the coefficients,
that is, the new single-particle wave function is written as a linear
expansion in terms of a fixed chosen orthogonal basis (for example
the well-known harmonic oscillator functions or the hydrogen-like
functions etc). We define our new Hartree-Fock single-particle basis
by performing a unitary transformation on our previous basis
(labelled with greek indices) as

$$\psi_{p\alpha} = \sum_{\lambda} C_{p\lambda} \phi_{\lambda}, \quad (13)$$

In this case we vary the coefficients \( C_{p\lambda} \). If the basis has infinitely
many solutions, we need to truncate the above sum. We assume
that the basis \( \phi_{\lambda} \) is orthogonal. A unitary transformation keeps the
orthogonality, as discussed in exercise 1 below.

More on linear algebra

In the previous slide we stated that a unitary transformation keeps
the orthogonality, as discussed in exercise 1 below. To see this
consider first a basis of vectors \( v_i \),

$$v_i = \begin{bmatrix} v_{i1} \\ \vdots \\ v_{in} \end{bmatrix}.$$

We assume that the basis is orthogonal, that is

$$v^T_i v_j = \delta_{ij}.$$

An orthogonal or unitary transformation

$$w_i = U v_i,$$

preserves the dot product and orthogonality since

$$w^T_i w_j = (U v_i)^T U v_j = v^T_i U^T U v_j = v^T_i v_j = \delta_{ij}.$$
More Basic Matrix Features, a general $n \times n$ determinant

We can generalize this to an $n \times n$ matrix and have

$$\begin{pmatrix}
\phi_{11} & \phi_{12} & \cdots & \phi_{1n} \\
\phi_{21} & \phi_{22} & \cdots & \phi_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
\phi_{n1} & \phi_{n2} & \cdots & \phi_{nn}
\end{pmatrix} = \sum_{k=1}^{n} \phi_{k} \phi_{k}(x)$$

This is a property we will use in our Hartree-Fock discussions.

A general Slater determinant

With our definition of the new basis in terms of an orthogonal basis we have

$$\psi_{\lambda}(x) = \sum_{\lambda} C_{\lambda} \phi_{\lambda}(x)$$

If the coefficients $C_{\lambda}$ belong to an orthogonal or unitary matrix, the new basis is also orthogonal. Our Slater determinant in the new basis $\psi_{\lambda}(x)$ is written as

$$\begin{pmatrix}
\psi_{1}(x) & \psi_{2}(x) & \cdots & \psi_{n}(x) \\
\psi_{1}(x) & \psi_{2}(x) & \cdots & \psi_{n}(x) \\
\vdots & \vdots & \ddots & \vdots \\
\psi_{1}(x) & \psi_{2}(x) & \cdots & \psi_{n}(x)
\end{pmatrix} = \sum_{\lambda=1}^{n} C_{\lambda} C_{\lambda}(x)$$

which is nothing but $\det(C)\det(\Phi)$, with $\det(\Phi)$ being the determinant given by the basis functions $\phi_{\lambda}(x)$.

Hartree-Fock by varying the coefficients of a wave function expansion

In Eq. (12), restated here

$$E[\Phi] = \sum_{\rho=1}^{\lambda} \sum_{\mu=1}^{\lambda} \langle \rho | \hat{v} | \mu \rangle A_{\rho}$$

we found the expression for the energy functional in terms of the basis function $\phi_{\lambda}(r)$. We then varied the above energy functional with respect to the basis functions $\langle \rho |$. Now we are interested in defining a new basis defined in terms of a chosen basis as defined in Eq. (13). We can then rewrite the energy functional as

$$E[\Phi^{HF}] = \sum_{\rho=1}^{\lambda} \sum_{\mu=1}^{\lambda} \langle \rho | \hat{v} | \mu \rangle + \frac{1}{2} \sum_{\rho=1}^{\lambda} \sum_{\mu=1}^{\lambda} \langle \rho | \hat{v} | \mu \rangle A_{\rho}$$

where $\Phi^{HF}$ is the new Slater determinant defined by the new basis of Eq. (13).
Using Eq. (13) we can rewrite Eq. (14) as
\[ E'[\Psi] = \sum_{i=1}^{A} \sum_{\alpha}\sum_{\beta} C_i^\alpha C_i^\beta \langle \alpha | h | \beta \rangle + \frac{1}{2} \sum_{j=1}^{A} \sum_{\alpha'} \sum_{\beta'} C_j^\alpha C_j^\beta C_i^\alpha C_i^\beta \langle \alpha | \hat{v} | \beta \rangle \delta_{\alpha\beta} \delta_{\alpha'\beta'} \]

(15)

Minimizing with respect to \( C_i^\alpha \), remembering that the equations for \( C_i^\alpha \) and \( C_i^\beta \) can be written as two independent equations, we obtain
\[ \frac{d}{dC_i^\alpha} E'[\Psi] = \sum_{j=1}^{A} \sum_{\alpha'} \sum_{\beta'} C_j^\alpha C_j^\beta \langle \alpha | \hat{v} | \beta \rangle \delta_{\alpha\beta} \delta_{\alpha'\beta'} = 0, \]

which yields for every single-particle state \( i \) and index \( \alpha \) (recalling that the coefficients \( C_i^\alpha \) are matrix elements of a unitary (or orthogonal for a real symmetric matrix) matrix) the following Hartree-Fock equations
\[ \sum_{\beta} C_i^\alpha \langle \alpha | h | \beta \rangle + \frac{1}{2} \sum_{j=1}^{A} \sum_{\alpha'} \sum_{\beta'} C_j^\alpha C_j^\beta C_i^\alpha C_i^\beta \langle \alpha | \hat{v} | \beta \rangle \delta_{\alpha\beta} \delta_{\alpha'\beta'} = \epsilon_{HF}^i C_i^\alpha. \]

(16)

We wish now to minimize the above functional. We introduce again a set of Lagrange multipliers, noting that since \( \langle i | j \rangle = \delta_{ij} \) and \( \langle \alpha | \beta \rangle = \delta_{\alpha\beta} \), the coefficients \( C_i^\alpha \) obey the relation
\[ \langle i | C_i^\alpha \rangle = \delta_{i\alpha} = \sum_{\beta} C_i^\alpha C_i^\beta \langle \alpha | \hat{v} | \beta \rangle \delta_{\alpha\beta}, \]

which allows us to define a functional to be minimized that reads
\[ F[\Phi^{HF}] = E[\Phi^{HF}] - \sum_{i=1}^{A} \epsilon_i \sum_{\alpha} C_i^\alpha C_i^\alpha. \]

(16)

We can rewrite this equation as (changing dummy variables)
\[ \sum_{\beta} \left( \langle \alpha | h | \beta \rangle + \sum_{j=1}^{A} C_j^\alpha C_j^\beta \langle \alpha | \hat{v} | \beta \rangle \delta_{\alpha\beta} \right) C_i^\beta = \epsilon_{HF}^i C_i^\alpha. \]

Note that the sums over greek indices run over the number of basis set functions (in principle an infinite number).

Defining
\[ \hat{M}^{HF}_{\alpha\beta} = \langle \alpha | h | \beta \rangle + \sum_{j=1}^{A} C_j^\alpha C_j^\beta \langle \alpha | \hat{v} | \beta \rangle \delta_{\alpha\beta} \]
we can rewrite the new equations as
\[ \sum_{\beta} \hat{M}^{HF}_{\alpha\beta} C_i^\beta = \epsilon_{HF}^i C_i^\alpha. \]

(17)

The latter is nothing but a standard eigenvalue problem. It suffices to tabulate the matrix elements \( \langle \alpha | h | \beta \rangle \) and \( \langle \alpha | \hat{v} | \beta \rangle \delta_{\alpha\beta} \) once and for all. Successive iterations require thus only a look-up in tables over one-body and two-body matrix elements. These details will be discussed below when we solve the Hartree-Fock equations numerically.
Hartree-Fock algorithm

Normally we assume that the single-particle basis \( |\beta\rangle \) forms an eigenbasis for the operator \( \hat{h}_0 \), meaning that the Hartree-Fock matrix becomes

\[
\hat{h}^\text{HF}_\alpha\beta = \epsilon_\alpha \delta_{\alpha\beta} \quad + \sum_{j=1}^A \sum_{\gamma\delta} C^{(1)}_{\gamma\beta} C^{(1)}_{\delta\gamma} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{\text{AS}}.
\]

The Hartree-Fock eigenvalue problem

\[
\sum_{\alpha} \hat{h}^\text{HF}_\alpha\beta C_{\alpha\beta} = \epsilon^\text{HF}_{\beta} C_{\alpha\beta},
\]

can be written out in a more compact form as

\[
\hat{h}^\text{HF} \hat{C} = \epsilon^\text{HF} \hat{C}.
\]

Hartree-Fock algorithm

Solving the Hartree-Fock eigenvalue problem yields new eigenvectors \( C^{(1)}_{\gamma\beta} \) and eigenvalues \( \epsilon^{\text{HF}} \). With the new eigenvectors we can set up a new Hartree-Fock potential

\[
\hat{h}^\text{HF}\beta\gamma = \epsilon_{\gamma\delta} \delta_{\gamma\delta} + \sum_{j=1}^A \sum_{\gamma\delta} C^{(1)}_{\gamma\beta} C^{(1)}_{\delta\gamma} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{\text{AS}}.
\]

The diagonalization with the new Hartree-Fock potential yields new eigenvectors and eigenvalues. This process is continued till for example

\[
\sum_{\alpha} |\lambda^\alpha|^2 \leq \lambda_m
\]

where \( \lambda \) is a user prefixed quantity (\( \lambda \sim 10^{-3} \) or smaller) and \( m \) runs over all calculated single-particle energies and \( m \) is the number of single-particle states.

Analysis of Hartree-Fock equations and Koopman’s theorem

Using our definition of the Hartree-Fock single-particle energies we obtain then the following expression for the total ground-state energy

\[
E_0^{\text{HF}} = \sum_{j \neq F} \frac{\lambda_j}{2} + \frac{1}{2} \sum_{j \neq F} \sum_{i \neq j} \langle |j\rangle |i\rangle - \langle |i\rangle |j\rangle.
\]

This form will be used in our discussion of Koopman’s theorem.

Hartree-Fock algorithm

The Hartree-Fock equations are, in their simplest form, solved in an iterative way, starting with a guess for the coefficients \( C_{\alpha\beta} \). We label the coefficients as \( C_{\alpha\beta}^{(n)} \), where the subscript \( n \) stands for iteration \( n \). To set up the algorithm we can proceed as follows:

- We start with a guess \( C_{\alpha\beta}^{(0)} = \hat{h}_0 \). Alternatively, we could have used random starting values as long as the vectors are normalized. Another possibility is to give states below the Fermi level a larger weight.
- The Hartree-Fock matrix simplifies then to (assuming that the coefficients \( C_{\alpha\beta} \) are real)

\[
\hat{h}^\text{HF}\beta\gamma = \epsilon_{\gamma\delta} \delta_{\gamma\delta} + \sum_{j=1}^A \sum_{\gamma\delta} C^{(1)}_{\gamma\beta} C^{(1)}_{\delta\gamma} \langle \alpha\gamma | \hat{v} | \beta\delta \rangle_{\text{AS}}.
\]

Analysis of Hartree-Fock equations and Koopman’s theorem

We can rewrite the ground state energy by adding and subtracting \( \hat{U}^{\text{HF}}(\nu) \)

\[
E_0^{\text{HF}} = \langle \Phi_0 | \hat{h}_0 | \Phi_0 \rangle - \frac{1}{2} \sum_{j=1}^A \sum_{i \neq j} \langle |j\rangle |i\rangle - \langle |i\rangle |j\rangle - \sum_{j \neq F} \frac{\lambda_j}{2}.
\]

which results in

\[
E_0^{\text{HF}} = \sum_{j \neq F} \langle |j\rangle |j\rangle - \frac{1}{2} \sum_{j \neq F} \sum_{i \neq j} \langle |j\rangle |i\rangle - \langle |i\rangle |j\rangle - \sum_{j \neq F} \frac{\lambda_j}{2}.
\]

Our single-particle states \( |j\rangle \) are now single-particle states obtained from the solution of the Hartree-Fock equations.  

Atomic physics case

We have

\[
E[\Phi^{\text{HF}}(N-I)] = \sum_{j \neq F} \langle |j\rangle |j\rangle + \frac{1}{2} \sum_{j \neq F} \langle |j\rangle |j\rangle_{\text{AS}},
\]

where \( \Phi^{\text{HF}}(N-I) \) is the new Slater determinant defined by the new basis of Eq. (13) for \( N \) electrons (same \( Z \)). If we assume that the single-particle wave functions in the new basis do not change when we remove one electron or add one electron, we can then define the corresponding energy for the \( N-1 \) systems as

\[
E[\Phi^{\text{HF}}(N-I)] = \sum_{j \neq F} \langle |j\rangle |j\rangle + \frac{1}{2} \sum_{j \neq F} \langle |j\rangle |j\rangle_{\text{AS}}.
\]

where we have removed a single-particle state \( k \leq F \), that is a state below the Fermi level.
As an example, consider a simple model for atomic sodium, Na. Neutral sodium has eleven electrons, with the weakest bound one being confined the 3s single-particle quantum numbers. The energy needed to remove an electron from neutral sodium is rather small, 5.1391 eV, a feature which pertains to all alkali metals. Having performed a Hartree-Fock calculation for neutral sodium would then allow us to compute the ionization energy by using the single-particle energy for the 3s states, namely $E_{HF}^{3s}$. From these considerations, we see that Hartree-Fock theory allows us to make a connection between experimental observables (here ionization and affinity energies) and the underlying interactions between particles. In this sense, we are now linking the dynamics and structure of a many-body system with the laws of motion which govern the system. Our approach is a reductionist one, meaning that we want to understand the laws of motion in terms of the particles or degrees of freedom which we believe are the fundamental ones. Our Slater determinant, being constructed as the product of various single-particle functions, follows this philosophy. 

Similarly, we can now compute the difference (we label the single-particle states above the Fermi level as $ab > F$)

$$E[\Phi^{HF}(N+1)] - E[\Phi^{HF}(N)] = E_{HF}^{N+1} - E_{HF}^{N}$$

These two equations can thus be used to the electron affinity or ionization energies, respectively. Koopman’s theorem states that for example the ionization energy of a closed-shell system is given by the energy of the highest occupied single-particle state. If we assume that changing the number of electrons from $N$ to $N + 1$ does not change the Hartree-Fock single-particle energies and eigenfunctions, then Koopman’s theorem simply states that the ionization energy of an atom is given by the single-particle energy of the last bound state. In a similar way, we can also define the electron affinities.

Calculating the difference

$$E[\Phi^{HF}(N)] - E[\Phi^{HF}(N-1)] = \sum_{j=1}^{n} \langle k | \hat{h}_j | k \rangle + \frac{1}{2} \sum_{j=1}^{n} \sum_{k=1}^{n} \langle k | \hat{h}_j | k \rangle_{AS}$$

we obtain

$$E[\Phi^{HF}(N)] - E[\Phi^{HF}(N-1)] = \frac{1}{2} \sum_{j=1}^{n} \langle k | \hat{h}_j | k \rangle_{AS}$$

which is just our definition of the Hartree-Fock single-particle energy $E[\Phi_{HF}^{N}] - E[\Phi_{HF}^{N-1}] = \epsilon_{HF}^{k}$

As an example, consider a simple model for atomic sodium, Na. Neutral sodium has eleven electrons, with the weakest bound one being confined the 3s single-particle quantum numbers. The energy needed to remove an electron from neutral sodium is rather small, 5.1391 eV, a feature which pertains to all alkali metals. Having performed a Hartree-Fock calculation for neutral sodium would then allow us to compute the ionization energy by using the single-particle energy for the 3s states, namely $E_{HF}^{3s}$. From these considerations, we see that Hartree-Fock theory allows us to make a connection between experimental observables (here ionization and affinity energies) and the underlying interactions between particles. In this sense, we are now linking the dynamics and structure of a many-body system with the laws of motion which govern the system. Our approach is a reductionist one, meaning that we want to understand the laws of motion in terms of the particles or degrees of freedom which we believe are the fundamental ones. Our Slater determinant, being constructed as the product of various single-particle functions, follows this philosophy.

Similarly, we can now compute the difference (recall that the single-particle states $ab > F$)

$$E[\Phi^{HF}(A+1)] - E[\Phi^{HF}(A)] = E_{HF}^{A+1} - E_{HF}^{A}$$

If we then recall that the binding energy differences

$$BE(A) = BE(A-1) \text{ and } BE(A+1) - BE(A),$$

define the separation energies, we see that the Hartree-Fock single-particle energies can be used to define separation energies. We have thus our first link between nuclear forces (included in the potential energy term) and an observable quantity defined by differences in binding energies.
Developing a Hartree-Fock program

The single-particle energies obtained by solving the Hartree-Fock equations can be directly related to experimental separation energies. Since Hartree-Fock theory is the starting point for several many-body techniques (density functional theory, random-phase approximation, shell-model etc.), the aim here is to develop a computer program to solve the Hartree-Fock equations in a given single-particle basis, here the harmonic oscillator.

Analysis of Hartree-Fock equations and Koopman’s theorem

We have thus the following interpretations (if the single-particle field do not change)

\[ BE(A) - BE(A - 1) \approx E[\Phi^\text{HF}(A)] - E[\Phi^\text{HF}(A - 1)] = e_i^{\text{HF}}, \]

and

\[ BE(A + 1) - BE(A) \approx E[\Phi^\text{HF}(A + 1)] - E[\Phi^\text{HF}(A)] = e_i^{\text{HF}}. \]

If we use \(^{16}\text{O}\) as our closed-shell nucleus, we could then interpret the separation energy

\[ BE(\text{Ne}) - BE(\text{O}) = \frac{\hbar^2}{2m} \sum_{i=1}^{N} \lambda_i. \]

We can continue like this for all \(N\) nuclei where \(N\) is a good closed-shell (or subshell closure) nucleus. Examples are \(^{22}\text{O}, \^{24}\text{O}, \^{40}\text{Ca}, \^{48}\text{Ca}, \^{52}\text{Ca}, \^{56}\text{Ni}, \^{58}\text{Ni}, \^{60}\text{Ni}, \^{88}\text{Sr}, \^{100}\text{Sn}, \^{120}\text{Sn}, \^{208}\text{Pb}, \) to mention some possible cases.

Analysis of Hartree-Fock equations and Koopman’s theorem

Similarly, we could interpret

\[ BE(\text{Ne}) - BE(\text{O}) \approx e_i^{\text{HF}}, \]

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\[ BE(\text{Ne}) - BE(\text{O}) \approx e_i^{\text{HF}}. \]

We can do this like this for all \(N\) nuclei where \(N\) is a good closed-shell (or subshell closure) nucleus. Examples are \(^{22}\text{O}, \^{24}\text{O}, \^{40}\text{Ca}, \^{48}\text{Ca}, \^{52}\text{Ca}, \^{56}\text{Ni}, \^{58}\text{Ni}, \^{60}\text{Ni}, \^{88}\text{Sr}, \^{100}\text{Sn}, \^{120}\text{Sn}, \^{208}\text{Pb}, \) to mention some possible cases.

Analysis of Hartree-Fock equations and Koopman’s theorem

We can thus make our first interpretation of the separation energies in terms of the simplest possible many-body theory. If we also recall that the so-called energy gap for neutrons (or protons) is defined as

\[ \Delta S_N = 2BE(N, Z) - BE(N - 1, Z) - BE(N + 1, Z), \]

for neutrons and the corresponding gap for protons

\[ \Delta S_p = 2BE(N, Z) - BE(N, Z - 1) - BE(N, Z + 1). \]

We can define the neutron and proton energy gaps for \(^{16}\text{O}\) as

\[ \Delta S_N = \frac{\hbar^2}{2m} \sum_{i=1}^{N} \lambda_i, \]

and

\[ \Delta S_p = \frac{\hbar^2}{2m} \sum_{i=1}^{N} \lambda_i. \]

Consider a Slater determinant built up of orthogonal single-particle orbitals \( \psi_\lambda \), with \( \lambda = 1, 2, \ldots, A \).

The unitary transformation

\[ \psi_\lambda = \sum_\alpha C_\alpha \psi_\lambda, \]

brings us into the new basis. The new basis has quantum numbers \( \alpha = 1, 2, \ldots, A \).

a) Show that the new basis is orthogonal.

b) Show that the new Slater determinant constructed from the new single-particle wave functions can be written as the determinant based on the previous basis and the determinant of the matrix \( C \).

c) Show that the old and the new Slater determinants are equal up to a complex constant with absolute value unity.

Hint: \( C \) is a unitary matrix.

Analysis of Hartree-Fock equations and Koopman’s theorem

The single-particle energies obtained by solving the Hartree-Fock equations can be directly related to experimental separation energies. Since Hartree-Fock theory is the starting point for several many-body techniques (density functional theory, random-phase approximation, shell-model etc.), the aim here is to develop a computer program to solve the Hartree-Fock equations in a given single-particle basis, here the harmonic oscillator.

Developing a Hartree-Fock program

The Hartree-Fock algorithm can be broken down as follows. We recall that our Hartree-Fock matrix is

\[ \hat{H}^\text{HF} = \langle \alpha | \hat{H} | \beta \rangle + \sum_{J=1}^{N} C_J | \alpha \rangle \langle \gamma | V | \beta \rangle_{AB}. \]

Normally we assume that the single-particle basis \( | \beta \rangle \) forms an eigenbasis for the operator \( \hat{H} \) (this is our case), meaning that the Hartree-Fock matrix becomes

\[ \hat{H}^\text{HF} = e_i | \alpha \rangle \langle \beta | + \sum_{J=1}^{N} C_J | \gamma \rangle \langle \gamma | V | \beta \rangle_{AB}. \]

The Hartree-Fock eigenvalue problem

\[ \sum_{\alpha} \hat{H}^\text{HF} | \alpha \rangle = e_i | \alpha \rangle, \]

can be written out in a more compact form as

\[ \hat{H}^\text{HF} \hat{\phi} = e_i \hat{\phi}. \]
Developing a Hartree-Fock program, the density matrix

The equations are often rewritten in terms of a so-called density matrix, which is defined as

$$\rho_{\alpha\beta} = \sum_{\gamma\delta} \langle \gamma | \hat{\rho} | \delta \rangle = \sum_{\gamma\delta} C_{\gamma} C_{\delta}.$$  \hspace{1cm} (18)

It means that we can rewrite the Hartree-Fock Hamiltonian as

$$\hat{H}^{HF}_{\gamma\delta} = \epsilon_{\alpha} C_{\gamma} + \sum_{\beta} \rho_{\alpha\beta} |\gamma\rangle |\beta\rangle_{AS}.$$

It is convenient to use the density matrix since we can precalculate in every iteration the product of two eigenvector components $C$.

Developing a Hartree-Fock program, a simple Python program

An example of a function written in python which performs the Hartree-Fock calculation is shown here. In setting up your code you will need to write a function which sets up the single-particle basis, the matrix elements $t_{\alpha\beta}$ of the one-body operator (called XO in the function below) and the antisymmetric TBMEs (called reninter in the code link below) and the density matrix elements $\rho_{\alpha\beta}$ (called densityMatrix below). The python program shows how one can, in a brute force way, read in matrix elements in m-scheme and compute the Hartree-Fock single-particle energies for four major shells. The interaction which has been used is the so-called NILO interaction of Machleidt and Entem using the Similarity Renormalization Group approach method to renormalize the interaction, using an oscillator energy $\hbar \omega = 10$ MeV.

The nucleon-nucleon two-body matrix elements are in m-scheme and are fully anti-symmetric. The Hartree-Fock programs uses the density matrix discussed above in order to compute the Hartree-Fock matrix. Here we display the Hartree-Fock part only.

Developing a Hartree-Fock program, additional considerations

Note that $\langle \alpha | \hat{h}_0 | \beta \rangle$ denotes the matrix elements of the one-body part of the starting hamiltonian. For self-bound nucleus $\langle \alpha | \hat{h}_0 | \beta \rangle$ is the kinetic energy, whereas for neutron drops, $\langle \alpha | \hat{h}_0 | \beta \rangle$ represents the harmonic oscillator hamiltonian since the system is confined in a harmonic trap. If we are working in a harmonic oscillator basis with the same $\omega$ as the trapping potential, then $\langle \alpha | \hat{h}_0 | \beta \rangle$ is diagonal.

Developing a Hartree-Fock program, input files

The input file spdata.dat contains the information of all single-particle quantum numbers needed to define this space. In total we have 40 single-particle states labeled by $n$, $\nu$, $j$ and $m$, where $m$ is the projection of the total single-particle angular momentum $j$. For every set of single-particle quantum numbers there is a unique number $p$ identifying them, meaning that the two-body matrix elements in the file twobody.dat are identified as $(\nu\nu|V|\nu\nu)$. You will need to read these two files and set up arrays which store the matrix elements while running the program.

Developing a Hartree-Fock program, analyzing the results

Running the program, one finds that the lowest-lying states for a nucleus like $^{16}$O, we see that the nucleon-nucleon force brings a natural spin-orbit splitting for the Qp states (or other states except the $s$-states). Since we are using the m-scheme for our calculations, we observe that there are several states with the same eigenvalues. The number of eigenvalues corresponds to the degeneracy $2j + 1$ and is well respected in our calculations, as seen from the table here.

The values of the lowest-lying states are $(\nu$ for protons and $\pi$ for neutrons)

<table>
<thead>
<tr>
<th>Quantum number</th>
<th>Energy (MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Qp, 0</td>
<td>-40.4602</td>
</tr>
<tr>
<td>Qp, 1</td>
<td>-40.4600</td>
</tr>
<tr>
<td>Qp, 2</td>
<td>-40.4626</td>
</tr>
<tr>
<td>Qp, 3</td>
<td>-40.4626</td>
</tr>
<tr>
<td>Qp, 4</td>
<td>-40.4632</td>
</tr>
<tr>
<td>Qp, 5</td>
<td>-40.4633</td>
</tr>
<tr>
<td>Qp, 6</td>
<td>-5.7373</td>
</tr>
<tr>
<td>Qp, 7</td>
<td>-5.7373</td>
</tr>
<tr>
<td>Qp, 8</td>
<td>-5.8403</td>
</tr>
<tr>
<td>Qp, 9</td>
<td>-5.8403</td>
</tr>
<tr>
<td>Qp, 10</td>
<td>-11.5886</td>
</tr>
</tbody>
</table>
Developing a Hartree-Fock program, separation energies

We can use these results to attempt our first link with experimental data, namely to compute the shell gap or the separation energies. The shell gap for neutrons is given by

$$\Delta S_n = 2BE(N, Z) - BE(N - 1, Z) - BE(N + 1, Z).$$

For $^{16}O$ we have an experimental value for the shell gap of 11.51 MeV for neutrons, while our Hartree-Fock calculations result in 25.65 MeV. This means that correlations beyond a simple Hartree-Fock calculation with a two-body force play an important role in nuclear physics. The splitting between the $^1S_0^+$ and the $^3S_1^-$ state is 4.88 MeV, while the experimental value for the gap between the ground state $^1S_0^+$ and the first excited $^3S_1^-$ state is 6.08 MeV. The two-nucleon spin-orbit force plays a central role here. In our discussion of nuclear forces we will see how the spin-orbit force comes into play here.

Reminder on definitions

The action of the creation and annihilation operators with respect to a reference state $\Phi_0$ are then given by $a_\alpha(\Phi_0) = |\Phi_0\rangle$ where a state labeled by $|\Phi_0\rangle$ means that a particle in a single-particle state $\alpha$ has been removed. Similarly, we have $a_\alpha^\dagger(\Phi_0) = |\Phi_0\rangle$, $a_\alpha |\Phi_0\rangle = 0$ and $a_\alpha a_\alpha |\Phi_0\rangle = 0$. With the above definitions, we write our Hamiltonian as

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

where the single-particle part is given by

$$\hat{H}_0 = \sum_{p,q} \langle p|\hat{h}_0|q\rangle a_\dagger_p a_q,$$

Finally, the three-body part of our Hamiltonian is defined by

$$\hat{W} = \frac{1}{3!} \sum_{pqrstuv} \langle pq|\hat{\omega}|rstuv\rangle a_\dagger_p a_\dagger_q a_\dagger_r a_s a_t a_u,$$

Adding a three-body interaction

where we have defined the antisymmetric matrix elements

$$\langle pq|\hat{\omega}|rstuv\rangle = \langle pq|\hat{\omega}|rstuv\rangle + \langle pq|\hat{\omega}|sruvt\rangle + \langle pq|\hat{\omega}|stuvr\rangle - \langle pq|\hat{\omega}|stuv\rangle.$$

We will in the discussions to come drop the $AS$ subscript, assuming thereby that all matrix elements are antisymmetrized.

Analyzing the results in terms of the nuclear force components

Our Hamiltonian contains one-body, two-body and three-body contributions and in the equations below, we label states below the Fermi level $F$ as $i, j, ...$ while states above the Fermi level are defined by $a, b, ...$. General single-particle states are given by the letters $p, q, ...$. The quantities $pq$ ... represent the quantum numbers of various single-particle states, namely $p = (\nu_p, \lambda_p, j_p, m_p, t_p)$. The commutation relations for creation and annihilation operators with respect to a given reference state are then given by

$$\{ a_p^\dagger, a_q \} = \delta_{pq}, \quad p, q \leq F$$

$$\{ a_p^\dagger, a_q \} = \delta_{pq}, \quad p, q > F.$$

A general Hamiltonian

This part of the Hamiltonian is commonly defined in terms of some external potential like the three-dimensional harmonic oscillator or a particular mean-field basis. Similarly, the two-body part of the Hamiltonian is given by

$$\hat{V} = \frac{1}{2} \sum_{pq} \langle pq|\hat{\mathcal{V}}|rs\rangle a_\dagger_p a_q a_\dagger_r a_s,$$

where we have employed antisymmetric matrix elements defined as

$$\langle pq|\hat{\mathcal{V}}|rs\rangle = \langle pq|\hat{\mathcal{V}}|rs\rangle - \langle pq|\hat{\mathcal{V}}|sr\rangle.$$

We will assume that the two-body operator $\hat{\mathcal{V}}$ is given by a nucleon-nucleon interaction.

An additional reminder

Introducing a reference state $|\Phi_0\rangle$ as our new vacuum state leads to a redefinition of the Hamiltonian in terms of a constant reference energy $E_0$ defined as

$$E_0 = \sum_{i,j} \langle i|\hat{h}_0|j\rangle + \frac{1}{2} \sum_{i,j} \langle j|\hat{\mathcal{V}}|i\rangle + \frac{1}{2} \sum_{i,j,k} \langle jk|\hat{\omega}|ij\rangle,$$

and a normal-ordered Hamiltonian

$$\hat{H}_0 = \sum_{p,q} \langle pq|\hat{\mathcal{V}}|pq\rangle a_\dagger_p a_q + \frac{1}{2} \sum_{p,q} \langle pq|\hat{\mathcal{V}}|pq\rangle a_\dagger_p a_\dagger_q a_q a_p + \frac{1}{3!} \sum_{pqstuv} \langle pq|\hat{\omega}|pqstuv\rangle a_\dagger_p a_\dagger_q a_\dagger_r a_s a_t a_u$$

where

$$\langle pq|\hat{\mathcal{V}}|pq\rangle = \langle pq|\hat{\mathcal{V}}|pq\rangle + \sum_{i,j} \langle pq|\hat{\mathcal{V}}|ij\rangle + \frac{1}{2} \sum_{i,j,k} \langle pq|\hat{\mathcal{V}}|jk\rangle.$$
The two-body matrix elements are now modified in order to account for medium-modified contributions from the three-body interaction, resulting in
\[
\langle \alpha \beta | \hat{v} | \gamma \delta \rangle = \langle \alpha \beta | \hat{v} | \gamma \delta \rangle + \sum_{\gamma \delta} \langle \alpha \beta | \hat{w} | \gamma \delta \rangle.
\]
In Eq. (19), the effective two-body interaction \( \hat{v} \) can contain both a standard two-nucleon interaction and a density dependent contribution stemming from a three-body interaction \( \hat{w} \).

More on the monopole term

The spherical single-particle states, provide an important ingredient for the formation of shells and interplay between spherical configurations and deformation in nuclei. Large shell gaps obtained for the formation of shells and interplay between spherical and deformed shapes, resulting in so-called monopole configurations and deformation in nuclei. Large shell gaps obtained for the formation of shells and interplay between spherical and deformed shapes.

The single-particle energy \( \epsilon_p \) resulting from for example a self-consistent Hartree-Fock field, or from first order in many-body perturbation theory, is given by (in an uncoupled basis)
\[
\epsilon_p = \langle \alpha | \hat{h}_0 | \alpha \rangle + \sum_{i \leq F} \langle \alpha | \hat{v} | \alpha \rangle + \frac{1}{2} \sum_{i < j \leq F} \langle \alpha | \hat{w} | \alpha \rangle.
\]
where we have included the three-body interaction as well.

Linking the monopole part with Hartree-Fock theory

We can rewrite this equation in an angular coupled basis (\( j \)-coupled basis) as
\[
\epsilon_p = \langle \alpha | \hat{h}_0 | \alpha \rangle + \frac{1}{2J+1} \sum_{\alpha \beta \gamma \delta} \left( \sum_{\gamma \delta} \langle \alpha \beta | \hat{v} | \gamma \delta \rangle + \frac{1}{2} \sum_{\gamma \delta} \langle \alpha \beta | \hat{w} | \gamma \delta \rangle \right),
\]
\[
\epsilon_p = \langle \alpha_1 | \hat{h}_0 | \alpha_1 \rangle + \frac{1}{2J+1} \sum_{\alpha_1 \alpha_2 \gamma \delta} \left( \sum_{\gamma \delta} \langle \alpha_1 \alpha_2 | \hat{v} | \gamma \delta \rangle + \frac{1}{2} \sum_{\gamma \delta} \langle \alpha_1 \alpha_2 | \hat{w} | \gamma \delta \rangle \right),
\]
where the first equation contains a two-body force only while Eq. (24) includes the medium-modified contribution from the three-body interaction as well.

Linking the monopole part with Hartree-Fock theory, angular momentum

In Eqs. (23) and (24), we have used a compact notation for the single-particle states, with the symbol \( \alpha \), \( \beta \), \( \gamma \), \( \delta \) representing all possible quantum numbers except the magnetic substates \( m_{\alpha \beta \gamma \delta} \), that is \( \alpha \beta \gamma \delta = (\alpha_1, \beta_1, \gamma_1, \delta_1) \). The symbol \( \alpha_1 \beta_1 \gamma_1 \delta_1 \) stands now for all single-particle states up to the Fermi level, excluding again the magnetic substates. In the above two-body interaction matrix elements \( \langle \alpha_1 \alpha_2 | \hat{v} | \gamma \delta \rangle \) or \( \langle \alpha_1 \alpha_2 | \hat{w} | \gamma \delta \rangle \) we have dropped additional quantum numbers like the isospin projection. Our interactions are diagonal in the projection of the total isospin but breaks both isospin symmetry and charge symmetry.
Final expressions for the monopole term

Using the definition of the single-particle energy in Eq. (23), the definition of the monopole matrix element in Eqs. (20) or (22) and Eq. (21), we can rewrite Eq. (23) as

$$\epsilon_{\alpha p} = \langle \alpha p | \hat{h}_0 | \alpha p \rangle + \sum_{n_i} \mathcal{C}_n \mathcal{P}_{n \alpha i}$$

with $N_{n_i} = 2n_i + 1$, and Eq. (24) as

$$\epsilon_{\alpha p} = \langle \alpha p | \hat{h}_0 | \alpha p \rangle + \sum_{n_i} \mathcal{N}_{n_i} \mathcal{P}_{n \alpha i}.$$

Analyzing our results, decomposing the Hamiltonian

One possible decomposition of the effective interaction is to express the $k$-th component of the interaction $\langle \nu | \hat{V} \alpha \rangle \langle \nu | \hat{V} \alpha \rangle_\nu$ in a $j-j$-coupled basis, where $\hat{v}_k$ is related to the matrix elements $\langle \nu | \hat{V} \alpha \rangle \langle \nu | \hat{V} \alpha \rangle_\nu$ or $\langle \nu | \hat{V} \alpha \rangle \langle \nu | \hat{V} \alpha \rangle_\nu$ through the relation

$$\langle \nu | \hat{V} \alpha \rangle \langle \nu | \hat{V} \alpha \rangle_\nu = (-1)^{2k+1} \sum_{L J S J'} \langle \nu | \hat{V} \alpha \rangle |L J S J\rangle \langle \nu | \hat{V} \alpha \rangle \langle J J' | \hat{v}_k | J K J' \rangle$$

\begin{align*}
&\quad \times \left\{ \sum_{L J S J'} (-1)^{j-j'} (2j+1) \begin{pmatrix} J & J' & L \end{pmatrix} \right\} \sum_{L J S J'} \langle \nu | \hat{V} \alpha \rangle \langle J J' | \hat{v}_k | J K J' \rangle \\
&\quad \times \langle \nu | \hat{V} \alpha \rangle \langle J J' | \hat{v}_k | J K J' \rangle \langle J J' | \hat{v}_k | J K J' \rangle \langle \nu | \hat{V} \alpha \rangle \langle J J' | \hat{v}_k | J K J' \rangle \langle \nu | \hat{V} \alpha \rangle \langle J J' | \hat{v}_k | J K J' \rangle. \tag{28}
\end{align*}

The transformation from an $LS$ basis to a $jj$-coupled scheme is then given by the relation

$$\langle \nu | \hat{V} \alpha \rangle = \sum_{L J S J} \langle \nu | \hat{V} \alpha \rangle |L J S J\rangle \langle \nu | \hat{V} \alpha \rangle,$$

where the symbol $\hat{v}_k \approx \nu$ refers to the quantum numbers in an $LS$ basis, that is $\nu_j = \{n_j, l_j, s_j, t_j\}$.

To derive Eq. (28), we have used the fact that the two-body matrix elements of $\hat{v}_k$ can also be interpreted in the representation of the $LS$-coupling scheme.