Many-body Hamiltonians, basic linear algebra and Second Quantization

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Jul 10, 2018

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 onebody part and a twobody part

$$\hat{H} = \hat{H}_0 + \hat{H}_I = \sum_{i=1}^{A} \hat{h}_0(x_i) + \sum_{i<j}^{A} \hat{v}(r_{ij}), \tag{1}$$

with

$$H_0 = \sum_{i=1}^{A} \hat{h}_0(x_i). \tag{2}$$

The onebody part $u_{\mathrm{ext}}(x_i)$ is normally approximated by a harmonic oscillator potential or 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.

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 $\Psi_\lambda(x_1, x_2, \dots, x_A)$ is an eigenfunction of $\hat{P}$ as well, that is

$$\hat{P}_{ij}\Psi_\lambda(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_A) = \beta\Psi_\lambda(x_1, x_2, \dots, x_i, \dots, x_j, \dots, x_A),$$

where β 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 $\beta = -1$.

In our case we assume that we can approximate the exact eigenfunction with a Slater determinant

$$\Phi(x_1, x_2, \dots, x_A, \alpha, \beta, \dots, \sigma) = \frac{1}{\sqrt{A!}} \begin{vmatrix} \psi_\alpha(x_1) & \psi_\alpha(x_2) & \dots & \dots & \psi_\alpha(x_A) \\ \psi_\beta(x_1) & \psi_\beta(x_2) & \dots & \dots & \psi_\beta(x_A) \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \psi_\sigma(x_1) & \psi_\sigma(x_2) & \dots & \dots & \psi_\sigma(x_A) \end{vmatrix}, \tag{3}$$

where x_i stand for the coordinates and spin values of a particle i and $\alpha, \beta, \dots, \gamma$ are quantum numbers needed to describe remaining quantum numbers.

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

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

A unitary matrix $\mathbf{A}$ is one whose inverse is its adjoint

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

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

$$\mathbf{A} = \mathbf{A}^\dagger.$$

Relations	Name	matrix elements
$A = A^T$	symmetric	$a_{ij} = a_{ji}$
$A = \left(A^T\right)^{-1}$	real orthogonal	$\sum_k a_{ik}a_{jk} = \sum_k a_{ki}a_{kj} = \delta_{ij}$
$A = A^*$	real matrix	$a_{ij} = a^*_{ij}$
$A = A^\dagger$	hermitian	$a_{ij} = a^*_{ji}$
$A = \left(A^\dagger\right)^{-1}$	unitary	$\sum_k a_{ik}a^*_{jk} = \sum_k a^*_{ki}a_{kj} = \delta_{ij}$

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 $\mathbf{A}$ we can write its determinant

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

in a more compact form as

$$|\mathbf{A}| = \sum_{i=1}^{n!} (-1)^{p_i} \hat{P}_i a_{11} a_{22} \dots a_{nn},$$

where $\hat{P}_i$ is a permutation operator which permutes the column indices $1, 2, 3, \dots, n$ and the sum runs over all $n!$ permutations. The quantity p_i represents the number of transpositions of column indices that are needed in order to bring a given permutation back to its initial ordering, in our case given by $a_{11} a_{22} \dots a_{nn}$ here.

A simple 2×2 determinant illustrates this. We have

$$det(\mathbf{A}) = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = (-1)^0 a_{11} a_{22} + (-1)^1 a_{12} a_{21},$$

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

Back to the derivation of the energy. The single-particle function $\psi_\alpha(x_i)$ are eigenfunctions of the onebody Hamiltonian h_i, that is

$$\hat{h}_0(x_i) = \hat{t}(x_i) + \hat{u}_{\text{ext}}(x_i),$$

with eigenvalues

$$\hat{h}_0(x_i)\psi_\alpha(x_i) = \left(\hat{t}(x_i) + \hat{u}_{\text{ext}}(x_i)\right) \psi_\alpha(x_i) = \varepsilon_\alpha \psi_\alpha(x_i).$$

The energies ε_α 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.

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

$$E_0 \leq E[\Phi] = \int \Phi^* \hat{H} \Phi d\tau$$

where Φ is a trial function which we assume to be normalized

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

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

In the Hartree-Fock method the trial function is the Slater determinant of Eq. (3) which can be rewritten as

$$\Phi(x_1, x_2, \dots, x_A, \alpha, \beta, \dots, \nu) = \frac{1}{\sqrt{A!}} \sum_P (-)^P \hat{P} \psi_\alpha(x_1) \psi_\beta(x_2) \dots \psi_\nu(x_A) = \sqrt{A!} \hat{A} \Phi_H,$$

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

It is defined as

$$\hat{A} = \frac{1}{A!} \sum_p (-)^p \hat{P}, \tag{4}$$

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

$$\Phi_H(x_1, x_2, \dots, x_A, \alpha, \beta, \dots, \nu) = \psi_\alpha(x_1) \psi_\beta(x_2) \dots \psi_\nu(x_A).$$

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

$$[H_0, \hat{A}] = [H_I, \hat{A}] = 0. \tag{5}$$

Furthermore, $\hat{A}$ satisfies

$$\hat{A}^2 = \hat{A}, \tag{6}$$

since every permutation of the Slater determinant reproduces it.

The expectation value of $\hat{H}_0$

$$\int \Phi^* \hat{H}_0 \Phi d\tau = A! \int \Phi_H^* \hat{A} \hat{H}_0 \hat{A} \Phi_H d\tau$$

is readily reduced to

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

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

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{i=1}^{A} \sum_p (-)^p \int \Phi_H^* \hat{h}_0 \hat{P} \Phi_H d\tau.$$

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

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{i=1}^{A} \int \Phi_H^* \hat{h}_0 \Phi_H d\tau.$$

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

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{\mu=1}^{A} \int \psi_\mu^*(x) \hat{h}_0 \psi_\mu(x) dx d\mathbf{r}. \tag{7}$$

We introduce the following shorthand for the above integral

$$\langle \mu | \hat{h}_0 | \mu \rangle = \int \psi_\mu^*(x) \hat{h}_0 \psi_\mu(x) dx,$$

and rewrite Eq. (7) as

$$\int \Phi^* \hat{H}_0 \Phi d\tau = \sum_{\mu=1}^{A} \langle \mu | \hat{h}_0 | \mu \rangle. \tag{8}$$

The expectation value of the two-body part of the Hamiltonian is obtained in a similar manner. We have

$$\int \Phi^* \hat{H}_I \Phi d\tau = A! \int \Phi_H^* \hat{A} \hat{H}_I \hat{A} \Phi_H d\tau,$$

which reduces to

$$\int \Phi^* \hat{H}_I \Phi d\tau = \sum_{i \leq j=1}^{A} \sum_{p} (-)^p \int \Phi_H^* \hat{v}(r_{ij}) \hat{P} \Phi_H d\tau,$$

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

$$\int \Phi^* \hat{H}_I \Phi d\tau = \sum_{i<j=1}^{A} \int \Phi_H^* \hat{v}(r_{ij})(1 - P_{ij}) \Phi_H d\tau.$$

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 obtain

$$\int \Phi^* \hat{H}_I \Phi d\tau = \frac{1}{2} \sum_{\mu=1}^{A} \sum_{\nu=1}^{A} \Big[\int \psi_\mu^*(x_i) \psi_\nu^*(x_j) \hat{v}(r_{ij}) \psi_\mu(x_i) \psi_\nu(x_j) dx_i dx_j \tag{9}$$

$$- \int \psi_\mu^*(x_i) \psi_\nu^*(x_j) \hat{v}(r_{ij}) \psi_\nu(x_i) \psi_\mu(x_j) dx_i dx_j \Big]. \tag{10}$$

The first term is the so-called direct term. It is frequently also called the Hartree term, while the second is due to the Pauli principle and is called the exchange

term or just the Fock term. The factor 1/2 is introduced because we now run over all pairs twice.

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

$$\psi_\alpha(x) = \langle x|\alpha\rangle.$$

We introduce the following shorthands for the above two integrals

$$\langle\mu\nu|\hat{v}|\mu\nu\rangle = \int \psi^*_\mu(x_i)\psi^*_\nu(x_j)\hat{v}(r_{ij})\psi_\mu(x_i)\psi_\nu(x_j)dx_i dx_j,$$

and

$$\langle\mu\nu|\hat{v}|\nu\mu\rangle = \int \psi^*_\mu(x_i)\psi^*_\nu(x_j)\hat{v}(r_{ij})\psi_\nu(x_i)\psi_\mu(x_j)dx_i dx_j.$$

Preparing for later studies: varying the coefficients of a wave function expansion and orthogonal transformations

It is common to 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 single-particle basis (this is a normal approach for Hartree-Fock theory) by performing a unitary transformation on our previous basis (labelled with greek indices) as

$$\psi^{new}_p = \sum_\lambda C_{p\lambda}\phi_\lambda. \tag{11}$$

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 ϕ_λ is orthogonal.

It is normal to choose a single-particle basis defined as the eigenfunctions of parts of the full Hamiltonian. The typical situation consists of the solutions of the one-body part of the Hamiltonian, that is we have

$$\hat{h}_0\phi_\lambda = \epsilon_\lambda\phi_\lambda.$$

The single-particle wave functions $\phi_\lambda(\mathbf{r})$, defined by the quantum numbers λ and $\mathbf{r}$ are defined as the overlap

$$\phi_\lambda(\mathbf{r}) = \langle\mathbf{r}|\lambda\rangle.$$

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 stated that a unitary transformation keeps the orthogonality. To see this consider first a basis of vectors $\mathbf{v}_i$,

$$\mathbf{v}_i = \begin{bmatrix} v_{i1} \\ \dots \\ \dots \\ v_{in} \end{bmatrix}$$

We assume that the basis is orthogonal, that is

$$\mathbf{v}_j^T \mathbf{v}_i = \delta_{ij}.$$

An orthogonal or unitary transformation

$$\mathbf{w}_i = \mathbf{U}\mathbf{v}_i,$$

preserves the dot product and orthogonality since

$$\mathbf{w}_j^T \mathbf{w}_i = (\mathbf{U}\mathbf{v}_j)^T \mathbf{U}\mathbf{v}_i = \mathbf{v}_j^T \mathbf{U}^T \mathbf{U}\mathbf{v}_i = \mathbf{v}_j^T \mathbf{v}_i = \delta_{ij}.$$

This means that if the coefficients $C_{p\lambda}$ belong to a unitary or orthogonal trasformation (using the Dirac bra-ket notation)

$$|p\rangle = \sum_\lambda C_{p\lambda} |\lambda\rangle,$$

orthogonality is preserved, that is $\langle\alpha|\beta\rangle = \delta_{\alpha\beta}$ and $\langle p|q\rangle = \delta_{pq}$.

This propertry is extremely useful when we build up a basis of many-body Stater determinant based states.

Note also that although a basis $|\alpha\rangle$ contains an infinity of states, for practical calculations we have always to make some truncations.

Before we develop for example the Hartree-Fock equations, there is another very useful property of determinants that we will use both in connection with Hartree-Fock calculations and later shell-model calculations.

Consider the following determinant

$$\begin{vmatrix} \alpha_1 b_{11} + \alpha_2 s b_{12} & a_{12} \\ \alpha_1 b_{21} + \alpha_2 b_{22} & a_{22} \end{vmatrix} = \alpha_1 \begin{vmatrix} b_{11} & a_{12} \\ b_{21} & a_{22} \end{vmatrix} + \alpha_2 \begin{vmatrix} b_{12} & a_{12} \\ b_{22} & a_{22} \end{vmatrix}$$

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

$$\begin{vmatrix} a_{11} & a_{12} & \dots & \sum_{k=1}^n c_k b_{1k} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & \sum_{k=1}^n c_k b_{2k} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & \sum_{k=1}^n c_k b_{nk} & \dots & a_{nn} \end{vmatrix} = \sum_{k=1}^n c_k \begin{vmatrix} a_{11} & a_{12} & \dots & b_{1k} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & b_{2k} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & b_{nk} & \dots & a_{nn} \end{vmatrix}.$$

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

We can generalize the previous results, now with all elements a_{ij} being given as functions of linear combinations of various coefficients c and elements b_{ij},

$$\begin{vmatrix} \sum_{k=1}^n b_{1k}c_{k1} & \sum_{k=1}^n b_{1k}c_{k2} & \dots & \sum_{k=1}^n b_{1k}c_{kj} & \dots & \sum_{k=1}^n b_{1k}c_{kn} \\ \sum_{k=1}^n b_{2k}c_{k1} & \sum_{k=1}^n b_{2k}c_{k2} & \dots & \sum_{k=1}^n b_{2k}c_{kj} & \dots & \sum_{k=1}^n b_{2k}c_{kn} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \sum_{k=1}^n b_{nk}c_{k1} & \sum_{k=1}^n b_{nk}c_{k2} & \dots & \sum_{k=1}^n b_{nk}c_{kj} & \dots & \sum_{k=1}^n b_{nk}c_{kn} \end{vmatrix} = det(\mathbf{C})det(\mathbf{B}),$$

where $det(\mathbf{C})$ and $det(\mathbf{B})$ are the determinants of $n \times n$ matrices with elements c_{ij} and b_{ij} respectively. This is a property we will use in our Hartree-Fock discussions. Convince yourself about the correctness of the above expression by setting $n = 2$.

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

$$\psi_p(x) = \sum_\lambda C_{p\lambda}\phi_\lambda(x).$$

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

$$\frac{1}{\sqrt{A!}}\begin{vmatrix} \psi_p(x_1) & \psi_p(x_2) & \dots & \dots & \psi_p(x_A) \\ \psi_q(x_1) & \psi_q(x_2) & \dots & \dots & \psi_q(x_A) \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \psi_t(x_1) & \psi_t(x_2) & \dots & \dots & \psi_t(x_A) \end{vmatrix} = \frac{1}{\sqrt{A!}}\begin{vmatrix} \sum_\lambda C_{p\lambda}\phi_\lambda(x_1) & \sum_\lambda C_{p\lambda}\phi_\lambda(x_2) & \dots & \dots & \sum_\lambda C_{p\lambda}\phi_\lambda(x \\ \sum_\lambda C_{q\lambda}\phi_\lambda(x_1) & \sum_\lambda C_{q\lambda}\phi_\lambda(x_2) & \dots & \dots & \sum_\lambda C_{q\lambda}\phi_\lambda(x \\ \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots \\ \sum_\lambda C_{t\lambda}\phi_\lambda(x_1) & \sum_\lambda C_{t\lambda}\phi_\lambda(x_2) & \dots & \dots & \sum_\lambda C_{t\lambda}\phi_\lambda(x \end{vmatrix}$$

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

In our discussions hereafter we will use our definitions of single-particle states above and below the Fermi (F) level given by the labels $ijkl\cdots \leq F$ for so-called single-hole states and $abcd\cdots > F$ for so-called particle states. For general single-particle states we employ the labels $pqrs\ldots$.

The energy functional is

$$E[\Phi] = \sum_{\mu=1}^A \langle\mu|h|\mu\rangle + \frac{1}{2}\sum_{\mu=1}^A\sum_{\nu=1}^A \langle\mu\nu|\hat{v}|\mu\nu\rangle_{AS},$$

we found the expression for the energy functional in terms of the basis function $\phi_\lambda(\mathbf{r})$. We then varied the above energy functional with respect to the basis functions $|\mu\rangle$. Now we are interested in defining a new basis defined in terms of a chosen basis as defined in Eq. (11). We can then rewrite the energy functional as

$$E[\Phi^{New}] = \sum_{i=1}^A \langle i|h|i\rangle + \frac{1}{2}\sum_{ij=1}^A \langle ij|\hat{v}|ij\rangle_{AS}, \tag{12}$$

where Φ^{New} is the new Slater determinant defined by the new basis of Eq. (11).

Using Eq. (11) we can rewrite Eq. (12) as

$$E[\Psi] = \sum_{i=1}^{A}\sum_{\alpha\beta} C_{i\alpha}^{*}C_{i\beta}\langle\alpha|h|\beta\rangle + \frac{1}{2}\sum_{ij=1}^{A}\sum_{\alpha\beta\gamma\delta} C_{i\alpha}^{*}C_{j\beta}^{*}C_{i\gamma}C_{j\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle_{AS}. \quad (13)$$

Definitions and Second quantization

We introduce the time-independent operators $a_\alpha^\dagger$ and a_α which create and annihilate, respectively, a particle in the single-particle state φ_α. We define the fermion creation operator $a_\alpha^\dagger$

$$a_\alpha^\dagger|0\rangle \equiv |\alpha\rangle, \quad (14)$$

and

$$a_\alpha^\dagger|\alpha_1\dots\alpha_n\rangle_{\rm AS} \equiv |\alpha\alpha_1\dots\alpha_n\rangle_{\rm AS} \quad (15)$$

In Eq. (14) the operator $a_\alpha^\dagger$ acts on the vacuum state $|0\rangle$, which does not contain any particles. Alternatively, we could define a closed-shell nucleus or atom as our new vacuum, but then we need to introduce the particle-hole formalism, see the discussion to come.

In Eq. (15) $a_\alpha^\dagger$ acts on an antisymmetric n-particle state and creates an antisymmetric $(n+1)$-particle state, where the one-body state φ_α is occupied, under the condition that $\alpha \neq \alpha_1, \alpha_2, \dots, \alpha_n$. It follows that we can express an antisymmetric state as the product of the creation operators acting on the vacuum state.

$$|\alpha_1\dots\alpha_n\rangle_{\rm AS} = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \dots a_{\alpha_n}^\dagger|0\rangle \quad (16)$$

It is easy to derive the commutation and anticommutation rules for the fermionic creation operators $a_\alpha^\dagger$. Using the antisymmetry of the states (16)

$$|\alpha_1\dots\alpha_i\dots\alpha_k\dots\alpha_n\rangle_{\rm AS} = -|\alpha_1\dots\alpha_k\dots\alpha_i\dots\alpha_n\rangle_{\rm AS} \quad (17)$$

we obtain

$$a_{\alpha_i}^\dagger a_{\alpha_k}^\dagger = -a_{\alpha_k}^\dagger a_{\alpha_i}^\dagger \quad (18)$$

Using the Pauli principle

$$|\alpha_1\dots\alpha_i\dots\alpha_i\dots\alpha_n\rangle_{\rm AS} = 0 \quad (19)$$

it follows that

$$a_{\alpha_i}^\dagger a_{\alpha_i}^\dagger = 0. \quad (20)$$

If we combine Eqs. (18) and (20), we obtain the well-known anti-commutation rule

$$a_\alpha^\dagger a_\beta^\dagger + a_\beta^\dagger a_\alpha^\dagger \equiv \{a_\alpha^\dagger, a_\beta^\dagger\} = 0 \quad (21)$$

The hermitian conjugate of $a_\alpha^\dagger$ is

$$a_\alpha = (a_\alpha^\dagger)^\dagger \quad (22)$$

If we take the hermitian conjugate of Eq. (21), we arrive at

$$\{a_\alpha, a_\beta\} = 0 \tag{23}$$

What is the physical interpretation of the operator a_α and what is the effect of a_α on a given state $|\alpha_1\alpha_2\dots\alpha_n\rangle_{\rm AS}$? Consider the following matrix element

$$\langle\alpha_1\alpha_2\dots\alpha_n|a_\alpha|\alpha'_1\alpha'_2\dots\alpha'_m\rangle \tag{24}$$

where both sides are antisymmetric. We distinguish between two cases. The first (1) is when $\alpha \in \{\alpha_i\}$. Using the Pauli principle of Eq. (19) it follows

$$\langle\alpha_1\alpha_2\dots\alpha_n|a_\alpha = 0 \tag{25}$$

The second (2) case is when $\alpha \notin \{\alpha_i\}$. It follows that an hermitian conjugation

$$\langle\alpha_1\alpha_2\dots\alpha_n|a_\alpha = \langle\alpha\alpha_1\alpha_2\dots\alpha_n| \tag{26}$$

Eq. (26) holds for case (1) since the lefthand side is zero due to the Pauli principle. We write Eq. (24) as

$$\langle\alpha_1\alpha_2\dots\alpha_n|a_\alpha|\alpha'_1\alpha'_2\dots\alpha'_m\rangle = \langle\alpha_1\alpha_2\dots\alpha_n|\alpha\alpha'_1\alpha'_2\dots\alpha'_m\rangle \tag{27}$$

Here we must have $m = n+1$ if Eq. (27) has to be trivially different from zero.

For the last case, the minus and plus signs apply when the sequence $\alpha, \alpha_1, \alpha_2, \dots, \alpha_n$ and $\alpha'_1, \alpha'_2, \dots, \alpha'_{n+1}$ are related to each other via even and odd permutations. If we assume that $\alpha \notin \{\alpha_i\}$ we obtain

$$\langle\alpha_1\alpha_2\dots\alpha_n|a_\alpha|\alpha'_1\alpha'_2\dots\alpha'_{n+1}\rangle = 0 \tag{28}$$

when $\alpha \in \{\alpha'_i\}$. If $\alpha \notin \{\alpha'_i\}$, we obtain

$$a_\alpha \underbrace{|\alpha'_1\alpha'_2\dots\alpha'_{n+1}\rangle}_{\neq\alpha} = 0 \tag{29}$$

and in particular

$$a_\alpha|0\rangle = 0 \tag{30}$$

If $\{\alpha\alpha_i\} = \{\alpha'_i\}$, performing the right permutations, the sequence $\alpha, \alpha_1, \alpha_2, \dots, \alpha_n$ is identical with the sequence $\alpha'_1, \alpha'_2, \dots, \alpha'_{n+1}$. This results in

$$\langle\alpha_1\alpha_2\dots\alpha_n|a_\alpha|\alpha\alpha_1\alpha_2\dots\alpha_n\rangle = 1 \tag{31}$$

and thus

$$a_\alpha|\alpha\alpha_1\alpha_2\dots\alpha_n\rangle = |\alpha_1\alpha_2\dots\alpha_n\rangle \tag{32}$$

The action of the operator a_α from the left on a state vector is to to remove one particle in the state α. If the state vector does not contain the single-particle state α, the outcome of the operation is zero. The operator a_α is normally called for a destruction or annihilation operator.

The next step is to establish the commutator algebra of $a^\dagger_\alpha$ and a_β.

The action of the anti-commutator $\{a^\dagger_\alpha,a_\alpha\}$ on a given n-particle state is

$$\begin{aligned} a^\dagger_\alpha a_\alpha \underbrace{|\alpha_1\alpha_2\ldots\alpha_n\rangle}_{\neq\alpha} &= 0 \\ a_\alpha a^\dagger_\alpha \underbrace{|\alpha_1\alpha_2\ldots\alpha_n\rangle}_{\neq\alpha} &= a_\alpha \underbrace{|\alpha\alpha_1\alpha_2\ldots\alpha_n\rangle}_{\neq\alpha} = \underbrace{|\alpha_1\alpha_2\ldots\alpha_n\rangle}_{\neq\alpha} \end{aligned} \tag{33}$$

if the single-particle state α is not contained in the state.

If it is present we arrive at

$$\begin{aligned} a^\dagger_\alpha a_\alpha|\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle &= a^\dagger_\alpha a_\alpha(-1)^k|\alpha\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle \\ &= (-1)^k|\alpha\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle = |\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle \\ a_\alpha a^\dagger_\alpha|\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle &= 0 \end{aligned} \tag{34}$$

From Eqs. (33) and (34) we arrive at

$$\{a^\dagger_\alpha, a_\alpha\} = a^\dagger_\alpha a_\alpha + a_\alpha a^\dagger_\alpha = 1 \tag{35}$$

The action of $\left\{a^\dagger_\alpha, a_\beta\right\}$, with $\alpha \neq \beta$ on a given state yields three possibilities. The first case is a state vector which contains both α and β, then either α or β and finally none of them.

The first case results in

$$\begin{aligned} a^\dagger_\alpha a_\beta|\alpha\beta\alpha_1\alpha_2\ldots\alpha_{n-2}\rangle &= 0 \\ a_\beta a^\dagger_\alpha|\alpha\beta\alpha_1\alpha_2\ldots\alpha_{n-2}\rangle &= 0 \end{aligned} \tag{36}$$

while the second case gives

$$\begin{aligned} a^\dagger_\alpha a_\beta|\beta \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle}_{\neq\alpha} &= |\alpha \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle}_{\neq\alpha} \\ a_\beta a^\dagger_\alpha|\beta \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle}_{\neq\alpha} &= a_\beta|\alpha\beta \underbrace{\beta\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle}_{\neq\alpha} \\ &= -|\alpha \underbrace{\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle}_{\neq\alpha} \end{aligned} \tag{37}$$

Finally if the state vector does not contain α and β

$$\begin{aligned} a^\dagger_\alpha a_\beta| \underbrace{\alpha_1\alpha_2\ldots\alpha_n\rangle}_{\neq\alpha,\beta} &= 0 \\ a_\beta a^\dagger_\alpha| \underbrace{\alpha_1\alpha_2\ldots\alpha_n\rangle}_{\neq\alpha,\beta} &= a_\beta|\alpha \underbrace{\alpha_1\alpha_2\ldots\alpha_n\rangle}_{\neq\alpha,\beta} = 0 \end{aligned} \tag{38}$$

For all three cases we have

$$\{a^\dagger_\alpha, a_\beta\} = a^\dagger_\alpha a_\beta + a_\beta a^\dagger_\alpha = 0, \quad \alpha \neq \beta \tag{39}$$

We can summarize our findings in Eqs. (35) and (39) as

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \tag{40}$$

with $\delta_{\alpha\beta}$ is the Kroenecker δ-symbol.

The properties of the creation and annihilation operators can be summarized as (for fermions)

$$a_\alpha^\dagger|0\rangle \equiv |\alpha\rangle,$$

and

$$a_\alpha^\dagger|\alpha_1 \ldots \alpha_n\rangle_{\rm AS} \equiv |\alpha\alpha_1 \ldots \alpha_n\rangle_{\rm AS}.$$

from which follows

$$|\alpha_1 \ldots \alpha_n\rangle_{\rm AS} = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \ldots a_{\alpha_n}^\dagger|0\rangle.$$

The hermitian conjugate has the folowing properties

$$a_\alpha = (a_\alpha^\dagger)^\dagger.$$

Finally we found

$$a_\alpha \underbrace{|\alpha_1'\alpha_2' \ldots \alpha_{n+1}'\rangle}_{\neq\alpha} = 0, \quad \text{in particular } a_\alpha|0\rangle = 0,$$

and

$$a_\alpha|\alpha\alpha_1\alpha_2 \ldots \alpha_n\rangle = |\alpha_1\alpha_2 \ldots \alpha_n\rangle,$$

and the corresponding commutator algebra

$$\{a_\alpha^\dagger, a_\beta^\dagger\} = \{a_\alpha, a_\beta\} = 0 \qquad \{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta}.$$

One-body operators in second quantization

A very useful operator is the so-called number-operator. Most physics cases we will study in this text conserve the total number of particles. The number operator is therefore a useful quantity which allows us to test that our many-body formalism conserves the number of particles. In for example (d, p) or (p, d) reactions it is important to be able to describe quantum mechanical states where particles get added or removed. A creation operator $a_\alpha^\dagger$ adds one particle to the single-particle state α of a give many-body state vector, while an annihilation operator a_α removes a particle from a single-particle state α.

Let us consider an operator proportional with $a_\alpha^\dagger a_\beta$ and $\alpha = \beta$. It acts on an n-particle state resulting in

$$a_\alpha^\dagger a_\alpha|\alpha_1\alpha_2 \ldots \alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ \\ |\alpha_1\alpha_2 \ldots \alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \tag{41}$$

Summing over all possible one-particle states we arrive at

$$\left(\sum_{\alpha} a_{\alpha}^{\dagger}a_{\alpha}\right)|\alpha_1\alpha_2\dots\alpha_n\rangle = n|\alpha_1\alpha_2\dots\alpha_n\rangle \tag{42}$$

The operator

$$\hat{N} = \sum_{\alpha} a_{\alpha}^{\dagger}a_{\alpha} \tag{43}$$

is called the number operator since it counts the number of particles in a give state vector when it acts on the different single-particle states. It acts on one single-particle state at the time and falls therefore under category one-body operators. Next we look at another important one-body operator, namely $\hat{H}_0$ and study its operator form in the occupation number representation.

We want to obtain an expression for a one-body operator which conserves the number of particles. Here we study the one-body operator for the kinetic energy plus an eventual external one-body potential. The action of this operator on a particular n-body state with its pertinent expectation value has already been studied in coordinate space. In coordinate space the operator reads

$$\hat{H}_0 = \sum_{i} \hat{h}_0(x_i) \tag{44}$$

and the anti-symmetric n-particle Slater determinant is defined as

$$\Phi(x_1, x_2, \dots, x_n, \alpha_1, \alpha_2, \dots, \alpha_n) = \frac{1}{\sqrt{n!}}\sum_{p}(-1)^p\hat{P}\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n).$$

Defining

$$\hat{h}_0(x_i)\psi_{\alpha_i}(x_i) = \sum_{\alpha_k'}\psi_{\alpha_k'}(x_i)\langle\alpha_k'|\hat{h}_0|\alpha_k\rangle \tag{45}$$

we can easily evaluate the action of $\hat{H}_0$ on each product of one-particle functions in Slater determinant. From Eq. (45) we obtain the following result without permuting any particle pair

$$\begin{aligned}
& \left(\sum_{i} \hat{h}_0(x_i)\right)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle\psi_{\alpha_1'}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n}(x_n) \\
+ & \sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle\psi_{\alpha_1}(x_1)\psi_{\alpha_2'}(x_2)\dots\psi_{\alpha_n}(x_n) \\
+ & \dots \\
+ & \sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\dots\psi_{\alpha_n'}(x_n)
\end{aligned} \tag{46}$$

If we interchange particles 1 and 2 we obtain

$$\begin{aligned}
&\left(\sum_i \hat{h}_0(x_i)\right)\psi_{\alpha_1}(x_2)\psi_{\alpha_1}(x_2)\dots\psi_{\alpha_n}(x_n)\\
=&\sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle\psi_{\alpha_1}(x_2)\psi_{\alpha_2'}(x_1)\dots\psi_{\alpha_n}(x_n)\\
+&\sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle\psi_{\alpha_1'}(x_2)\psi_{\alpha_2}(x_1)\dots\psi_{\alpha_n}(x_n)\\
+&\dots\\
+&\sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle\psi_{\alpha_1}(x_2)\psi_{\alpha_1}(x_2)\dots\psi_{\alpha_n'}(x_n) \qquad (47)
\end{aligned}$$

We can continue by computing all possible permutations. We rewrite also our Slater determinant in its second quantized form and skip the dependence on the quantum numbers x_i. Summing up all contributions and taking care of all phases $(-1)^p$ we arrive at

$$\begin{aligned}
\hat{H}_0|\alpha_1,\alpha_2,\dots,\alpha_n\rangle =&\sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle|\alpha_1'\alpha_2\dots\alpha_n\rangle\\
+&\sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle|\alpha_1\alpha_2'\dots\alpha_n\rangle\\
+&\dots\\
+&\sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle|\alpha_1\alpha_2\dots\alpha_n'\rangle \qquad (48)
\end{aligned}$$

In Eq. (48) we have expressed the action of the one-body operator of Eq. (44) on the n-body state in its second quantized form. This equation can be further manipulated if we use the properties of the creation and annihilation operator on each primed quantum number, that is

$$|\alpha_1\alpha_2\dots\alpha_k'\dots\alpha_n\rangle = a^\dagger_{\alpha_k'}a_{\alpha_k}|\alpha_1\alpha_2\dots\alpha_k\dots\alpha_n\rangle \qquad (49)$$

Inserting this in the right-hand side of Eq. (48) results in

$$\begin{aligned}
\hat{H}_0|\alpha_1\alpha_2\dots\alpha_n\rangle =&\sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle a^\dagger_{\alpha_1'}a_{\alpha_1}|\alpha_1\alpha_2\dots\alpha_n\rangle\\
+&\sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle a^\dagger_{\alpha_2'}a_{\alpha_2}|\alpha_1\alpha_2\dots\alpha_n\rangle\\
+&\dots\\
+&\sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle a^\dagger_{\alpha_n'}a_{\alpha_n}|\alpha_1\alpha_2\dots\alpha_n\rangle\\
=&\sum_{\alpha,\beta}\langle\alpha|\hat{h}_0|\beta\rangle a^\dagger_\alpha a_\beta|\alpha_1\alpha_2\dots\alpha_n\rangle \qquad (50)
\end{aligned}$$

In the number occupation representation or second quantization we get the following expression for a one-body operator which conserves the number of particles

$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_\alpha^\dagger a_\beta \tag{51}$$

Obviously, $\hat{H}_0$ can be replaced by any other one-body operator which preserved the number of particles. The stucture of the operator is therefore not limited to say the kinetic or single-particle energy only.

The opearator $\hat{H}_0$ takes a particle from the single-particle state β to the single-particle state α with a probability for the transition given by the expectation value $\langle \alpha | \hat{h}_0 | \beta \rangle$.

It is instructive to verify Eq. (51) by computing the expectation value of $\hat{H}_0$ between two single-particle states

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \langle 0 | a_{\alpha_1} a_\alpha^\dagger a_\beta a_{\alpha_2}^\dagger | 0 \rangle \tag{52}$$

Using the commutation relations for the creation and annihilation operators we have

$$a_{\alpha_1} a_\alpha^\dagger a_\beta a_{\alpha_2}^\dagger = (\delta_{\alpha\alpha_1} - a_\alpha^\dagger a_{\alpha_1})(\delta_{\beta\alpha_2} - a_{\alpha_2}^\dagger a_\beta), \tag{53}$$

which results in

$$\langle 0 | a_{\alpha_1} a_\alpha^\dagger a_\beta a_{\alpha_2}^\dagger | 0 \rangle = \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} \tag{54}$$

and

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} = \langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle \tag{55}$$

Two-body operators in second quantization

Let us now derive the expression for our two-body interaction part, which also conserves the number of particles. We can proceed in exactly the same way as for the one-body operator. In the coordinate representation our two-body interaction part takes the following expression

$$\hat{H}_I = \sum_{i<j} V(x_i, x_j) \tag{56}$$

where the summation runs over distinct pairs. The term V can be an interaction model for the nucleon-nucleon interaction or the interaction between two electrons. It can also include additional two-body interaction terms.

The action of this operator on a product of two single-particle functions is defined as

$$V(x_i, x_j) \psi_{\alpha_k}(x_i) \psi_{\alpha_l}(x_j) = \sum_{\alpha_k' \alpha_l'} \psi'_{\alpha_k}(x_i) \psi'_{\alpha_l}(x_j) \langle \alpha_k' \alpha_l' | \hat{v} | \alpha_k \alpha_l \rangle \tag{57}$$

We can now let $\hat{H}_I$ act on all terms in the linear combination for $|\alpha_1\alpha_2\ldots\alpha_n\rangle$. Without any permutations we have

$$\begin{aligned}
& \left(\sum_{i<j} V(x_i,x_j)\right)\psi_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha_1'\alpha_2'}\langle\alpha_1'\alpha_2'|\hat{v}|\alpha_1\alpha_2\rangle\psi'_{\alpha_1}(x_1)\psi'_{\alpha_2}(x_2)\ldots\psi_{\alpha_n}(x_n) \\
+ & \ldots \\
+ & \sum_{\alpha_1'\alpha_n'}\langle\alpha_1'\alpha_n'|\hat{v}|\alpha_1\alpha_n\rangle\psi'_{\alpha_1}(x_1)\psi_{\alpha_2}(x_2)\ldots\psi'_{\alpha_n}(x_n) \\
+ & \ldots \\
+ & \sum_{\alpha_2'\alpha_n'}\langle\alpha_2'\alpha_n'|\hat{v}|\alpha_2\alpha_n\rangle\psi_{\alpha_1}(x_1)\psi'_{\alpha_2}(x_2)\ldots\psi'_{\alpha_n}(x_n) \\
+ & \ldots
\end{aligned} \tag{58}$$

where on the rhs we have a term for each distinct pairs.

For the other terms on the rhs we obtain similar expressions and summing over all terms we obtain

$$\begin{aligned}
H_I|\alpha_1\alpha_2\ldots\alpha_n\rangle = & \sum_{\alpha_1',\alpha_2'}\langle\alpha_1'\alpha_2'|\hat{v}|\alpha_1\alpha_2\rangle|\alpha_1'\alpha_2'\ldots\alpha_n\rangle \\
+ & \ldots \\
+ & \sum_{\alpha_1',\alpha_n'}\langle\alpha_1'\alpha_n'|\hat{v}|\alpha_1\alpha_n\rangle|\alpha_1'\alpha_2\ldots\alpha_n'\rangle \\
+ & \ldots \\
+ & \sum_{\alpha_2',\alpha_n'}\langle\alpha_2'\alpha_n'|\hat{v}|\alpha_2\alpha_n\rangle|\alpha_1\alpha_2'\ldots\alpha_n'\rangle \\
+ & \ldots
\end{aligned} \tag{59}$$

We introduce second quantization via the relation

$$\begin{aligned}
& a^\dagger_{\alpha_k'}a^\dagger_{\alpha_l'}a_{\alpha_l}a_{\alpha_k}|\alpha_1\alpha_2\ldots\alpha_k\ldots\alpha_l\ldots\alpha_n\rangle \\
= & (-1)^{k-1}(-1)^{l-2}a^\dagger_{\alpha_k'}a^\dagger_{\alpha_l'}a_{\alpha_l}a_{\alpha_k}|\alpha_k\alpha_l\underbrace{\alpha_1\alpha_2\ldots\alpha_n}_{\neq\alpha_k,\alpha_l}\rangle \\
= & (-1)^{k-1}(-1)^{l-2}|\alpha_k'\alpha_l'\underbrace{\alpha_1\alpha_2\ldots\alpha_n}_{\neq\alpha_k',\alpha_l'}\rangle \\
= & |\alpha_1\alpha_2\ldots\alpha_k'\ldots\alpha_l'\ldots\alpha_n\rangle
\end{aligned} \tag{60}$$

Inserting this in (59) gives

$$\begin{aligned}
H_I|\alpha_1\alpha_2\ldots\alpha_n\rangle = & \sum_{\alpha_1',\alpha_2'}\langle\alpha_1'\alpha_2'|\hat{v}|\alpha_1\alpha_2\rangle a^\dagger_{\alpha_1'}a^\dagger_{\alpha_2'}a_{\alpha_2}a_{\alpha_1}|\alpha_1\alpha_2\ldots\alpha_n\rangle \\
+ & \quad\ldots \\
= & \sum_{\alpha_1',\alpha_n'}\langle\alpha_1'\alpha_n'|\hat{v}|\alpha_1\alpha_n\rangle a^\dagger_{\alpha_1'}a^\dagger_{\alpha_n'}a_{\alpha_n}a_{\alpha_1}|\alpha_1\alpha_2\ldots\alpha_n\rangle \\
+ & \quad\ldots \\
= & \sum_{\alpha_2',\alpha_n'}\langle\alpha_2'\alpha_n'|\hat{v}|\alpha_2\alpha_n\rangle a^\dagger_{\alpha_2'}a^\dagger_{\alpha_n'}a_{\alpha_n}a_{\alpha_2}|\alpha_1\alpha_2\ldots\alpha_n\rangle \\
+ & \quad\ldots \\
= & \sum_{\alpha,\beta,\gamma,\delta}{}'\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma|\alpha_1\alpha_2\ldots\alpha_n\rangle \qquad (61)
\end{aligned}$$

Here we let $\sum'$ indicate that the sums running over α and β run over all single-particle states, while the summations γ and δ run over all pairs of single-particle states. We wish to remove this restriction and since

$$\langle\alpha\beta|\hat{v}|\gamma\delta\rangle = \langle\beta\alpha|\hat{v}|\delta\gamma\rangle \qquad (62)$$

we get

$$\begin{aligned}
\sum_{\alpha\beta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma = & \sum_{\alpha\beta}\langle\beta\alpha|\hat{v}|\delta\gamma\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \qquad (63)\\
= & \sum_{\alpha\beta}\langle\beta\alpha|\hat{v}|\delta\gamma\rangle a^\dagger_\beta a^\dagger_\alpha a_\gamma a_\delta \qquad (64)
\end{aligned}$$

where we have used the anti-commutation rules.

Changing the summation indices α and β in (64) we obtain

$$\sum_{\alpha\beta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma = \sum_{\alpha\beta}\langle\alpha\beta|\hat{v}|\delta\gamma\rangle a^\dagger_\alpha a^\dagger_\beta a_\gamma a_\delta \qquad (65)$$

From this it follows that the restriction on the summation over γ and δ can be removed if we multiply with a factor $\frac{1}{2}$, resulting in

$$\hat{H}_I = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \qquad (66)$$

where we sum freely over all single-particle states α, β, γ og δ.

With this expression we can now verify that the second quantization form of $\hat{H}_I$ in Eq. (66) results in the same matrix between two anti-symmetrized two-particle states as its corresponding coordinate space representation. We have

$$\langle\alpha_1\alpha_2|\hat{H}_I|\beta_1\beta_2\rangle = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle\langle 0|a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1}a^\dagger_{\beta_2}|0\rangle. \qquad (67)$$

Using the commutation relations we get

$$\begin{aligned}
& a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1}a^\dagger_{\beta_2} \\
= \; & a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta(a_\delta\delta_{\gamma\beta_1}a^\dagger_{\beta_2} - a_\delta a^\dagger_{\beta_1}a_\gamma a^\dagger_{\beta_2}) \\
= \; & a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta(\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\gamma\beta_1}a^\dagger_{\beta_2}a_\delta - a_\delta a^\dagger_{\beta_1}\delta_{\gamma\beta_2} + a_\delta a^\dagger_{\beta_1}a^\dagger_{\beta_2}a_\gamma) \\
= \; & a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta(\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\gamma\beta_1}a^\dagger_{\beta_2}a_\delta \\
& -\delta_{\delta\beta_1}\delta_{\gamma\beta_2} + \delta_{\gamma\beta_2}a^\dagger_{\beta_1}a_\delta + a_\delta a^\dagger_{\beta_1}a^\dagger_{\beta_2}a_\gamma) \qquad (68)
\end{aligned}$$

The vacuum expectation value of this product of operators becomes

$$\begin{aligned}
& \langle 0|a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma a^\dagger_{\beta_1}a^\dagger_{\beta_2}|0\rangle \\
= \; & (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\delta\beta_1}\delta_{\gamma\beta_2})\langle 0|a_{\alpha_2}a_{\alpha_1}a^\dagger_\alpha a^\dagger_\beta|0\rangle \\
= \; & (\delta_{\gamma\beta_1}\delta_{\delta\beta_2} - \delta_{\delta\beta_1}\delta_{\gamma\beta_2})(\delta_{\alpha\alpha_1}\delta_{\beta\alpha_2} - \delta_{\beta\alpha_1}\delta_{\alpha\alpha_2}) \qquad (69)
\end{aligned}$$

Insertion of Eq. (69) in Eq. (67) results in

$$\begin{aligned}
\langle\alpha_1\alpha_2|\hat{H}_I|\beta_1\beta_2\rangle = \; & \frac{1}{2}\big[\langle\alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle - \langle\alpha_1\alpha_2|\hat{v}|\beta_2\beta_1\rangle \\
& -\langle\alpha_2\alpha_1|\hat{v}|\beta_1\beta_2\rangle + \langle\alpha_2\alpha_1|\hat{v}|\beta_2\beta_1\rangle\big] \\
= \; & \langle\alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle - \langle\alpha_1\alpha_2|\hat{v}|\beta_2\beta_1\rangle \\
= \; & \langle\alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle_{\rm AS}. \qquad (70)
\end{aligned}$$

The two-body operator can also be expressed in terms of the anti-symmetrized matrix elements we discussed previously as

$$\begin{aligned}
\hat{H}_I = \; & \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
= \; & \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\left[\langle\alpha\beta|\hat{v}|\gamma\delta\rangle - \langle\alpha\beta|\hat{v}|\delta\gamma\rangle\right] a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
= \; & \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle_{\rm AS} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \qquad (71)
\end{aligned}$$

The factors in front of the operator, either $\frac{1}{4}$ or $\frac{1}{2}$ tells whether we use antisymmetrized matrix elements or not.

We can now express the Hamiltonian operator for a many-fermion system in the occupation basis representation as

$$H = \sum_{\alpha,\beta}\langle\alpha|\hat{t} + \hat{u}_{\rm ext}|\beta\rangle a^\dagger_\alpha a_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma. \qquad (72)$$

This is the form we will use in the rest of these lectures, assuming that we work with anti-symmetrized two-body matrix elements.

Particle-hole formalism

Second quantization is a useful and elegant formalism for constructing many-body states and quantum mechanical operators. One can express and translate many physical processes into simple pictures such as Feynman diagrams. Expecation values of many-body states are also easily calculated. However, although the equations are seemingly easy to set up, from a practical point of view, that is the solution of Schroedinger's equation, there is no particular gain. The many-body equation is equally hard to solve, irrespective of representation. The cliche that there is no free lunch brings us down to earth again. Note however that a transformation to a particular basis, for cases where the interaction obeys specific symmetries, can ease the solution of Schroedinger's equation.

But there is at least one important case where second quantization comes to our rescue. It is namely easy to introduce another reference state than the pure vacuum $|0\rangle$, where all single-particle states are active. With many particles present it is often useful to introduce another reference state than the vacuum state$|0\rangle$. We will label this state $|c\rangle$ (c for core) and as we will see it can reduce considerably the complexity and thereby the dimensionality of the many-body problem. It allows us to sum up to infinite order specific many-body correlations. The particle-hole representation is one of these handy representations.

In the original particle representation these states are products of the creation operators $a^\dagger_{\alpha_i}$ acting on the true vacuum $|0\rangle$. Following Eq. (16) we have

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}|0\rangle \tag{73}$$

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}a^\dagger_{\alpha_{n+1}}|0\rangle \tag{74}$$

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}|0\rangle \tag{75}$$

If we use Eq. (73) as our new reference state, we can simplify considerably the representation of this state

$$|c\rangle \equiv |\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}\dots a^\dagger_{\alpha_{n-1}}a^\dagger_{\alpha_n}|0\rangle \tag{76}$$

The new reference states for the $n+1$ and $n-1$ states can then be written as

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\alpha_n\alpha_{n+1}\rangle = (-1)^n a^\dagger_{\alpha_{n+1}}|c\rangle \equiv (-1)^n|\alpha_{n+1}\rangle_c \tag{77}$$

$$|\alpha_1\alpha_2\dots\alpha_{n-1}\rangle = (-1)^{n-1}a_{\alpha_n}|c\rangle \equiv (-1)^{n-1}|\alpha_{n-1}\rangle_c \tag{78}$$

The first state has one additional particle with respect to the new vacuum state $|c\rangle$ and is normally referred to as a one-particle state or one particle added to the many-body reference state. The second state has one particle less than the reference vacuum state $|c\rangle$ and is referred to as a one-hole state. When dealing with a new reference state it is often convenient to introduce new creation and annihilation operators since we have from Eq. (78)

$$a_\alpha|c\rangle \neq 0 \tag{79}$$

since α is contained in $|c\rangle$, while for the true vacuum we have $a_\alpha|0\rangle = 0$ for all α.

The new reference state leads to the definition of new creation and annihilation operators which satisfy the following relations

$$b_\alpha|c\rangle = 0 \tag{80}$$

$$\{b_\alpha^\dagger, b_\beta^\dagger\} = \{b_\alpha, b_\beta\} = 0$$

$$\{b_\alpha^\dagger, b_\beta\} = \delta_{\alpha\beta} \tag{81}$$

We assume also that the new reference state is properly normalized

$$\langle c|c\rangle = 1 \tag{82}$$

The physical interpretation of these new operators is that of so-called quasiparticle states. This means that a state defined by the addition of one extra particle to a reference state $|c\rangle$ may not necesseraly be interpreted as one particle coupled to a core. We define now new creation operators that act on a state α creating a new quasiparticle state

$$b_\alpha^\dagger|c\rangle = \begin{cases} a_\alpha^\dagger|c\rangle = |\alpha\rangle, & \alpha > F \\ \\ a_\alpha|c\rangle = |\alpha^{-1}\rangle, & \alpha \leq F \end{cases} \tag{83}$$

where F is the Fermi level representing the last occupied single-particle orbit of the new reference state $|c\rangle$.

The annihilation is the hermitian conjugate of the creation operator

$$b_\alpha = (b_\alpha^\dagger)^\dagger,$$

resulting in

$$b_\alpha^\dagger = \begin{cases} a_\alpha^\dagger & \alpha > F \\ \\ a_\alpha & \alpha \leq F \end{cases} \qquad b_\alpha = \begin{cases} a_\alpha & \alpha > F \\ \\ a_\alpha^\dagger & \alpha \leq F \end{cases} \tag{84}$$

With the new creation and annihilation operator we can now construct many-body quasiparticle states, with one-particle-one-hole states, two-particle-two-hole states etc in the same fashion as we previously constructed many-particle states. We can write a general particle-hole state as

$$|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \equiv \underbrace{b_{\beta_1}^\dagger b_{\beta_2}^\dagger \dots b_{\beta_{n_p}}^\dagger}_{>F} \underbrace{b_{\gamma_1}^\dagger b_{\gamma_2}^\dagger \dots b_{\gamma_{n_h}}^\dagger}_{\leq F} |c\rangle \tag{85}$$

We can now rewrite our one-body and two-body operators in terms of the new creation and annihilation operators. The number operator becomes

$$\hat{N} = \sum_\alpha a_\alpha^\dagger a_\alpha = \sum_{\alpha>F} b_\alpha^\dagger b_\alpha + n_c - \sum_{\alpha\leq F} b_\alpha^\dagger b_\alpha \tag{86}$$

where n_c is the number of particle in the new vacuum state $|c\rangle$. The action of $\hat{N}$ on a many-body state results in

$$N|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle = (n_p + n_c - n_h)|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \tag{87}$$

Here $n = n_p + n_c - n_h$ is the total number of particles in the quasi-particle state of Eq. (85). Note that $\hat{N}$ counts the total number of particles present

$$N_{qp} = \sum_\alpha b_\alpha^\dagger b_\alpha, \tag{88}$$

gives us the number of quasi-particles as can be seen by computing

$$N_{qp} = |\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle = (n_p + n_h)|\beta_1\beta_2\dots\beta_{n_p}\gamma_1^{-1}\gamma_2^{-1}\dots\gamma_{n_h}^{-1}\rangle \tag{89}$$

where $n_{qp} = n_p + n_h$ is the total number of quasi-particles.

We express the one-body operator $\hat{H}_0$ in terms of the quasi-particle creation and annihilation operators, resulting in

$$\begin{aligned}\hat{H}_0 = & \sum_{\alpha\beta>F}\langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta + \sum_{\alpha>F,\beta\le F}\Big[\langle\alpha|\hat{h}_0|\beta\rangle b_\alpha^\dagger b_\beta^\dagger + \langle\beta|\hat{h}_0|\alpha\rangle b_\beta b_\alpha\Big] \\ + & \sum_{\alpha\le F}\langle\alpha|\hat{h}_0|\alpha\rangle - \sum_{\alpha\beta\le F}\langle\beta|\hat{h}_0|\alpha\rangle b_\alpha^\dagger b_\beta\end{aligned} \tag{90}$$

The first term gives contribution only for particle states, while the last one contributes only for holestates. The second term can create or destroy a set of quasi-particles and the third term is the contribution from the vacuum state $|c\rangle$.

Before we continue with the expressions for the two-body operator, we introduce a nomenclature we will use for the rest of this text. It is inspired by the notation used in quantum chemistry. We reserve the labels $i, j, k, \dots$ for hole states and $a, b, c, \dots$ for states above F, viz. particle states. This means also that we will skip the constraint $\le F$ or $> F$ in the summation symbols. Our operator $\hat{H}_0$ reads now

$$\begin{aligned}\hat{H}_0 = & \sum_{ab}\langle a|\hat{h}|b\rangle b_a^\dagger b_b + \sum_{ai}\Big[\langle a|\hat{h}|i\rangle b_a^\dagger b_i^\dagger + \langle i|\hat{h}|a\rangle b_i b_a\Big] \\ + & \sum_i\langle i|\hat{h}|i\rangle - \sum_{ij}\langle j|\hat{h}|i\rangle b_i^\dagger b_j\end{aligned} \tag{91}$$

The two-particle operator in the particle-hole formalism is more complicated since we have to translate four indices $\alpha\beta\gamma\delta$ to the possible combinations of particle and hole states. When performing the commutator algebra we can regroup the operator in five different terms

$$\hat{H}_I = \hat{H}_I^{(a)} + \hat{H}_I^{(b)} + \hat{H}_I^{(c)} + \hat{H}_I^{(d)} + \hat{H}_I^{(e)} \tag{92}$$

Using anti-symmetrized matrix elements, bthe term $\hat{H}_I^{(a)}$ is

$$\hat{H}_I^{(a)} = \frac{1}{4}\sum_{abcd}\langle ab|\hat{V}|cd\rangle b_a^\dagger b_b^\dagger b_d b_c \tag{93}$$

The next term $\hat{H}_I^{(b)}$ reads

$$\hat{H}_I^{(b)} = \frac{1}{4}\sum_{abci}\Big(\langle ab|\hat{V}|ci\rangle b_a^\dagger b_b^\dagger b_i^\dagger b_c + \langle ai|\hat{V}|cb\rangle b_a^\dagger b_i b_b b_c\Big) \tag{94}$$

This term conserves the number of quasiparticles but creates or removes a three-particle-one-hole state. For $\hat{H}_I^{(c)}$ we have

$$\begin{aligned}\hat{H}_I^{(c)} = \quad & \frac{1}{4}\sum_{abij}\Big(\langle ab|\hat{V}|ij\rangle b_a^\dagger b_b^\dagger b_j^\dagger b_i^\dagger + \langle ij|\hat{V}|ab\rangle b_a b_b b_j b_i\Big) + \\ & \frac{1}{2}\sum_{abij}\langle ai|\hat{V}|bj\rangle b_a^\dagger b_j^\dagger b_b b_i + \frac{1}{2}\sum_{abi}\langle ai|\hat{V}|bi\rangle b_a^\dagger b_b. \end{aligned}\tag{95}$$

The first line stands for the creation of a two-particle-two-hole state, while the second line represents the creation to two one-particle-one-hole pairs while the last term represents a contribution to the particle single-particle energy from the hole states, that is an interaction between the particle states and the hole states within the new vacuum state. The fourth term reads

$$\begin{aligned}\hat{H}_I^{(d)} = \quad & \frac{1}{4}\sum_{aijk}\Big(\langle ai|\hat{V}|jk\rangle b_a^\dagger b_k^\dagger b_j^\dagger b_i + \langle ji|\hat{V}|ak\rangle b_k^\dagger b_j b_i b_a\Big) + \\ & \frac{1}{4}\sum_{aij}\Big(\langle ai|\hat{V}|ji\rangle b_a^\dagger b_j^\dagger + \langle ji|\hat{V}|ai\rangle - \langle ji|\hat{V}|ia\rangle b_j b_a\Big). \end{aligned}\tag{96}$$

The terms in the first line stand for the creation of a particle-hole state interacting with hole states, we will label this as a two-hole-one-particle contribution. The remaining terms are a particle-hole state interacting with the holes in the vacuum state. Finally we have

$$\hat{H}_I^{(e)} = \frac{1}{4}\sum_{ijkl}\langle kl|\hat{V}|ij\rangle b_i^\dagger b_j^\dagger b_l b_k + \frac{1}{2}\sum_{ijk}\langle ij|\hat{V}|kj\rangle b_k^\dagger b_i + \frac{1}{2}\sum_{ij}\langle ij|\hat{V}|ij\rangle \tag{97}$$

The first terms represents the interaction between two holes while the second stands for the interaction between a hole and the remaining holes in the vacuum state. It represents a contribution to single-hole energy to first order. The last term collects all contributions to the energy of the ground state of a closed-shell system arising from hole-hole correlations.

Summarizing and defining a normal-ordered Hamiltonian

$$\Phi_{AS}(\alpha_1,\dots,\alpha_A;x_1,\dots x_A) = \frac{1}{\sqrt{A}}\sum_{\hat{P}}(-1)^P\hat{P}\prod_{i=1}^{A}\psi_{\alpha_i}(x_i),$$

which is equivalent with $|\alpha_1 \dots \alpha_A\rangle = a^\dagger_{\alpha_1} \dots a^\dagger_{\alpha_A}|0\rangle$. We have also

$$a^\dagger_p|0\rangle = |p\rangle, \quad a_p|q\rangle = \delta_{pq}|0\rangle$$

$$\delta_{pq} = \left\{a_p, a^\dagger_q\right\},$$

and

$$0 = \left\{a^\dagger_p, a_q\right\} = \{a_p, a_q\} = \left\{a^\dagger_p, a^\dagger_q\right\}$$
$$|\Phi_0\rangle = |\alpha_1 \dots \alpha_A\rangle, \quad \alpha_1, \dots, \alpha_A \leq \alpha_F$$

$$\left\{a^\dagger_p, a_q\right\} = \delta_{pq}, p, q \leq \alpha_F$$
$$\left\{a_p, a^\dagger_q\right\} = \delta_{pq}, p, q > \alpha_F$$

with $i, j, \dots \leq \alpha_F, \quad a, b, \dots > \alpha_F, \quad p, q, \dots -$ any

$$a_i|\Phi_0\rangle = |\Phi_i\rangle, \qquad a^\dagger_a|\Phi_0\rangle = |\Phi^a\rangle$$

and

$$a^\dagger_i|\Phi_0\rangle = 0 \qquad a_a|\Phi_0\rangle = 0$$

The one-body operator is defined as

$$\hat{F} = \sum_{pq}\langle p|\hat{f}|q\rangle a^\dagger_p a_q$$

while the two-body opreator is defined as

$$\hat{V} = \frac{1}{4}\sum_{pqrs}\langle pq|\hat{v}|rs\rangle_{AS} a^\dagger_p a^\dagger_q a_s a_r$$

where we have defined the antisymmetric matrix elements

$$\langle pq|\hat{v}|rs\rangle_{AS} = \langle pq|\hat{v}|rs\rangle - \langle pq|\hat{v}|sr\rangle.$$

We can also define a three-body operator

$$\hat{V}_3 = \frac{1}{36}\sum_{pqrstu}\langle pqr|\hat{v}_3|stu\rangle_{AS} a^\dagger_p a^\dagger_q a^\dagger_r a_u a_t a_s$$

with the antisymmetrized matrix element

$$\langle pqr|\hat{v}_3|stu\rangle_{AS} = \langle pqr|\hat{v}_3|stu\rangle + \langle pqr|\hat{v}_3|tus\rangle + \langle pqr|\hat{v}_3|ust\rangle - \langle pqr|\hat{v}_3|sut\rangle - \langle pqr|\hat{v}_3|tsu\rangle - \langle pqr|\hat{v}_3|uts\rangle. \tag{98}$$

Hartree-Fock in second quantization and stability of HF solution

We wish now to derive the Hartree-Fock equations using our second-quantized formalism and study the stability of the equations. Our ansatz for the ground state of the system is approximated as (this is our representation of a Slater determinant in second quantization)

$$|\Phi_0\rangle = |c\rangle = a_i^\dagger a_j^\dagger \dots a_l^\dagger |0\rangle.$$

We wish to determine $\hat{u}^{HF}$ so that $E_0^{HF} = \langle c|\hat{H}|c\rangle$ becomes a local minimum.

In our analysis here we will need Thouless' theorem, which states that an arbitrary Slater determinant $|c'\rangle$ which is not orthogonal to a determinant $|c\rangle = \prod_{i=1}^{n} a_{\alpha_i}^\dagger |0\rangle$, can be written as

$$|c'\rangle = exp\left\{\sum_{a>F}\sum_{i\leq F} C_{ai} a_a^\dagger a_i\right\}|c\rangle$$

Let us give a simple proof of Thouless' theorem. The theorem states that we can make a linear combination av particle-hole excitations with respect to a given reference state $|c\rangle$. With this linear combination, we can make a new Slater determinant $|c'\rangle$ which is not orthogonal to $|c\rangle$, that is

$$\langle c|c'\rangle \neq 0.$$

To show this we need some intermediate steps. The exponential product of two operators $\exp\hat{A} \times \exp\hat{B}$ is equal to $\exp(\hat{A}+\hat{B})$ only if the two operators commute, that is

$$[\hat{A}, \hat{B}] = 0.$$

Thouless' theorem

If the operators do not commute, we need to resort to the Baker-Campbell-Hauersdorf. This relation states that

$$\exp\hat{C} = \exp\hat{A}\exp\hat{B},$$

with

$$\hat{C} = \hat{A} + \hat{B} + \frac{1}{2}[\hat{A}, \hat{B}] + \frac{1}{12}[[\hat{A}, \hat{B}], \hat{B}] - \frac{1}{12}[[\hat{A}, \hat{B}], \hat{A}] + \dots$$

From these relations, we note that in our expression for $|c'\rangle$ we have commutators of the type

$$[a_a^\dagger a_i, a_b^\dagger a_j],$$

and it is easy to convince oneself that these commutators, or higher powers thereof, are all zero. This means that we can write out our new representation of a Slater determinant as

$$|c'\rangle = exp\left\{\sum_{a>F}\sum_{i\leq F} C_{ai}a_a^\dagger a_i\right\}|c\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i + \left(\sum_{a>F} C_{ai}a_a^\dagger a_i\right)^2 + \dots\right\}|c\rangle$$

We note that

$$\prod_i \sum_{a>F} C_{ai}a_a^\dagger a_i \sum_{b>F} C_{bi}a_b^\dagger a_i|c\rangle = 0,$$

and all higher-order powers of these combinations of creation and annihilation operators disappear due to the fact that $(a_i)^n|c\rangle = 0$ when $n > 1$. This allows us to rewrite the expression for $|c'\rangle$ as

$$|c'\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i\right\}|c\rangle,$$

which we can rewrite as

$$|c'\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i\right\}|a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_n}^\dagger|0\rangle.$$

The last equation can be written as

$$|c'\rangle = \prod_i\left\{1+\sum_{a>F} C_{ai}a_a^\dagger a_i\right\}|a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_n}^\dagger|0\rangle = \left(1+\sum_{a>F} C_{ai_1}a_a^\dagger a_{i_1}\right)a_{i_1}^\dagger \quad (99)$$

$$\times\left(1+\sum_{a>F} C_{ai_2}a_a^\dagger a_{i_2}\right)a_{i_2}^\dagger \dots|0\rangle = \prod_i\left(a_i^\dagger + \sum_{a>F} C_{ai}a_a^\dagger\right)|0\rangle. \quad (100)$$

New operators

If we define a new creation operator

$$b_i^\dagger = a_i^\dagger + \sum_{a>F} C_{ai}a_a^\dagger, \quad (101)$$

we have

$$|c'\rangle = \prod_i b_i^\dagger|0\rangle = \prod_i\left(a_i^\dagger + \sum_{a>F} C_{ai}a_a^\dagger\right)|0\rangle,$$

meaning that the new representation of the Slater determinant in second quantization, $|c'\rangle$, looks like our previous ones. However, this representation is not general enough since we have a restriction on the sum over single-particle states in Eq. (101). The single-particle states have all to be above the Fermi level. The

question then is whether we can construct a general representation of a Slater determinant with a creation operator

$$\tilde{b}_i^\dagger = \sum_p f_{ip} a_p^\dagger,$$

where f_{ip} is a matrix element of a unitary matrix which transforms our creation and annihilation operators $a^\dagger$ and a to $\tilde{b}^\dagger$ and $\tilde{b}$. These new operators define a new representation of a Slater determinant as

$$|\tilde{c}\rangle = \prod_i \tilde{b}_i^\dagger |0\rangle.$$

Showing that $|\tilde{c}\rangle = |c'\rangle$

We need to show that $|\tilde{c}\rangle = |c'\rangle$. We need also to assume that the new state is not orthogonal to $|c\rangle$, that is $\langle c|\tilde{c}\rangle \neq 0$. From this it follows that

$$\langle c|\tilde{c}\rangle = \langle 0|a_{i_n} \dots a_{i_1} \left(\sum_{p=i_1}^{i_n} f_{i_1 p} a_p^\dagger\right) \left(\sum_{q=i_1}^{i_n} f_{i_2 q} a_q^\dagger\right) \dots \left(\sum_{t=i_1}^{i_n} f_{i_n t} a_t^\dagger\right) |0\rangle,$$

which is nothing but the determinant $det(f_{ip})$ which we can, using the intermediate normalization condition, normalize to one, that is

$$det(f_{ip}) = 1,$$

meaning that f has an inverse defined as (since we are dealing with orthogonal, and in our case unitary as well, transformations)

$$\sum_k f_{ik} f_{kj}^{-1} = \delta_{ij},$$

and

$$\sum_j f_{ij}^{-1} f_{jk} = \delta_{ik}.$$

Using these relations we can then define the linear combination of creation (and annihilation as well) operators as

$$\sum_i f_{ki}^{-1} \tilde{b}_i^\dagger = \sum_i f_{ki}^{-1} \sum_{p=i_1}^{\infty} f_{ip} a_p^\dagger = a_k^\dagger + \sum_i \sum_{p=i_{n+1}}^{\infty} f_{ki}^{-1} f_{ip} a_p^\dagger.$$

Defining

$$c_{kp} = \sum_{i \leq F} f_{ki}^{-1} f_{ip},$$

we can redefine

$$a_k^\dagger + \sum_i \sum_{p=i_{n+1}}^{\infty} f_{ki}^{-1} f_{ip} a_p^\dagger = a_k^\dagger + \sum_{p=i_{n+1}}^{\infty} c_{kp} a_p^\dagger = b_k^\dagger,$$

our starting point. We have shown that our general representation of a Slater determinant

$$|\tilde{c}\rangle = \prod_i \tilde{b}_i^\dagger |0\rangle = |c'\rangle = \prod_i b_i^\dagger |0\rangle,$$

with

$$b_k^\dagger = a_k^\dagger + \sum_{p=i_{n+1}}^{\infty} c_{kp} a_p^\dagger.$$

This means that we can actually write an ansatz for the ground state of the system as a linear combination of terms which contain the ansatz itself $|c\rangle$ with an admixture from an infinity of one-particle-one-hole states. The latter has important consequences when we wish to interpret the Hartree-Fock equations and their stability. We can rewrite the new representation as

$$|c'\rangle = |c\rangle + |\delta c\rangle,$$

where $|\delta c\rangle$ can now be interpreted as a small variation. If we approximate this term with contributions from one-particle-one-hole (*1p-1h*) states only, we arrive at

$$|c'\rangle = \left(1 + \sum_{ai} \delta C_{ai} a_a^\dagger a_i\right) |c\rangle.$$

In our derivation of the Hartree-Fock equations we have shown that

$$\langle \delta c | \hat{H} | c \rangle = 0,$$

which means that we have to satisfy

$$\langle c | \sum_{ai} \delta C_{ai} \left\{ a_a^\dagger a_i \right\} \hat{H} | c \rangle = 0.$$

With this as a background, we are now ready to study the stability of the Hartree-Fock equations.

Hartree-Fock in second quantization and stability of HF solution

The variational condition for deriving the Hartree-Fock equations guarantees only that the expectation value $\langle c|\hat{H}|c\rangle$ has an extreme value, not necessarily a minimum. To figure out whether the extreme value we have found is a minimum, we can use second quantization to analyze our results and find a criterion for the above expectation value to a local minimum. We will use Thouless' theorem and show that

$$\frac{\langle c'|\hat{H}|c'\rangle}{\langle c'|c'\rangle} \geq \langle c|\hat{H}|c\rangle = E_0,$$

with

$$|c'\rangle = |c\rangle + |\delta c\rangle.$$

Using Thouless' theorem we can write out $|c'\rangle$ as

$$|c'\rangle = \exp\left\{\sum_{a>F}\sum_{i\leq F}\delta C_{ai}a_a^\dagger a_i\right\}|c\rangle \tag{102}$$

$$= \left\{1 + \sum_{a>F}\sum_{i\leq F}\delta C_{ai}a_a^\dagger a_i + \frac{1}{2!}\sum_{ab>F}\sum_{ij\leq F}\delta C_{ai}\delta C_{bj}a_a^\dagger a_i a_b^\dagger a_j + \ldots\right\} \tag{103}$$

where the amplitudes δC are small.

The norm of $|c'\rangle$ is given by (using the intermediate normalization condition $\langle c'|c\rangle = 1$)

$$\langle c'|c'\rangle = 1 + \sum_{a>F}\sum_{i\leq F}|\delta C_{ai}|^2 + O(\delta C_{ai}^3).$$

The expectation value for the energy is now given by (using the Hartree-Fock condition)

$$\langle c'|\hat{H}|c'\rangle = \langle c|\hat{H}|c\rangle + \sum_{ab>F}\sum_{ij\leq F}\delta C_{ai}^*\delta C_{bj}\langle c|a_i^\dagger a_a\hat{H}a_b^\dagger a_j|c\rangle +$$

$$\frac{1}{2!}\sum_{ab>F}\sum_{ij\leq F}\delta C_{ai}\delta C_{bj}\langle c|\hat{H}a_a^\dagger a_i a_b^\dagger a_j|c\rangle + \frac{1}{2!}\sum_{ab>F}\sum_{ij\leq F}\delta C_{ai}^*\delta C_{bj}^*\langle c|a_j^\dagger a_b a_i^\dagger a_a\hat{H}|c\rangle + \ldots$$

We have already calculated the second term on the right-hand side of the previous equation

$$\langle c|\left(\{a_i^\dagger a_a\}\hat{H}\{a_b^\dagger a_j\}\right)|c\rangle = \sum_{pq}\sum_{ijab}\delta C_{ai}^*\delta C_{bj}\langle p|\hat{h}_0|q\rangle\langle c|\left(\{a_i^\dagger a_a\}\{a_p^\dagger a_q\}\{a_b^\dagger a_j\}\right)|c\rangle \tag{104}$$

$$+\frac{1}{4}\sum_{pqrs}\sum_{ijab}\delta C_{ai}^*\delta C_{bj}\langle pq|\hat{v}|rs\rangle\langle c|\left(\{a_i^\dagger a_a\}\{a_p^\dagger a_q^\dagger a_s a_r\}\{a_b^\dagger a_j\}\right)|c\rangle, \tag{105}$$

resulting in

$$E_0\sum_{ai}|\delta C_{ai}|^2 + \sum_{ai}|\delta C_{ai}|^2(\varepsilon_a - \varepsilon_i) - \sum_{ijab}\langle aj|\hat{v}|bi\rangle\delta C_{ai}^*\delta C_{bj}.$$

$$\frac{1}{2!}\langle c|\left(\{a_j^\dagger a_b\}\{a_i^\dagger a_a\}\hat{V}_N\right)|c\rangle = \frac{1}{2!}\langle c|\left(\hat{V}_N\{a_a^\dagger a_i\}\{a_b^\dagger a_j\}\right)^\dagger|c\rangle$$

which is nothing but

$$\frac{1}{2!}\langle c|\left(\hat{V}_N\{a_a^\dagger a_i\}\{a_b^\dagger a_j\}\right)|c\rangle^* = \frac{1}{2}\sum_{ijab}(\langle ij|\hat{v}|ab\rangle)^*\delta C_{ai}^*\delta C_{bj}^*$$

or

$$\frac{1}{2}\sum_{ijab}(\langle ab|\hat{v}|ij\rangle)\delta C^*_{ai}\delta C^*_{bj}$$

where we have used the relation

$$\langle a|\hat{A}|b\rangle = (\langle b|\hat{A}^\dagger|a\rangle)^*$$

due to the hermiticity of $\hat{H}$ and $\hat{V}$.

We define two matrix elements

$$A_{ai,bj} = -\langle aj|\hat{v}bi\rangle$$

and

$$B_{ai,bj} = \langle ab|\hat{v}|ij\rangle$$

both being anti-symmetrized.

With these definitions we write out the energy as

$$\langle c'|H|c'\rangle = \left(1 + \sum_{ai}|\delta C_{ai}|^2\right)\langle c|H|c\rangle + \sum_{ai}|\delta C_{ai}|^2(\varepsilon^{HF}_a - \varepsilon^{HF}_i) + \sum_{ijab}A_{ai,bj}\delta C^*_{ai}\delta C_{bj} + \tag{106}$$

$$\frac{1}{2}\sum_{ijab}B^*_{ai,bj}\delta C_{ai}\delta C_{bj} + \frac{1}{2}\sum_{ijab}B_{ai,bj}\delta C^*_{ai}\delta C^*_{bj} + O(\delta C^3_{ai}), \tag{107}$$

which can be rewritten as

$$\langle c'|H|c'\rangle = \left(1 + \sum_{ai}|\delta C_{ai}|^2\right)\langle c|H|c\rangle + \Delta E + O(\delta C^3_{ai}),$$

and skipping higher-order terms we arrived

$$\frac{\langle c'|\hat{H}|c'\rangle}{\langle c'|c'\rangle} = E_0 + \frac{\Delta E}{(1 + \sum_{ai}|\delta C_{ai}|^2)}.$$

We have defined

$$\Delta E = \frac{1}{2}\langle\chi|\hat{M}|\chi\rangle$$

with the vectors

$$\chi = [\delta C \;\; \delta C^*]^T$$

and the matrix

$$\hat{M} = \begin{pmatrix} \Delta + A & B \\ B^* & \Delta + A^* \end{pmatrix},$$

with $\Delta_{ai,bj} = (\varepsilon_a - \varepsilon_i)\delta_{ab}\delta_{ij}$.

The condition

$$\Delta E = \frac{1}{2}\langle\chi|\hat{M}|\chi\rangle \geq 0$$

for an arbitrary vector

$$\chi = [\delta C \;\; \delta C^*]^T$$

means that all eigenvalues of the matrix have to be larger than or equal zero. A necessary (but no sufficient) condition is that the matrix elements (for all ai)

$$(\varepsilon_a - \varepsilon_i)\delta_{ab}\delta_{ij} + A_{ai,bj} \geq 0.$$

This equation can be used as a first test of the stability of the Hartree-Fock equation.

Operators in second quantization

In the build-up of a shell-model or FCI code that is meant to tackle large dimensionalities is the action of the Hamiltonian $\hat{H}$ on a Slater determinant represented in second quantization as

$$|\alpha_1 \dots \alpha_n\rangle = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_n}|0\rangle.$$

The time consuming part stems from the action of the Hamiltonian on the above determinant,

$$\left(\sum_{\alpha\beta}\langle\alpha|t+u|\beta\rangle a^\dagger_\alpha a_\beta + \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma\right) a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_n}|0\rangle.$$

A practically useful way to implement this action is to encode a Slater determinant as a bit pattern.

Assume that we have at our disposal n different single-particle orbits $\alpha_0, \alpha_2, \dots, \alpha_{n-1}$ and that we can distribute among these orbits $N \leq n$ particles.

A Slater determinant can then be coded as an integer of n bits. As an example, if we have $n = 16$ single-particle states $\alpha_0, \alpha_1, \dots, \alpha_{15}$ and $N = 4$ fermions occupying the states α_3, α_6, α_{10} and α_{13} we could write this Slater determinant as

$$\Phi_\Lambda = a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}}|0\rangle.$$

The unoccupied single-particle states have bit value 0 while the occupied ones are represented by bit state 1. In the binary notation we would write this 16 bits long integer as

α_0	α_1	α_2	α_3	α_4	α_5	α_6	α_7	α_8	α_9	α_{10}	α_{11}	α_{12}	α_{13}	α_{14}	α_{15}
0	0	0	1	0	0	1	0	0	0	1	0	0	1	0	0

which translates into the decimal number

$$2^3 + 2^6 + 2^{10} + 2^{13} = 9288.$$

We can thus encode a Slater determinant as a bit pattern.

With N particles that can be distributed over n single-particle states, the total number of Slater determinats (and defining thereby the dimensionality of the system) is

$$\dim(\mathcal{H}) = \left(\begin{array}{c} n \\ N \end{array} \right).$$

The total number of bit patterns is 2^n.

We assume again that we have at our disposal n different single-particle orbits $\alpha_0, \alpha_2, \ldots, \alpha_{n-1}$ and that we can distribute among these orbits $N \leq n$ particles. The ordering among these states is important as it defines the order of the creation operators. We will write the determinant

$$\Phi_\Lambda = a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

in a more compact way as

$$\Phi_{3,6,10,13} = |0001001000100100\rangle.$$

The action of a creation operator is thus

$$a^\dagger_{\alpha_4} \Phi_{3,6,10,13} = a^\dagger_{\alpha_4} |0001001000100100\rangle = a^\dagger_{\alpha_4} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_3} a^\dagger_{\alpha_4} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = -|0001101000100100\rangle.$$

Similarly

$$a^\dagger_{\alpha_6} \Phi_{3,6,10,13} = a^\dagger_{\alpha_6} |0001001000100100\rangle = a^\dagger_{\alpha_6} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_4} (a^\dagger_{\alpha_6})^2 a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = 0!$$

This gives a simple recipe:

- If one of the bits b_j is 1 and we act with a creation operator on this bit, we return a null vector
- If $b_j = 0$, we set it to 1 and return a sign factor $(-1)^l$, where l is the number of bits set before bit j.

Consider the action of $a^\dagger_{\alpha_2}$ on various slater determinants:

$$\begin{array}{lll}
a^\dagger_{\alpha_2} \Phi_{00111} & = a^\dagger_{\alpha_2} |00111\rangle & = 0 \times |00111\rangle \\
a^\dagger_{\alpha_2} \Phi_{01011} & = a^\dagger_{\alpha_2} |01011\rangle & = (-1) \times |01111\rangle \\
a^\dagger_{\alpha_2} \Phi_{01101} & = a^\dagger_{\alpha_2} |01101\rangle & = 0 \times |01101\rangle \\
a^\dagger_{\alpha_2} \Phi_{01110} & = a^\dagger_{\alpha_2} |01110\rangle & = 0 \times |01110\rangle \\
a^\dagger_{\alpha_2} \Phi_{10011} & = a^\dagger_{\alpha_2} |10011\rangle & = (-1) \times |10111\rangle \\
a^\dagger_{\alpha_2} \Phi_{10101} & = a^\dagger_{\alpha_2} |10101\rangle & = 0 \times |10101\rangle \\
a^\dagger_{\alpha_2} \Phi_{10110} & = a^\dagger_{\alpha_2} |10110\rangle & = 0 \times |10110\rangle \\
a^\dagger_{\alpha_2} \Phi_{11001} & = a^\dagger_{\alpha_2} |11001\rangle & = (+1) \times |11101\rangle \\
a^\dagger_{\alpha_2} \Phi_{11010} & = a^\dagger_{\alpha_2} |11010\rangle & = (+1) \times |11110\rangle
\end{array}$$

What is the simplest way to obtain the phase when we act with one annihilation(creation) operator on the given Slater determinant representation?

We have an SD representation

$$\Phi_\Lambda = a^\dagger_{\alpha_0} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

in a more compact way as

$$\Phi_{0,3,6,10,13} = |1001001000100100\rangle.$$

The action of

$$a^\dagger_{\alpha_4} a_{\alpha_0} \Phi_{0,3,6,10,13} = a^\dagger_{\alpha_4} |0001001000100100\rangle = a^\dagger_{\alpha_4} a^\dagger_{\alpha_3} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle,$$

which becomes

$$-a^\dagger_{\alpha_3} a^\dagger_{\alpha_4} a^\dagger_{\alpha_6} a^\dagger_{\alpha_{10}} a^\dagger_{\alpha_{13}} |0\rangle = -|0001101000100100\rangle.$$

The action

$$a_{\alpha_0} \Phi_{0,3,6,10,13} = |0001001000100100\rangle,$$

can be obtained by subtracting the logical sum (AND operation) of $\Phi_{0,3,6,10,13}$ and a word which represents only α_0, that is

$$|1000000000000000\rangle,$$

from $\Phi_{0,3,6,10,13} = |1001001000100100\rangle$.

This operation gives $|0001001000100100\rangle$.

Similarly, we can form $a^\dagger_{\alpha_4} a_{\alpha_0} \Phi_{0,3,6,10,13}$, say, by adding $|0000100000000000\rangle$ to $a_{\alpha_0} \Phi_{0,3,6,10,13}$, first checking that their logical sum is zero in order to make sure that orbital α_4 is not already occupied.

It is trickier however to get the phase $(-1)^l$. One possibility is as follows

- Let S_1 be a word that represents the $1-$bit to be removed and all others set to zero.

In the previous example $S_1 = |1000000000000000\rangle$

- Define S_2 as the similar word that represents the bit to be added, that is in our case

$S_2 = |0000100000000000\rangle$.

- Compute then $S = S_1 - S_2$, which here becomes

$$S = |0111000000000000\rangle$$

- Perform then the logical AND operation of S with the word containing

$$\Phi_{0,3,6,10,13} = |1001001000100100\rangle,$$

which results in $|0001000000000000\rangle$. Counting the number of $1-$bits gives the phase. Here you need however an algorithm for bitcounting. Several efficient ones available.

*

Exercise 1: Relation between basis functions

This exercise serves to convince you about the relation between two different single-particle bases, where one could be our new Hartree-Fock basis and the other a harmonic oscillator basis.

Consider a Slater determinant built up of single-particle orbitals ψ_λ, with $\lambda = 1, 2, \ldots, A$. The unitary transformation

$$\psi_a = \sum_\lambda C_{a\lambda}\phi_\lambda,$$

brings us into the new basis. The new basis has quantum numbers $a = 1, 2, \ldots, A$. Show that the new basis is orthonormal. 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. 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).

Starting with the second quantization representation of the Slater determinant

$$\Phi_0 = \prod_{i=1}^{n} a^\dagger_{\alpha_i}|0\rangle,$$

use Wick's theorem to compute the normalization integral $\langle\Phi_0|\Phi_0\rangle$.

*

Exercise 2: Matrix elements

Calculate the matrix elements

$$\langle\alpha_1\alpha_2|\hat{F}|\alpha_1\alpha_2\rangle$$

and

$$\langle\alpha_1\alpha_2|\hat{G}|\alpha_1\alpha_2\rangle$$

with

$$|\alpha_1\alpha_2\rangle = a^\dagger_{\alpha_1}a^\dagger_{\alpha_2}|0\rangle,$$

$$\hat{F} = \sum_{\alpha\beta}\langle\alpha|\hat{f}|\beta\rangle a^\dagger_\alpha a_\beta,$$

$$\langle\alpha|\hat{f}|\beta\rangle = \int \psi^*_\alpha(x)f(x)\psi_\beta(x)dx,$$

$$\hat{G} = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{g}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma,$$

and

$$\langle\alpha\beta|\hat{g}|\gamma\delta\rangle = \int\int \psi^*_\alpha(x_1)\psi^*_\beta(x_2)g(x_1,x_2)\psi_\gamma(x_1)\psi_\delta(x_2)dx_1dx_2$$

Compare these results with those from exercise 3c).

*

Exercise 3: Normal-ordered one-body operator

Show that the onebody part of the Hamiltonian

$$\hat{H}_0 = \sum_{pq} \langle p|\hat{h}_0|q\rangle a_p^\dagger a_q,$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\hat{H}_0 = \sum_{pq} \langle p|\hat{h}_0|q\rangle \left\{a_p^\dagger a_q\right\} + \sum_i \langle i|\hat{h}_0|i\rangle.$$

Explain the meaning of the various symbols. Which reference vacuum has been used?

*

Exercise 4: Normal-ordered two-body operator

Show that the twobody part of the Hamiltonian

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle a_p^\dagger a_q^\dagger a_s a_r,$$

can be written, using standard annihilation and creation operators, in normal-ordered form as

$$\hat{H}_I = \frac{1}{4}\sum_{pqrs} \langle pq|\hat{v}|rs\rangle \left\{a_p^\dagger a_q^\dagger a_s a_r\right\} + \sum_{pqi} \langle pi|\hat{v}|qi\rangle \left\{a_p^\dagger a_q\right\} + \frac{1}{2}\sum_{ij} \langle ij|\hat{v}|ij\rangle.$$

Explain again the meaning of the various symbols.

This exercise is optional: Derive the normal-ordered form of the threebody part of the Hamiltonian.

$$\hat{H}_3 = \frac{1}{36}\sum_{\substack{pqr\\stu}} \langle pqr|\hat{v}_3|stu\rangle a_p^\dagger a_q^\dagger a_r^\dagger a_u a_t a_s,$$

and specify the contributions to the twobody, onebody and the scalar part.

*

Exercise 5: Matrix elements using the Slater-Condon rule

The aim of this exercise is to set up specific matrix elements that will turn useful when we start our discussions of the nuclear shell model. In particular you will notice, depending on the character of the operator, that many matrix elements will actually be zero.

Consider three N-particle Slater determinants $|\Phi_0\rangle$, $|\Phi_i^a\rangle$ and $|\Phi_{ij}^{ab}\rangle$, where the notation means that Slater determinant $|\Phi_i^a\rangle$ differs from $|\Phi_0\rangle$ by one single-particle state, that is a single-particle state ψ_i is replaced by a single-particle

state ψ_a. It is often interpreted as a so-called one-particle-one-hole excitation. Similarly, the Slater determinant $|\Phi_{ij}^{ab}\rangle$ differs by two single-particle states from $|\Phi_0\rangle$ and is normally thought of as a two-particle-two-hole excitation. We assume also that $|\Phi_0\rangle$ represents our new vacuum reference state and the labels $ijk\ldots$ represent single-particle states below the Fermi level and $abc\ldots$ represent states above the Fermi level, so-called particle states. We define thereafter a general onebody normal-ordered (with respect to the new vacuum state) operator as

$$\hat{F}_N = \sum_{pq} \langle p|f|\beta\rangle \left\{a_p^\dagger a_q\right\},$$

with

$$\langle p|f|q\rangle = \int \psi_p^*(x) f(x) \psi_q(x) dx,$$

and a general normal-ordered two-body operator

$$\hat{G}_N = \frac{1}{4}\sum_{pqrs} \langle pq|g|rs\rangle_{AS} \left\{a_p^\dagger a_q^\dagger a_s a_r\right\},$$

with for example the direct matrix element given as

$$\langle pq|g|rs\rangle = \int\int \psi_p^*(x_1)\psi_q^*(x_2) g(x_1,x_2)\psi_r(x_1)\psi_s(x_2) dx_1 dx_2$$

with g being invariant under the interchange of the coordinates of two particles. The single-particle states ψ_i are not necessarily eigenstates of $\hat{f}$. The curly brackets mean that the operators are normal-ordered with respect to the new vacuum reference state.

How would you write the above Slater determinants in a second quantization formalism, utilizing the fact that we have defined a new reference state?

Use thereafter Wick's theorem to find the expectation values of

$$\langle\Phi_0|\hat{F}_N|\Phi_0\rangle,$$

and

$$\langle\Phi_0\hat{G}_N|\Phi_0\rangle.$$

Find thereafter

$$\langle\Phi_0|\hat{F}_N|\Phi_i^a\rangle,$$

and

$$\langle\Phi_0|\hat{G}_N|\Phi_i^a\rangle,$$

Finally, find

$$\langle\Phi_0|\hat{F}_N|\Phi_{ij}^{ab}\rangle,$$

and

$$\langle\Phi_0|\hat{G}_N|\Phi_{ij}^{ab}\rangle.$$

What happens with the two-body operator if we have a transition probability of the type

$$\langle\Phi_0|\hat{G}_N|\Phi_{ijk}^{abc}\rangle,$$

where the Slater determinant to the right of the operator differs by more than two single-particle states?

*

Exercise 6: Program to set up Slater determinants

Write a program which sets up all possible Slater determinants given $N = 4$ eletrons which can occupy the atomic single-particle states defined by the $1s$, $2s2p$ and $3s3p3d$ shells. How many single-particle states n are there in total? Include the spin degrees of freedom as well.

*

Exercise 7: Using sympy to compute matrix elements

Compute the matrix element

$$\langle \alpha_1\alpha_2\alpha_3|\hat{G}|\alpha_1'\alpha_2'\alpha_3'\rangle,$$

using Wick's theorem and express the two-body operator G in the occupation number (second quantization) representation.

*

Exercise 8: Using sympy to compute matrix elements

The last exercise can be solved using the symbolic Python package called *SymPy*. SymPy is a Python package for general purpose symbolic algebra. There is a physics module with several interesting submodules. Among these, the submodule called *secondquant*, contains several functionalities that allow us to test our algebraic manipulations using Wick's theorem and operators for second quantization.

```
from sympy import *
from sympy.physics.secondquant import *

i, j = symbols('i,j', below_fermi=True)
a, b = symbols('a,b', above_fermi=True)
p, q = symbols('p,q')
print simplify(wicks(Fd(i)*F(a)*Fd(p)*F(q)*Fd(b)*F(j), keep_only_fully_contracted=True))
```

The code defines single-particle states above and below the Fermi level, in addition to the genereal symbols pq which can refer to any type of state below or above the Fermi level. Wick's theorem is implemented between the creation and annihilation operators Fd and F, respectively. Using the simplify option, one can lump together several Kronecker-δ functions.

*

Exercise 9: Using sympy to compute matrix elements

We can expand the above Python code by defining one-body and two-body operators using the following SymPy code

```
# This code sets up a two-body Hamiltonian for fermions
from sympy import symbols, latex, WildFunction, collect, Rational
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO
```

```
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
f = AntiSymmetricTensor('f',(p,),(q,))
pr = NO((Fd(p)*F(q)))
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = NO(Fd(p)*Fd(q)*F(s)*F(r))
Hamiltonian=f*pr + Rational(1)/Rational(4)*v*pqsr
print "Hamiltonian defined as:", latex(Hamiltonian)
```

Here we have used the *AntiSymmetricTensor* functionality, together with normal-ordering defined by the *NO* function. Using the *latex* option, this program produces the following output

$$f^p_q \left\{a^\dagger_p a_q\right\} - \frac{1}{4} v^{qp}_{sr} \left\{a^\dagger_p a^\dagger_q a_r a_s\right\}$$

*

Exercise 10: Using sympy to compute matrix elements

We can now use this code to compute the matrix elements between two two-body Slater determinants using Wick's theorem.

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO, e
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
f = AntiSymmetricTensor('f',(p,),(q,))
pr = NO((Fd(p)*F(q)))
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = NO(Fd(p)*Fd(q)*F(s)*F(r))
Hamiltonian=f*pr + Rational(1)/Rational(4)*v*pqsr
c,d = symbols('c, d',above_fermi=True)
a,b = symbols('a, b',above_fermi=True)

expression = wicks(F(b)*F(a)*Hamiltonian*Fd(c)*Fd(d),keep_only_fully_contracted=True, simplify_kro
expression = evaluate_deltas(expression)
expression = simplify(expression)
print "Hamiltonian defined as:", latex(expression)
```

The result is as expected,

$$\delta_{ac} f^b_d - \delta_{ad} f^b_c - \delta_{bc} f^a_d + \delta_{bd} f^a_c + v^{ab}_{cd}.$$

*

Exercise 11: Using sympy to compute matrix elements

We can continue along these lines and define a normal-ordered Hamiltonian with respect to a given reference state. In our first step we just define the Hamiltonian

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO, e
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
```

```
f = AntiSymmetricTensor('f',(p,),(q,))
pr = Fd(p)*F(q)
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = Fd(p)*Fd(q)*F(s)*F(r)
#define the Hamiltonian
Hamiltonian = f*pr + Rational(1)/Rational(4)*v*pqsr
#define indices for states above and below the Fermi level
index_rule = {
     'below':  'kl',
     'above':  'cd',
     'general': 'pqrs'
     }
Hnormal = substitute_dummies(Hamiltonian,new_indices=True, pretty_indices=index_rule)
print "Hamiltonian defined as:", latex(Hnormal)
```

which results in

$$f_p^q a_q^\dagger a_p + \frac{1}{4} v_{qp}^{sr} a_s^\dagger a_r^\dagger a_p a_q$$

*

Exercise 12: Using sympy to compute matrix elements

In our next step we define the reference energy E_0 and redefine the Hamiltonian by subtracting the reference energy and collecting the coefficients for all normal-ordered products (given by the *NO* function).

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO, e
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)
f = AntiSymmetricTensor('f',(p,),(q,))
pr = Fd(p)*F(q)
v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = Fd(p)*Fd(q)*F(s)*F(r)
#define the Hamiltonian
Hamiltonian=f*pr + Rational(1)/Rational(4)*v*pqsr
#define indices for states above and below the Fermi level
index_rule = {
     'below':  'kl',
     'above':  'cd',
     'general': 'pqrs'
     }
Hnormal = substitute_dummies(Hamiltonian,new_indices=True, pretty_indices=index_rule)
E0 = wicks(Hnormal,keep_only_fully_contracted=True)
Hnormal = Hnormal-E0
w = WildFunction('w')
Hnormal = collect(Hnormal, NO(w))
Hnormal = evaluate_deltas(Hnormal)
print latex(Hnormal)
```

which gives us

$$-f_i^i + f_p^q a_q^\dagger a_p - \frac{1}{4} v_{ii}^{ii} - \frac{1}{4} v_{ii}^{ii} + \frac{1}{4} v_{qp}^{sr} a_r^\dagger a_s^\dagger a_q a_p,$$

again as expected, with the reference energy to be subtracted.

*

Exercise 13: Using sympy to compute matrix elements

We can now go back to exercise 7 and define the Hamiltonian and the second-quantized representation of a three-body Slater determinant.

```
from sympy import symbols, latex, WildFunction, collect, Rational, simplify
from sympy.physics.secondquant import F, Fd, wicks, AntiSymmetricTensor, substitute_dummies, NO, e
# setup hamiltonian
p,q,r,s = symbols('p q r s',dummy=True)

v = AntiSymmetricTensor('v',(p,q),(r,s))
pqsr = NO(Fd(p)*Fd(q)*F(s)*F(r))
Hamiltonian=Rational(1)/Rational(4)*v*pqsr
a,b,c,d,e,f = symbols('a,b, c, d, e, f',above_fermi=True)

expression = wicks(F(c)*F(b)*F(a)*Hamiltonian*Fd(d)*Fd(e)*Fd(f),keep_only_fully_contracted=True, s
expression = evaluate_deltas(expression)
expression = simplify(expression)
print latex(expression)
```

resulting in nine terms (as expected),

$$-\delta_{ad}v^{cb}_{ef} - \delta_{ae}v^{cb}_{fd} + \delta_{af}v^{cb}_{ed} - \delta_{bd}v^{ac}_{ef} - \delta_{be}v^{ac}_{fd} + \delta_{bf}v^{ac}_{ed} + \delta_{cd}v^{ab}_{ef} + \delta_{ce}v^{ab}_{fd} - \delta_{cf}v^{ab}_{ed}$$

*

Exercise 14: Diagrammatic representation of Hartree-Fock equations

What is the diagrammatic representation of the HF equation?

$$-\langle\alpha_k|u^{HF}|\alpha_i\rangle + \sum_{j=1}^{n}[\langle\alpha_k\alpha_j|\hat{v}|\alpha_i\alpha_j\rangle - \langle\alpha_k\alpha_j|v|\alpha_j\alpha_i\rangle] = 0$$

(Represent $(-u^{HF})$ by the symbol $---$X .)

*

Exercise 15: Derivation of Hartree-Fock equations

Consider the ground state $|\Phi\rangle$ of a bound many-particle system of fermions. Assume that we remove one particle from the single-particle state λ and that our system ends in a new state $|\Phi_n\rangle$. Define the energy needed to remove this particle as

$$E_\lambda = \sum_n |\langle\Phi_n|a_\lambda|\Phi\rangle|^2(E_0 - E_n),$$

where E_0 and E_n are the ground state energies of the states $|\Phi\rangle$ and $|\Phi_n\rangle$, respectively.

- Show that

$$E_\lambda = \langle\Phi|a^\dagger_\lambda\,[a_\lambda, H]\,|\Phi\rangle,$$

where H is the Hamiltonian of this system.

- If we assume that Φ is the Hartree-Fock result, find the

relation between E_λ and the single-particle energy ε_λ for states $\lambda \leq F$ and $\lambda > F$, with

$$\varepsilon_\lambda = \langle \lambda | \hat{t} + \hat{u} | \lambda \rangle,$$

and

$$\langle \lambda | \hat{u} | \lambda \rangle = \sum_{\beta \leq F} \langle \lambda \beta | \hat{v} | \lambda \beta \rangle.$$

We have assumed an antisymmetrized matrix element here. Discuss the result.

The Hamiltonian operator is defined as

$$H = \sum_{\alpha\beta} \langle \alpha | \hat{t} | \beta \rangle a_\alpha^\dagger a_\beta + \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma.$$