

Week 35: Ansatzes for fermions and bosons and second quantization

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Week 35

- ▶ Topics to be covered
 1. Thursday: Fermion and Boson state functions and computation of expectation values in first quantization, continuation from last week (see slides from last week)
 2. Video of lecture at https://youtu.be/ND3nkwTq_w0
 3. Whiteboard notes at <https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/HandwrittenNotes/2025/FYS4480August28.pdf>
 4. Friday: Second quantization
 5. Video of lecture at <https://youtu.be/XluU1E4uxjU>
 6. Whiteboard notes at <https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/HandwrittenNotes/2025/FYS4480August29.pdf>
- ▶ Lecture Material: These slides, slides from week 34 and Szabo and Ostlund chapters 1 and 2.
- ▶ Second exercise set

Definitions and second quantization

We introduce the time-independent operators a_{α}^{\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_{α}^{\dagger}

$$a_{\alpha}^{\dagger}|0\rangle \equiv |\alpha\rangle, \quad (1)$$

and

$$a_{\alpha}^{\dagger}|\alpha_1 \dots \alpha_n\rangle_{\text{AS}} \equiv |\alpha\alpha_1 \dots \alpha_n\rangle_{\text{AS}} \quad (2)$$

Second quantization

In Eq. (1) the operator a_{α}^{\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. (2) a_{α}^{\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.

$$|\alpha_1 \dots \alpha_n\rangle_{\text{AS}} = a_{\alpha_1}^{\dagger} a_{\alpha_2}^{\dagger} \dots a_{\alpha_n}^{\dagger} |0\rangle \quad (3)$$

Commutation rules

It is easy to derive the commutation and anticommutation rules for the fermionic creation operators a_{α}^{\dagger} . Using the antisymmetry of the states (3)

$$|\alpha_1 \dots \alpha_i \dots \alpha_k \dots \alpha_n\rangle_{AS} = -|\alpha_1 \dots \alpha_k \dots \alpha_i \dots \alpha_n\rangle_{AS} \quad (4)$$

we obtain

$$a_{\alpha_i}^{\dagger} a_{\alpha_k}^{\dagger} = -a_{\alpha_k}^{\dagger} a_{\alpha_i}^{\dagger} \quad (5)$$

More on commutation rules

Using the Pauli principle

$$|\alpha_1 \dots \alpha_i \dots \alpha_i \dots \alpha_n\rangle_{\text{AS}} = 0 \quad (6)$$

it follows that

$$a_{\alpha_i}^\dagger a_{\alpha_i}^\dagger = 0. \quad (7)$$

If we combine Eqs. (5) and (7), we obtain the well-known anti-commutation rule

$$a_\alpha^\dagger a_\beta^\dagger + a_\beta^\dagger a_\alpha^\dagger \equiv \{a_\alpha^\dagger, a_\beta^\dagger\} = 0 \quad (8)$$

Hermitian conjugate

The hermitian conjugate of a_{α}^{\dagger} is

$$a_{\alpha} = (a_{\alpha}^{\dagger})^{\dagger} \quad (9)$$

If we take the hermitian conjugate of Eq. (8), we arrive at

$$\{a_{\alpha}, a_{\beta}\} = 0 \quad (10)$$

Physical interpretation

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

$$\langle\alpha_1\alpha_2\ldots\alpha_n|a_\alpha|\alpha'_1\alpha'_2\ldots\alpha'_m\rangle \quad (11)$$

where both sides are antisymmetric.

Two specific cases

We distinguish between two cases. The first (1) is when $\alpha \in \{\alpha_i\}$. Using the Pauli principle of Eq. (6) it follows

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha = 0 \quad (12)$$

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

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha = \langle \alpha \alpha_1 \alpha_2 \dots \alpha_n | \quad (13)$$

More derivations

Eq. (13) holds for case (1) since the lefthand side is zero due to the Pauli principle. We write Eq. (11) as

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha | \alpha'_1 \alpha'_2 \dots \alpha'_m \rangle = \langle \alpha_1 \alpha_2 \dots \alpha_n | \alpha \alpha'_1 \alpha'_2 \dots \alpha'_m \rangle \quad (14)$$

Here we must have $m = n + 1$ if Eq. (14) has to be trivially different from zero.

Even and odd permutations

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

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha | \alpha'_1 \alpha'_2 \dots \alpha'_{n+1} \rangle = 0 \quad (15)$$

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

$$a_\alpha \underbrace{|\alpha'_1 \alpha'_2 \dots \alpha'_{n+1}\rangle}_{\neq \alpha} = 0 \quad (16)$$

and in particular

$$a_\alpha |0\rangle = 0 \quad (17)$$

Even and odd permutations

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

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha | \alpha \alpha_1 \alpha_2 \dots \alpha_n \rangle = 1 \quad (18)$$

and thus

$$a_\alpha | \alpha \alpha_1 \alpha_2 \dots \alpha_n \rangle = | \alpha_1 \alpha_2 \dots \alpha_n \rangle \quad (19)$$

Annihilation operators

The action of the operator a_α from the left on a state vector is 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_α^\dagger and a_β .

Action of anti-commutator

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

$$\begin{aligned} a_\alpha^\dagger a_\alpha \underbrace{|\alpha_1 \alpha_2 \dots \alpha_n\rangle}_{\neq \alpha} &= 0 \\ a_\alpha a_\alpha^\dagger \underbrace{|\alpha_1 \alpha_2 \dots \alpha_n\rangle}_{\neq \alpha} &= a_\alpha \underbrace{|\alpha \alpha_1 \alpha_2 \dots \alpha_n\rangle}_{\neq \alpha} = \underbrace{|\alpha_1 \alpha_2 \dots \alpha_n\rangle}_{\neq \alpha} \end{aligned} \quad (20)$$

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

Anti-commutation rule for Fermions

If it is present we arrive at

$$\begin{aligned}a_{\alpha}^{\dagger}a_{\alpha}|\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle &= a_{\alpha}^{\dagger}a_{\alpha}(-1)^k|\alpha\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle \\&= (-1)^k|\alpha\alpha_1\alpha_2\ldots\alpha_{n-1}\rangle = |\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle \\a_{\alpha}a_{\alpha}^{\dagger}|\alpha_1\alpha_2\ldots\alpha_k\alpha\alpha_{k+1}\ldots\alpha_{n-1}\rangle &= 0\end{aligned}\tag{21}$$

From Eqs. (20) and (21) we arrive at

$$\{a_{\alpha}^{\dagger}, a_{\alpha}\} = a_{\alpha}^{\dagger}a_{\alpha} + a_{\alpha}a_{\alpha}^{\dagger} = 1\tag{22}$$

Three possible outcomes

The action of $\{a_\alpha^\dagger, a_\beta\}$, 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

$$\begin{aligned}a_\alpha^\dagger a_\beta |\alpha \beta \alpha_1 \alpha_2 \dots \alpha_{n-2}\rangle &= 0 \\a_\beta a_\alpha^\dagger |\alpha \beta \alpha_1 \alpha_2 \dots \alpha_{n-2}\rangle &= 0\end{aligned}\tag{23}$$

Second case

The second case gives

$$\begin{aligned} a_{\alpha}^{\dagger} a_{\beta} |\beta \underbrace{\alpha_1 \alpha_2 \dots \alpha_{n-1}}_{\neq \alpha} \rangle &= |\alpha \underbrace{\alpha_1 \alpha_2 \dots \alpha_{n-1}}_{\neq \alpha} \rangle \\ a_{\beta} a_{\alpha}^{\dagger} |\beta \underbrace{\alpha_1 \alpha_2 \dots \alpha_{n-1}}_{\neq \alpha} \rangle &= a_{\beta} |\alpha \beta \underbrace{\alpha_1 \alpha_2 \dots \alpha_{n-1}}_{\neq \alpha} \rangle \\ &= - |\alpha \underbrace{\alpha_1 \alpha_2 \dots \alpha_{n-1}}_{\neq \alpha} \rangle \end{aligned} \quad (24)$$

Third case

Finally if the state vector does not contain α and β

$$\begin{aligned} a_{\alpha}^{\dagger} a_{\beta} | \underbrace{\alpha_1 \alpha_2 \dots \alpha_n}_{\neq \alpha, \beta} \rangle &= 0 \\ a_{\beta} a_{\alpha}^{\dagger} | \underbrace{\alpha_1 \alpha_2 \dots \alpha_n}_{\neq \alpha, \beta} \rangle &= a_{\beta} | \alpha \underbrace{\alpha_1 \alpha_2 \dots \alpha_n}_{\neq \alpha, \beta} \rangle = 0 \end{aligned} \quad (25)$$

For all three cases we have

$$\{a_{\alpha}^{\dagger}, a_{\beta}\} = a_{\alpha}^{\dagger} a_{\beta} + a_{\beta} a_{\alpha}^{\dagger} = 0, \quad \alpha \neq \beta \quad (26)$$

Summarizing

We can summarize our findings in Eqs. (22) and (26) as

$$\{a_{\alpha}^{\dagger}, a_{\beta}\} = \delta_{\alpha\beta} \quad (27)$$

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

Properties of creation and annihilation operators

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

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

and

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

from which follows

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

Hermitian conjugate or just adjoint

The hermitian conjugate has the following properties

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

Finally we found

$$a_{\alpha} \underbrace{|\alpha'_1 \alpha'_2 \dots \alpha'_{n+1}\rangle}_{\neq \alpha} = 0, \quad \text{in particular } a_{\alpha} |0\rangle = 0,$$

and

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

and the corresponding commutator algebra

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

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_{α}^{\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 .

Getting started

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

$$a_{\alpha}^{\dagger}a_{\alpha}|\alpha_1\alpha_2\ldots\alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ |\alpha_1\alpha_2\ldots\alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \quad (28)$$

Summing over all possible one-particle states we arrive at

$$\left(\sum_{\alpha} a_{\alpha}^{\dagger}a_{\alpha}\right)|\alpha_1\alpha_2\ldots\alpha_n\rangle = n|\alpha_1\alpha_2\ldots\alpha_n\rangle \quad (29)$$

The number operator

The operator

$$\hat{N} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \quad (30)$$

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.

Preserving the number of particles

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

$$\hat{H}_0 = \sum_i \hat{h}_0(x_i) \quad (31)$$

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

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

One-body operator in second quantization

Defining

$$\hat{h}_0(x_i)\psi_{\alpha_i}(x_i) = \sum_{\alpha'_k} \psi_{\alpha'_k}(x_i) \langle \alpha'_k | \hat{h}_0 | \alpha_k \rangle \quad (32)$$

we can easily evaluate the action of \hat{H}_0 on each product of one-particle functions in Slater determinant. From Eq. (32) we obtain the following result without permuting any particle pair

$$\begin{aligned} & \left(\sum_i \hat{h}_0(x_i) \right) \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ = & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle \psi_{\alpha'_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ + & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle \psi_{\alpha_1}(x_1) \psi_{\alpha'_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ + & \dots \\ + & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha'_n}(x_n) \end{aligned} \quad (33)$$

Interchange particles 1 and 2

If we interchange particles 1 and 2 we obtain

$$\begin{aligned} & \left(\sum_i \hat{h}_0(x_i) \right) \psi_{\alpha_1}(x_2) \psi_{\alpha_1}(x_2) \dots \psi_{\alpha_n}(x_n) \\ = & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle \psi_{\alpha_1}(x_2) \psi_{\alpha'_2}(x_1) \dots \psi_{\alpha_n}(x_n) \\ + & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle \psi_{\alpha'_1}(x_2) \psi_{\alpha_2}(x_1) \dots \psi_{\alpha_n}(x_n) \\ + & \dots \\ + & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle \psi_{\alpha_1}(x_2) \psi_{\alpha_1}(x_2) \dots \psi_{\alpha'_n}(x_n) \end{aligned} \quad (34)$$

Including all possible permutations

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

$$\begin{aligned}\hat{H}_0|\alpha_1, \alpha_2, \dots, \alpha_n\rangle = & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle |\alpha'_1 \alpha_2 \dots \alpha_n\rangle \\ & + \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle |\alpha_1 \alpha'_2 \dots \alpha_n\rangle \\ & + \dots \\ & + \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle |\alpha_1 \alpha_2 \dots \alpha'_n\rangle\end{aligned}\quad (35)$$

More operations

In Eq. (35) we have expressed the action of the one-body operator of Eq. (31) 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

$$|\alpha_1 \alpha_2 \dots \alpha'_k \dots \alpha_n\rangle = a_{\alpha'_k}^\dagger a_{\alpha_k} |\alpha_1 \alpha_2 \dots \alpha_k \dots \alpha_n\rangle \quad (36)$$

Inserting this in the right-hand side of Eq. (35) results in

$$\begin{aligned} \hat{H}_0 |\alpha_1 \alpha_2 \dots \alpha_n\rangle &= \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle a_{\alpha'_1}^\dagger a_{\alpha_1} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\ &+ \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle a_{\alpha'_2}^\dagger a_{\alpha_2} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\ &+ \dots \\ &+ \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle a_{\alpha'_n}^\dagger a_{\alpha_n} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\ &= \sum_{\alpha \beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_\alpha^\dagger a_\beta |\alpha_1 \alpha_2 \dots \alpha_n\rangle \quad (37) \end{aligned}$$

Final expression for the one-body operator

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

$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} \quad (38)$$

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

The operator \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 $\langle \alpha | \hat{h}_0 | \beta \rangle$.

Applying the new expression

It is instructive to verify Eq. (38) by computing the expectation value of \hat{H}_0 between two single-particle states

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \langle 0 | a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} | 0 \rangle \quad (39)$$

Explicit results

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

$$a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} = (\delta_{\alpha\alpha_1} - a_{\alpha}^{\dagger} a_{\alpha_1})(\delta_{\beta\alpha_2} - a_{\alpha_2}^{\dagger} a_{\beta}), \quad (40)$$

which results in

$$\langle 0 | a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} | 0 \rangle = \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} \quad (41)$$

and

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} = \langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle \quad (42)$$

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

$$\hat{H}_I = \sum_{i < j} V(x_i, x_j) \quad (43)$$

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

$$V(x_i, x_j) \psi_{\alpha_k}(x_i) \psi_{\alpha_l}(x_j) = \sum_{\alpha'_k \alpha'_l} \psi'_{\alpha'_k}(x_i) \psi'_{\alpha'_l}(x_j) \langle \alpha'_k \alpha'_l | \hat{V} | \alpha_k \alpha_l \rangle \quad (44)$$

More operations

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

$$\begin{aligned}
 & \left(\sum_{i < j} V(x_i, x_j) \right) \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \ldots \psi_{\alpha_n}(x_n) \\
 = & \sum_{\alpha'_1 \alpha'_2} \langle \alpha'_1 \alpha'_2 | \hat{V} | \alpha_1 \alpha_2 \rangle \psi'_{\alpha'_1}(x_1) \psi'_{\alpha'_2}(x_2) \ldots \psi_{\alpha_n}(x_n) \\
 + & \hspace{15em} \ldots \\
 + & \sum_{\alpha'_1 \alpha'_n} \langle \alpha'_1 \alpha'_n | \hat{V} | \alpha_1 \alpha_n \rangle \psi'_{\alpha'_1}(x_1) \psi_{\alpha_2}(x_2) \ldots \psi'_{\alpha'_n}(x_n) \\
 + & \hspace{15em} \ldots \\
 + & \sum_{\alpha'_2 \alpha'_n} \langle \alpha'_2 \alpha'_n | \hat{V} | \alpha_2 \alpha_n \rangle \psi_{\alpha_1}(x_1) \psi'_{\alpha'_2}(x_2) \ldots \psi'_{\alpha'_n}(x_n) \\
 + & \hspace{15em} \ldots \hspace{1em} (45)
 \end{aligned}$$

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

Summing over all terms

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

$$\begin{aligned} H_I |\alpha_1 \alpha_2 \dots \alpha_n\rangle = & \sum_{\alpha'_1, \alpha'_2} \langle \alpha'_1 \alpha'_2 | \hat{V} | \alpha_1 \alpha_2 \rangle | \alpha'_1 \alpha'_2 \dots \alpha_n \rangle \\ & + \dots \\ & + \sum_{\alpha'_1, \alpha'_n} \langle \alpha'_1 \alpha'_n | \hat{V} | \alpha_1 \alpha_n \rangle | \alpha'_1 \alpha_2 \dots \alpha'_n \rangle \\ & + \dots \\ & + \sum_{\alpha'_2, \alpha'_n} \langle \alpha'_2 \alpha'_n | \hat{V} | \alpha_2 \alpha_n \rangle | \alpha_1 \alpha'_2 \dots \alpha'_n \rangle \\ & + \dots \end{aligned} \quad (46)$$

Introducing second quantization

We introduce second quantization via the relation

$$\begin{aligned}
 & a_{\alpha'_k}^\dagger a_{\alpha'_l}^\dagger a_{\alpha_l} a_{\alpha_k} |\alpha_1 \alpha_2 \dots \alpha_k \dots \alpha_l \dots \alpha_n\rangle \\
 = & (-1)^{k-1} (-1)^{l-2} a_{\alpha'_k}^\dagger a_{\alpha'_l}^\dagger a_{\alpha_l} a_{\alpha_k} |\alpha_k \alpha_l \underbrace{\alpha_1 \alpha_2 \dots \alpha_n}_{\neq \alpha_k, \alpha_l}\rangle \\
 = & (-1)^{k-1} (-1)^{l-2} |\alpha'_k \alpha'_l \underbrace{\alpha_1 \alpha_2 \dots \alpha_n}_{\neq \alpha'_k, \alpha'_l}\rangle \\
 = & |\alpha_1 \alpha_2 \dots \alpha'_k \dots \alpha'_l \dots \alpha_n\rangle \quad (47)
 \end{aligned}$$

Inserting back

Inserting this in (46) gives

$$\begin{aligned}
 H_I |\alpha_1 \alpha_2 \dots \alpha_n\rangle &= \sum_{\alpha'_1, \alpha'_2} \langle \alpha'_1 \alpha'_2 | \hat{V} | \alpha_1 \alpha_2 \rangle a_{\alpha'_1}^\dagger a_{\alpha'_2}^\dagger a_{\alpha_2} a_{\alpha_1} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\
 &+ \dots \\
 &= \sum_{\alpha'_1, \alpha'_n} \langle \alpha'_1 \alpha'_n | \hat{V} | \alpha_1 \alpha_n \rangle a_{\alpha'_1}^\dagger a_{\alpha'_n}^\dagger a_{\alpha_n} a_{\alpha_1} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\
 &+ \dots \\
 &= \sum_{\alpha'_2, \alpha'_n} \langle \alpha'_2 \alpha'_n | \hat{V} | \alpha_2 \alpha_n \rangle a_{\alpha'_2}^\dagger a_{\alpha'_n}^\dagger a_{\alpha_n} a_{\alpha_2} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\
 &+ \dots \\
 &= \sum_{\alpha, \beta, \gamma, \delta}^I \langle \alpha \beta | \hat{V} | \gamma \delta \rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma |\alpha_1 \alpha_2 \dots \alpha_n\rangle
 \end{aligned}
 \tag{48}$$

Removing restrictions

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

$$\langle \alpha\beta | \hat{v} | \gamma\delta \rangle = \langle \beta\alpha | \hat{v} | \delta\gamma \rangle \quad (49)$$

we get

$$\sum_{\alpha\beta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} = \sum_{\alpha\beta} \langle \beta\alpha | \hat{v} | \delta\gamma \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \quad (50)$$

$$= \sum_{\alpha\beta} \langle \beta\alpha | \hat{v} | \delta\gamma \rangle a_{\beta}^{\dagger} a_{\alpha}^{\dagger} a_{\gamma} a_{\delta} \quad (51)$$

where we have used the anti-commutation rules.

Changing summation indices

Changing the summation indices α and β in (51) we obtain

$$\sum_{\alpha\beta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} = \sum_{\alpha\beta} \langle \alpha\beta | \hat{v} | \delta\gamma \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} \quad (52)$$

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

$$\hat{H}_I = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \quad (53)$$

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

Using the new operator expressions

With this expression we can now verify that the second quantization form of \hat{H}_I in Eq. (53) results in the same matrix between two anti-symmetrized two-particle states as its corresponding coordinate space representation. We have

$$\langle \alpha_1 \alpha_2 | \hat{H}_I | \beta_1 \beta_2 \rangle = \frac{1}{2} \sum_{\alpha \beta \gamma \delta} \langle \alpha \beta | \hat{v} | \gamma \delta \rangle \langle 0 | a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} | 0 \rangle. \quad (54)$$

Two-body state

Using the commutation relations we get

$$\begin{aligned} & a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} \\ = & a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} (a_{\delta} \delta_{\gamma\beta_1} a_{\beta_2}^{\dagger} - a_{\delta} a_{\beta_1}^{\dagger} a_{\gamma} a_{\beta_2}^{\dagger}) \\ = & a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\gamma\beta_1} a_{\beta_2}^{\dagger} a_{\delta} - a_{\delta} a_{\beta_1}^{\dagger} \delta_{\gamma\beta_2} + a_{\delta} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} a_{\gamma}) \\ = & a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\gamma\beta_1} a_{\beta_2}^{\dagger} a_{\delta} \\ & - \delta_{\delta\beta_1} \delta_{\gamma\beta_2} + \delta_{\gamma\beta_2} a_{\beta_1}^{\dagger} a_{\delta} + a_{\delta} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} a_{\gamma}) \end{aligned} \quad (55)$$

Expectation value

The vacuum expectation value of this product of operators becomes

$$\begin{aligned} & \langle 0 | a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} | 0 \rangle \\ = & (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\delta\beta_1} \delta_{\gamma\beta_2}) \langle 0 | a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} | 0 \rangle \\ = & (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\delta\beta_1} \delta_{\gamma\beta_2}) (\delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} - \delta_{\beta\alpha_1} \delta_{\alpha\alpha_2}) \quad (56) \end{aligned}$$

Final expression

Insertion of Eq. (56) in Eq. (54) results in

$$\begin{aligned}\langle\alpha_1\alpha_2|\hat{H}_I|\beta_1\beta_2\rangle &= \frac{1}{2}\left[\langle\alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle - \langle\alpha_1\alpha_2|\hat{v}|\beta_2\beta_1\rangle\right. \\ &\quad \left.- \langle\alpha_2\alpha_1|\hat{v}|\beta_1\beta_2\rangle + \langle\alpha_2\alpha_1|\hat{v}|\beta_2\beta_1\rangle\right] \\ &= \langle\alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle - \langle\alpha_1\alpha_2|\hat{v}|\beta_2\beta_1\rangle \\ &= \langle\alpha_1\alpha_2|\hat{v}|\beta_1\beta_2\rangle_{\text{AS}}.\end{aligned}\quad (57)$$

Rewriting the two-body operator

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

$$\begin{aligned}\hat{H}_I &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \\ &= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} [\langle \alpha\beta | \hat{v} | \gamma\delta \rangle - \langle \alpha\beta | \hat{v} | \delta\gamma \rangle] a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \\ &= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{AS} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \quad (58)\end{aligned}$$

Antisymmetrized matrix elements

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

$$H = \sum_{\alpha, \beta} \langle \alpha | \hat{t} + \hat{u}_{\text{ext}} | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{4} \sum_{\alpha \beta \gamma \delta} \langle \alpha \beta | \hat{v} | \gamma \delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}. \quad (59)$$

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