

Week 36: Operators in second quantization, computation of expectation values and Wick's theorem

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Week 36

- Topics to be covered
 1. Thursday: Second quantization, operators in second quantization and diagrammatic representation
 2. [Video of lecture](#)
 3. Friday: Second quantization and Wick's theorem
 4. [Video of lecture](#)
- Lecture Material: These slides, handwritten notes and Szabo and Ostlund sections 2.3 and 2.4.
- [Second exercise set](#)

Second quantization, brief summary from week 35

We can summarize our findings from last week as

$$\{a_{\alpha}^{\dagger}, a_{\beta}\} = \delta_{\alpha\beta} \quad (1)$$

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

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

from which follows

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

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 .

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

$$a_\alpha^\dagger a_\alpha |\alpha_1 \alpha_2 \dots \alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ |\alpha_1 \alpha_2 \dots \alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \quad (2)$$

Summing over all possible one-particle states we arrive at

$$\left(\sum_\alpha a_\alpha^\dagger a_\alpha \right) |\alpha_1 \alpha_2 \dots \alpha_n\rangle = n |\alpha_1 \alpha_2 \dots \alpha_n\rangle \quad (3)$$

The operator

$$\hat{N} = \sum_\alpha a_\alpha^\dagger a_\alpha \quad (4)$$

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

$$\hat{H}_0 = \sum_i \hat{h}_0(x_i) \quad (5)$$

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

$$\hat{h}_0(x_i) \psi_{\alpha_i}(x_i) = \sum_{\alpha'_k} \psi_{\alpha'_k}(x_i) \langle \alpha'_k | \hat{h}_0 | \alpha_k \rangle \quad (6)$$

we can easily evaluate the action of \hat{H}_0 on each product of one-particle functions in Slater determinant. From Eq. (6) we obtain the following result without permuting any particle pair

$$\begin{aligned} & \left(\sum_i \hat{h}_0(x_i) \right) \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ = & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle \psi_{\alpha'_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ + & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle \psi_{\alpha_1}(x_1) \psi_{\alpha'_2}(x_2) \dots \psi_{\alpha_n}(x_n) \\ + & \dots \\ + & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \dots \psi_{\alpha'_n}(x_n) \end{aligned} \quad (7)$$

If we interchange particles 1 and 2 we obtain

$$\begin{aligned}
& \left(\sum_i \hat{h}_0(x_i) \right) \psi_{\alpha_1}(x_2) \psi_{\alpha_1}(x_2) \dots \psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle \psi_{\alpha_1}(x_2) \psi_{\alpha'_2}(x_1) \dots \psi_{\alpha_n}(x_n) \\
+ & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle \psi_{\alpha'_1}(x_2) \psi_{\alpha_2}(x_1) \dots \psi_{\alpha_n}(x_n) \\
+ & \dots \\
+ & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle \psi_{\alpha_1}(x_2) \psi_{\alpha_1}(x_2) \dots \psi_{\alpha'_n}(x_n) \quad (8)
\end{aligned}$$

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

$$\begin{aligned}
\hat{H}_0 |\alpha_1, \alpha_2, \dots, \alpha_n\rangle = & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle |\alpha'_1 \alpha_2 \dots \alpha_n\rangle \\
+ & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle |\alpha_1 \alpha'_2 \dots \alpha_n\rangle \\
+ & \dots \\
+ & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle |\alpha_1 \alpha_2 \dots \alpha'_n\rangle \quad (9)
\end{aligned}$$

In Eq. (9) we have expressed the action of the one-body operator of Eq. (5) 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

$$|\alpha_1 \alpha_2 \dots \alpha'_k \dots \alpha_n\rangle = a_{\alpha'_k}^\dagger a_{\alpha_k} |\alpha_1 \alpha_2 \dots \alpha_k \dots \alpha_n\rangle \quad (10)$$

Inserting this in the right-hand side of Eq. (9) results in

$$\begin{aligned}
\hat{H}_0 |\alpha_1 \alpha_2 \dots \alpha_n\rangle = & \sum_{\alpha'_1} \langle \alpha'_1 | \hat{h}_0 | \alpha_1 \rangle a_{\alpha'_1}^\dagger a_{\alpha_1} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\
+ & \sum_{\alpha'_2} \langle \alpha'_2 | \hat{h}_0 | \alpha_2 \rangle a_{\alpha'_2}^\dagger a_{\alpha_2} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\
+ & \dots \\
+ & \sum_{\alpha'_n} \langle \alpha'_n | \hat{h}_0 | \alpha_n \rangle a_{\alpha'_n}^\dagger a_{\alpha_n} |\alpha_1 \alpha_2 \dots \alpha_n\rangle \\
= & \sum_{\alpha, \beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_\alpha^\dagger a_\beta |\alpha_1 \alpha_2 \dots \alpha_n\rangle \quad (11)
\end{aligned}$$

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

$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} \quad (12)$$

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

It is instructive to verify Eq. (12) by computing the expectation value of \hat{H}_0 between two single-particle states

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \langle 0 | a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} | 0 \rangle \quad (13)$$

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

$$a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} = (\delta_{\alpha\alpha_1} - a_{\alpha}^{\dagger} a_{\alpha_1}) (\delta_{\beta\alpha_2} - a_{\alpha_2}^{\dagger} a_{\beta}), \quad (14)$$

which results in

$$\langle 0 | a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta} a_{\alpha_2}^{\dagger} | 0 \rangle = \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} \quad (15)$$

and

$$\langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle \delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} = \langle \alpha_1 | \hat{h}_0 | \alpha_2 \rangle \quad (16)$$

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

$$\hat{H}_I = \sum_{i < j} V(x_i, x_j) \quad (17)$$

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

$$V(x_i, x_j) \psi_{\alpha_k}(x_i) \psi_{\alpha_l}(x_j) = \sum_{\alpha'_k \alpha'_l} \psi'_{\alpha'_k}(x_i) \psi'_{\alpha'_l}(x_j) \langle \alpha'_k \alpha'_l | \hat{v} | \alpha_k \alpha_l \rangle \quad (18)$$

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

$$\begin{aligned}
& \left(\sum_{i < j} V(x_i, x_j) \right) \psi_{\alpha_1}(x_1) \psi_{\alpha_2}(x_2) \ldots \psi_{\alpha_n}(x_n) \\
= & \sum_{\alpha'_1 \alpha'_2} \langle \alpha'_1 \alpha'_2 | \hat{v} | \alpha_1 \alpha_2 \rangle \psi'_{\alpha'_1}(x_1) \psi'_{\alpha'_2}(x_2) \ldots \psi_{\alpha_n}(x_n) \\
& + \ldots \\
& + \sum_{\alpha'_1 \alpha'_n} \langle \alpha'_1 \alpha'_n | \hat{v} | \alpha_1 \alpha_n \rangle \psi'_{\alpha'_1}(x_1) \psi_{\alpha_2}(x_2) \ldots \psi'_{\alpha'_n}(x_n) \\
& + \ldots \\
& + \sum_{\alpha'_2 \alpha'_n} \langle \alpha'_2 \alpha'_n | \hat{v} | \alpha_2 \alpha_n \rangle \psi_{\alpha_1}(x_1) \psi'_{\alpha'_2}(x_2) \ldots \psi'_{\alpha'_n}(x_n) \\
& + \ldots
\end{aligned} \tag{19}$$

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

$$\begin{aligned}
H_I |\alpha_1 \alpha_2 \ldots \alpha_n\rangle = & \sum_{\alpha'_1, \alpha'_2} \langle \alpha'_1 \alpha'_2 | \hat{v} | \alpha_1 \alpha_2 \rangle |\alpha'_1 \alpha'_2 \ldots \alpha_n\rangle \\
& + \ldots \\
& + \sum_{\alpha'_1, \alpha'_n} \langle \alpha'_1 \alpha'_n | \hat{v} | \alpha_1 \alpha_n \rangle |\alpha'_1 \alpha_2 \ldots \alpha'_n\rangle \\
& + \ldots \\
& + \sum_{\alpha'_2, \alpha'_n} \langle \alpha'_2 \alpha'_n | \hat{v} | \alpha_2 \alpha_n \rangle |\alpha_1 \alpha'_2 \ldots \alpha'_n\rangle \\
& + \ldots
\end{aligned} \tag{20}$$

We introduce second quantization via the relation

$$\begin{aligned}
& a_{\alpha'_k}^\dagger a_{\alpha'_l}^\dagger a_{\alpha_l} a_{\alpha_k} |\alpha_1 \alpha_2 \ldots \alpha_k \ldots \alpha_l \ldots \alpha_n\rangle \\
= & (-1)^{k-1} (-1)^{l-2} a_{\alpha'_k}^\dagger a_{\alpha'_l}^\dagger a_{\alpha_l} a_{\alpha_k} |\alpha_k \alpha_l \underbrace{\alpha_1 \alpha_2 \ldots \alpha_n}_{\neq \alpha_k, \alpha_l}\rangle \\
= & (-1)^{k-1} (-1)^{l-2} |\alpha'_k \alpha'_l \underbrace{\alpha_1 \alpha_2 \ldots \alpha_n}_{\neq \alpha'_k, \alpha'_l}\rangle \\
= & |\alpha_1 \alpha_2 \ldots \alpha'_k \ldots \alpha'_l \ldots \alpha_n\rangle
\end{aligned} \tag{21}$$

Inserting this in (20) gives

$$\begin{aligned}
H_I|\alpha_1\alpha_2\ldots\alpha_n\rangle &= \sum_{\alpha'_1,\alpha'_2} \langle\alpha'_1\alpha'_2|\hat{v}|\alpha_1\alpha_2\rangle a_{\alpha'_1}^\dagger a_{\alpha'_2}^\dagger a_{\alpha_2} a_{\alpha_1} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \ldots \\
&= \sum_{\alpha'_1,\alpha'_n} \langle\alpha'_1\alpha'_n|\hat{v}|\alpha_1\alpha_n\rangle a_{\alpha'_1}^\dagger a_{\alpha'_n}^\dagger a_{\alpha_n} a_{\alpha_1} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \ldots \\
&= \sum_{\alpha'_2,\alpha'_n} \langle\alpha'_2\alpha'_n|\hat{v}|\alpha_2\alpha_n\rangle a_{\alpha'_2}^\dagger a_{\alpha'_n}^\dagger a_{\alpha_n} a_{\alpha_2} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
&+ \ldots \\
&= \sum'_{\alpha,\beta,\gamma,\delta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma |\alpha_1\alpha_2\ldots\alpha_n\rangle \quad (22)
\end{aligned}$$

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

$$\langle\alpha\beta|\hat{v}|\gamma\delta\rangle = \langle\beta\alpha|\hat{v}|\delta\gamma\rangle \quad (23)$$

we get

$$\sum_{\alpha\beta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = \sum_{\alpha\beta} \langle\beta\alpha|\hat{v}|\delta\gamma\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \quad (24)$$

$$= \sum_{\alpha\beta} \langle\beta\alpha|\hat{v}|\delta\gamma\rangle a_\beta^\dagger a_\alpha^\dagger a_\gamma a_\delta \quad (25)$$

where we have used the anti-commutation rules.

Changing the summation indices α and β in (25) we obtain

$$\sum_{\alpha\beta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma = \sum_{\alpha\beta} \langle\alpha\beta|\hat{v}|\delta\gamma\rangle a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta \quad (26)$$

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

$$\hat{H}_I = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma \quad (27)$$

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

With this expression we can now verify that the second quantization form of \hat{H}_I in Eq. (27) results in the same matrix between two anti-symmetrized two-particle states as its corresponding coordinate space representation. We have

$$\langle\alpha_1\alpha_2|\hat{H}_I|\beta_1\beta_2\rangle = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\hat{v}|\gamma\delta\rangle \langle 0|a_{\alpha_2} a_{\alpha_1} a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_{\beta_1}^\dagger a_{\beta_2}^\dagger|0\rangle. \quad (28)$$

Using the commutation relations we get

$$\begin{aligned}
& a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} \\
= & a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} (a_{\delta} \delta_{\gamma\beta_1} a_{\beta_2}^{\dagger} - a_{\delta} a_{\beta_1}^{\dagger} a_{\gamma} a_{\beta_2}^{\dagger}) \\
= & a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\gamma\beta_1} a_{\beta_2}^{\dagger} a_{\delta} - a_{\delta} a_{\beta_1}^{\dagger} \delta_{\gamma\beta_2} + a_{\delta} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} a_{\gamma}) \\
= & a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\gamma\beta_1} a_{\beta_2}^{\dagger} a_{\delta} \\
& - \delta_{\delta\beta_1} \delta_{\gamma\beta_2} + \delta_{\gamma\beta_2} a_{\beta_1}^{\dagger} a_{\delta} + a_{\delta} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} a_{\gamma}) \quad (29)
\end{aligned}$$

The vacuum expectation value of this product of operators becomes

$$\begin{aligned}
& \langle 0 | a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} a_{\beta_1}^{\dagger} a_{\beta_2}^{\dagger} | 0 \rangle \\
= & (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\delta\beta_1} \delta_{\gamma\beta_2}) \langle 0 | a_{\alpha_2} a_{\alpha_1} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} | 0 \rangle \\
= & (\delta_{\gamma\beta_1} \delta_{\delta\beta_2} - \delta_{\delta\beta_1} \delta_{\gamma\beta_2}) (\delta_{\alpha\alpha_1} \delta_{\beta\alpha_2} - \delta_{\beta\alpha_1} \delta_{\alpha\alpha_2}) \quad (30)
\end{aligned}$$

Insertion of Eq. (30) in Eq. (28) results in

$$\begin{aligned}
\langle \alpha_1 \alpha_2 | \hat{H}_I | \beta_1 \beta_2 \rangle &= \frac{1}{2} [\langle \alpha_1 \alpha_2 | \hat{v} | \beta_1 \beta_2 \rangle - \langle \alpha_1 \alpha_2 | \hat{v} | \beta_2 \beta_1 \rangle \\
&\quad - \langle \alpha_2 \alpha_1 | \hat{v} | \beta_1 \beta_2 \rangle + \langle \alpha_2 \alpha_1 | \hat{v} | \beta_2 \beta_1 \rangle] \\
&= \langle \alpha_1 \alpha_2 | \hat{v} | \beta_1 \beta_2 \rangle - \langle \alpha_1 \alpha_2 | \hat{v} | \beta_2 \beta_1 \rangle \\
&= \langle \alpha_1 \alpha_2 | \hat{v} | \beta_1 \beta_2 \rangle_{\text{AS}}. \quad (31)
\end{aligned}$$

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

$$\begin{aligned}
\hat{H}_I &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \\
&= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} [\langle \alpha\beta | \hat{v} | \gamma\delta \rangle - \langle \alpha\beta | \hat{v} | \delta\gamma \rangle] a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \\
&= \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle_{\text{AS}} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma} \quad (32)
\end{aligned}$$

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

$$H = \sum_{\alpha,\beta} \langle \alpha | \hat{t} + \hat{u}_{\text{ext}} | \beta \rangle a_{\alpha}^{\dagger} a_{\beta} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle \alpha\beta | \hat{v} | \gamma\delta \rangle a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\delta} a_{\gamma}. \quad (33)$$

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

Wick's theorem

See handwritten notes for week 36