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

Morten Hjorth-Jensen

Department of Physics and Center for Computing in Science Education, University of Oslo, Norway

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Week 36

- Topics to be covered
  1. Thursday: Second quantization, operators in second quantization and diagrammatic representation
  2. Friday: Second quantization and Wick's theorem
- Lecture Material: These slides, handwritten notes and Szabo and Ostlund sections 2.3 and 2.4.
- Third exercise set

Second quantization, brief summary from week 35

We can summarize our findings from last week as

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \tag{1}$$

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

Properties of operators

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

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

and

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

from which follows

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

Hermitian conjugate

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

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

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 $a_\alpha^\dagger$ 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.

Getting started

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

$$a^\dagger_\alpha a_\alpha |\alpha_1 \alpha_2 \dots \alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ \\ |\alpha_1 \alpha_2 \dots \alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \tag{2}$$

Summing over all possible one-particle states we arrive at

$$\left(\sum_\alpha a^\dagger_\alpha a_\alpha \right) |\alpha_1 \alpha_2 \dots \alpha_n\rangle = n |\alpha_1 \alpha_2 \dots \alpha_n\rangle \tag{3}$$

The number operator

The operator

$$\hat{N} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha} \tag{4}$$

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.

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

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

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

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

One-body operator in second quantitazion

Defining

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

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

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

Interchange particles 1 and 2

If we interchange particles 1 and 2 we obtain

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

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

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

More operations

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

$$|\alpha_1\alpha_2\dots\alpha_k'\dots\alpha_n\rangle = a^{\dagger}_{\alpha_k'} a_{\alpha_k}|\alpha_1\alpha_2\dots\alpha_k\dots\alpha_n\rangle \tag{10}$$

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

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

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

$$\hat{H}_0 = \sum_{\alpha\beta} \langle \alpha | \hat{h}_0 | \beta \rangle a^\dagger_\alpha a_\beta \tag{12}$$

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

Applying the new expression

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

$$\langle\alpha_1|\hat{h}_0|\alpha_2\rangle = \sum_{\alpha\beta}\langle\alpha|\hat{h}_0|\beta\rangle\langle 0|a_{\alpha_1}a^{\dagger}_{\alpha}a_{\beta}a^{\dagger}_{\alpha_2}|0\rangle \tag{13}$$

Explicit results

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

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

which results in

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

and

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

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

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

More operations

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

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

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

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

Introducing second quantization

We introduce second quantization via the relation

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

Inserting back

Inserting this in (20) gives

$$
\begin{aligned}
H_I|\alpha_1\alpha_2\ldots\alpha_n\rangle = & \sum_{\alpha_1',\alpha_2'} \langle\alpha_1'\alpha_2'|\hat{v}|\alpha_1\alpha_2\rangle a^\dagger_{\alpha_1'} a^\dagger_{\alpha_2'} a_{\alpha_2} a_{\alpha_1} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
+ & \qquad \ldots \\
= & \sum_{\alpha_1',\alpha_n'} \langle\alpha_1'\alpha_n'|\hat{v}|\alpha_1\alpha_n\rangle a^\dagger_{\alpha_1'} a^\dagger_{\alpha_n'} a_{\alpha_n} a_{\alpha_1} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
+ & \qquad \ldots \\
= & \sum_{\alpha_2',\alpha_n'} \langle\alpha_2'\alpha_n'|\hat{v}|\alpha_2\alpha_n\rangle a^\dagger_{\alpha_2'} a^\dagger_{\alpha_n'} a_{\alpha_n} a_{\alpha_2} |\alpha_1\alpha_2\ldots\alpha_n\rangle \\
+ & \qquad \ldots \\
= & \sum_{\alpha,\beta,\gamma,\delta}{}' \langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma |\alpha_1\alpha_2\ldots\alpha_n\rangle
\end{aligned}
\tag{22}
$$

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

$$\langle \alpha\beta|\hat{v}|\gamma\delta\rangle = \langle \beta\alpha|\hat{v}|\delta\gamma\rangle \tag{23}$$

we get

$$\begin{aligned}\sum_{\alpha\beta}\langle \alpha\beta|\hat{v}|\gamma\delta\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma &= \sum_{\alpha\beta}\langle \beta\alpha|\hat{v}|\delta\gamma\rangle a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma &(24)\\ &= \sum_{\alpha\beta}\langle \beta\alpha|\hat{v}|\delta\gamma\rangle a_\beta^\dagger a_\alpha^\dagger a_\gamma a_\delta &(25)\end{aligned}$$

where we have used the anti-commutation rules.

Changing summation indices

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

$$\sum_{\alpha\beta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^{\dagger}_{\alpha}a^{\dagger}_{\beta}a_{\delta}a_{\gamma} = \sum_{\alpha\beta}\langle\alpha\beta|\hat{v}|\delta\gamma\rangle a^{\dagger}_{\alpha}a^{\dagger}_{\beta}a_{\gamma}a_{\delta} \tag{26}$$

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

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

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. (27) results in the same matrix between two anti-symmetrized two-particle states as its corresponding coordinate space representation. We have

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

Two-body state

Using the commutation relations we get

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

Expectation value

The vacuum expectation value of this product of operators becomes

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

Final expression

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

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

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

$$
\begin{aligned}
\hat{H}_I = & \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
= & \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\left[\langle\alpha\beta|\hat{v}|\gamma\delta\rangle - \langle\alpha\beta|\hat{v}|\delta\gamma\rangle\right] a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \\
= & \frac{1}{4}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle_{\mathrm{AS}} a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma \qquad (32)
\end{aligned}
$$

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

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

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

Wick's theorem is based on two fundamental concepts, namely *normal ordering* and *contraction*. The normal-ordered form of $\widehat{\mathbf{A}}\widehat{\mathbf{B}}..\widehat{\mathbf{X}}\widehat{\mathbf{Y}}$, where the individual terms are either a creation or annihilation operator, is defined as

$$\left\{\widehat{\mathbf{A}}\widehat{\mathbf{B}}..\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\right\} \equiv (-1)^p \, [\text{creation operators}] \cdot [\text{annihilation operators}] \, . \tag{34}$$

The p subscript denotes the number of permutations that is needed to transform the original string into the normal-ordered form. A contraction between to arbitrary operators $\widehat{\mathbf{X}}$ and $\widehat{\mathbf{Y}}$ is defined as

$$\overbracket{\widehat{\mathbf{X}}\widehat{\mathbf{Y}}} \equiv \langle 0|\widehat{\mathbf{X}}\widehat{\mathbf{Y}}|0\rangle . \tag{35}$$

Wick's theorem

It is also possible to contract operators inside a normal ordered products. We define the original relative position between two operators in a normal ordered product as p, the so-called permutation number. This is the number of permutations needed to bring one of the two operators next to the other one. A contraction between two operators with $p \neq 0$ inside a normal ordered is defined as

$$\left\{\overbracket{\widehat{\mathbf{A}}\widehat{\mathbf{B}}..\widehat{\mathbf{X}}}\widehat{\mathbf{Y}}\right\} = (-1)^p \left\{\overbracket{\widehat{\mathbf{A}}\widehat{\mathbf{B}}}..\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\right\}. \tag{36}$$

In the general case with m contractions, the procedure is similar, and the prefactor changes to

$$(-1)^{p_1+p_2+..+p_m}. \tag{37}$$

Wick's theorem

Wick's theorem states that every string of creation and annihilation operators can be written as a sum of normalordered products with all possible ways of contractions,

$$\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z} = \left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\} \tag{38}$$

$$+ \sum_{(1)} \left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\} \tag{39}$$

$$+ \sum_{(2)} \left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\} \tag{40}$$

$$+ \ldots \tag{41}$$

$$+ \sum_{[\frac{N}{2}]} \left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\}. \tag{42}$$

Wick's theorem

The $\sum_{(m)}$ means the sum over all terms with m contractions, while $\left[\frac{N}{2}\right]$ means the largest integer that not do not exceeds $\frac{N}{2}$ where N is the number of creation and annihilation operators. When N is even,

$$\left[\frac{N}{2}\right] = \frac{N}{2}, \tag{43}$$

and the last sum in Eq. (38) is over fully contracted terms. When N is odd,

$$\left[\frac{N}{2}\right] \neq \frac{N}{2}, \tag{44}$$

and none of the terms in Eq. (38) are fully contracted

Wick's theorem

An important extension of Wick's theorem allow us to define contractions between normal-ordered strings of operators. This is the so-called generalized Wick's theorem,

$$\left\{\hat{A}\hat{B}\hat{C}\hat{D}..\right\}\left\{\hat{R}\hat{X}\hat{Y}\hat{Z}..\right\} = \left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\} \tag{45}$$

$$+\sum_{(1)}\left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\} \tag{46}$$

$$+\sum_{(2)}\left\{\hat{A}\hat{B}\hat{C}\hat{D}..\hat{R}\hat{X}\hat{Y}\hat{Z}\right\} \tag{47}$$

$$+\ldots \tag{48}$$

Wick's theorem

Turning back to the many-body problem, the vacuum expectation value of products of creation and annihilation operators can be written, according to Wick's theoren in Eq. (38), as a sum over normal ordered products with all possible numbers and combinations of contractions,

$$\langle 0|\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}|0\rangle = \langle 0|\left\{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}\right\}|0\rangle \tag{49}$$

$$+\sum_{(1)}\langle 0|\left\{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}\right\}|0\rangle \tag{50}$$

$$+\sum_{(2)}\langle 0|\left\{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}\right\}|0\rangle \tag{51}$$

$$+\ldots \tag{52}$$

$$+\sum_{[\frac{N}{2}]}\langle 0|\left\{\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\ \widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}\right\}|0\rangle. \tag{53}$$

Wick's theorem

All vacuum expectation values of normal ordered products without fully contracted terms are zero. Hence, the only contributions to the expectation value are those terms that *is* fully contracted,

$$\langle 0|\widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}|0\rangle = \sum_{(all)} \langle 0| \left\{ \widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\ \widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}} \right\} |0\rangle \tag{54}$$

$$= \sum_{(all)} \widehat{\mathbf{A}}\widehat{\mathbf{B}}\widehat{\mathbf{C}}\widehat{\mathbf{D}}..\ \widehat{\mathbf{R}}\widehat{\mathbf{X}}\widehat{\mathbf{Y}}\widehat{\mathbf{Z}}. \tag{55}$$

Wick's theorem

To obtain fully contracted terms, Eq. (43) must hold. When the number of creation and annihilation operators is odd, the vacuum expectation value can be set to zero at once. When the number is even, the expectation value is simply the sum of terms with all possible combinations of fully contracted terms. Observing that the only contractions that give nonzero contributions are

$$
\contraction{}{a}{_\alpha}{a} a_\alpha a^\dagger_\beta = \delta_{\alpha\beta}, \tag{56}
$$

the terms that contribute are reduced even more.

Wick's theorem provides us with an algebraic method for easy determination of the terms that contribute to the matrix element. Our next step is the particle-hole formalism, which is a very useful formalism in many-body systems. This topic will be discussed next week.

Wick's Theorem (Time-Independent) – Formal Proof in Many-Body Theory

In a more compact notation (using $:AB\dots XZ:$ for normalordering and dropping hats for operators)

$$ABCD =: ABCD: + \sum_{\text{singles}} :ABCD: + \sum_{\text{doubles}} :ABCD: + \cdots,$$

and similarly for any longer string.
In general, if n is even the final term will be the full contraction (product of $n/2$ contraction pairs, yielding a c-number), and if n is odd the last term will contain one unpaired operator (which remains in the normal-ordered form) . All possible distinct contraction pairings are included in the expansion, with appropriate sign factors for fermionic operators (each contraction effectively corresponds to commuting an annihilation past a creation operator).