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/XluUlE4uxjU
  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 $a_\alpha^\dagger$ and a_α which create and annihilate, respectively, a particle in the single-particle state φ_α. We define the fermion creation operator $a_\alpha^\dagger$

$$a_\alpha^\dagger|0\rangle \equiv |\alpha\rangle, \tag{1}$$

and

$$a_\alpha^\dagger|\alpha_1 \dots \alpha_n\rangle_{\mathrm{AS}} \equiv |\alpha\alpha_1 \dots \alpha_n\rangle_{\mathrm{AS}} \tag{2}$$

Second quantization

In Eq. (1) the operator $a^\dagger_\alpha$ 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) $a^\dagger_\alpha$ 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 $\alpha \ne \alpha_1, \alpha_2, \dots, \alpha_n$. It follows that we can express an antisymmetric state as the product of the creation operators acting on the vacuum state.

$$|\alpha_1 \dots \alpha_n\rangle_{\mathrm{AS}} = a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_n} |0\rangle \tag{3}$$

Commutation rules

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

$$|\alpha_1 \dots \alpha_i \dots \alpha_k \dots \alpha_n\rangle_{\mathrm{AS}} = -|\alpha_1 \dots \alpha_k \dots \alpha_i \dots \alpha_n\rangle_{\mathrm{AS}} \tag{4}$$

we obtain

$$a_{\alpha_i}^\dagger a_{\alpha_k}^\dagger = -a_{\alpha_k}^\dagger a_{\alpha_i}^\dagger \tag{5}$$

More on commutation rules

Using the Pauli principle

$$|\alpha_1 \ldots \alpha_i \ldots \alpha_i \ldots \alpha_n\rangle_{\mathrm{AS}} = 0 \tag{6}$$

it follows that

$$a^\dagger_{\alpha_i} a^\dagger_{\alpha_i} = 0. \tag{7}$$

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

$$a^\dagger_\alpha a^\dagger_\beta + a^\dagger_\beta a^\dagger_\alpha \equiv \{a^\dagger_\alpha, a^\dagger_\beta\} = 0 \tag{8}$$

Hermitian conjugate

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

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

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

$$\{a_\alpha, a_\beta\} = 0 \tag{10}$$

Physical interpretation

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

$$\langle\alpha_1\alpha_2\dots\alpha_n|a_\alpha|\alpha'_1\alpha'_2\dots\alpha'_m\rangle \tag{11}$$

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

$$\langle \alpha_1 \alpha_2 \ldots \alpha_n | a_\alpha = 0 \qquad (12)$$

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

$$\langle \alpha_1 \alpha_2 \ldots \alpha_n | a_\alpha = \langle \alpha \alpha_1 \alpha_2 \ldots \alpha_n | \qquad (13)$$

More derivations

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

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

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 $\alpha, \alpha_1, \alpha_2, \ldots, \alpha_n$ and $\alpha'_1, \alpha'_2, \ldots, \alpha'_{n+1}$ are related to each other via even and odd permutations. If we assume that $\alpha \notin \{\alpha_i\}$ we obtain

$$\langle \alpha_1 \alpha_2 \ldots \alpha_n | a_\alpha | \alpha'_1 \alpha'_2 \ldots \alpha'_{n+1} \rangle = 0 \tag{15}$$

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

$$a_\alpha \underbrace{|\alpha'_1 \alpha'_2 \ldots \alpha'_{n+1}\rangle}_{\neq \alpha} = 0 \tag{16}$$

and in particular

$$a_\alpha |0\rangle = 0 \tag{17}$$

Even and odd permutations

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

$$\langle\alpha_1\alpha_2\ldots\alpha_n|a_\alpha|\alpha\alpha_1\alpha_2\ldots\alpha_n\rangle = 1 \tag{18}$$

and thus

$$a_\alpha|\alpha\alpha_1\alpha_2\ldots\alpha_n\rangle = |\alpha_1\alpha_2\ldots\alpha_n\rangle \tag{19}$$

Annihilation operators

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 $a_\alpha^\dagger$ 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

$$a_\alpha^\dagger a_\alpha \underbrace{|\alpha_1\alpha_2 \ldots \alpha_n\rangle}_{\neq\alpha} = 0$$

$$a_\alpha a_\alpha^\dagger \underbrace{|\alpha_1\alpha_2 \ldots \alpha_n\rangle}_{\neq\alpha} = a_\alpha \underbrace{|\alpha\alpha_1\alpha_2 \ldots \alpha_n\rangle}_{\neq\alpha} = \underbrace{|\alpha_1\alpha_2 \ldots \alpha_n\rangle}_{\neq\alpha} \tag{20}$$

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 $\left\{a_\alpha^\dagger, a_\beta\right\}$, 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

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

Second case

The second case gives

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

Third case

Finally if the state vector does not contain α and β

$$\begin{aligned} a^\dagger_\alpha a_\beta|\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle &= 0 \\ a_\beta a^\dagger_\alpha|\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle &= a_\beta|\alpha\underbrace{\alpha_1\alpha_2\dots\alpha_n}_{\neq\alpha,\beta}\rangle = 0 \end{aligned} \tag{25}$$

For all three cases we have

$$\{a^\dagger_\alpha, a_\beta\} = a^\dagger_\alpha a_\beta + a_\beta a^\dagger_\alpha = 0, \quad \alpha \neq \beta \tag{26}$$

Summarizing

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

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \tag{27}$$

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

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

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 or just adjoint

The hermitian conjugate has the folowing 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 $a_\alpha^\dagger$ 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 $a_\alpha^\dagger a_\beta$ and $\alpha = \beta$. It acts on an n-particle state resulting in

$$a_\alpha^\dagger a_\alpha |\alpha_1\alpha_2\dots\alpha_n\rangle = \begin{cases} 0 & \alpha \notin \{\alpha_i\} \\ \\ |\alpha_1\alpha_2\dots\alpha_n\rangle & \alpha \in \{\alpha_i\} \end{cases} \tag{28}$$

Summing over all possible one-particle states we arrive at

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

The number operator

The operator

$$\hat{N} = \sum_{\alpha} a^{\dagger}_{\alpha} a_{\alpha} \tag{30}$$

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

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

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

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

One-body operator in second quantitazion

Defining

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

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

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

Interchange particles 1 and 2

If we interchange particles 1 and 2 we obtain

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

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

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

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

$$|\alpha_1\alpha_2\dots\alpha_k'\dots\alpha_n\rangle = a^\dagger_{\alpha_k'}a_{\alpha_k}|\alpha_1\alpha_2\dots\alpha_k\dots\alpha_n\rangle \tag{36}$$

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

$$\begin{aligned}
\hat{H}_0|\alpha_1\alpha_2\dots\alpha_n\rangle = & \sum_{\alpha_1'}\langle\alpha_1'|\hat{h}_0|\alpha_1\rangle a^\dagger_{\alpha_1'}a_{\alpha_1}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
+ & \sum_{\alpha_2'}\langle\alpha_2'|\hat{h}_0|\alpha_2\rangle a^\dagger_{\alpha_2'}a_{\alpha_2}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
+ & \qquad\qquad\qquad\dots \\
+ & \sum_{\alpha_n'}\langle\alpha_n'|\hat{h}_0|\alpha_n\rangle a^\dagger_{\alpha_n'}a_{\alpha_n}|\alpha_1\alpha_2\dots\alpha_n\rangle \\
= & \sum_{\alpha,\beta}\langle\alpha|\hat{h}_0|\beta\rangle a^\dagger_{\alpha}a_{\beta}|\alpha_1\alpha_2\dots\alpha_n\rangle
\end{aligned} \tag{37}$$

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

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

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. (38) by computing the expectation value of $\hat{H}_0$ between two single-particle states

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

Explicit results

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

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

which results in

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

and

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