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

In Eq. (2) $a_\alpha^\dagger$ acts on an antisymmetric n-particle state and creates an antisymmetric $(n+1)$-particle state, where the one-body state φ_α is occupied, under the condition that $\alpha \ne \alpha_1, \alpha_2, \dots, \alpha_n$. It follows that we can express an antisymmetric state as the product of the creation operators acting on the vacuum state.

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

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 $|\alpha_1\alpha_2\ldots\alpha_n\rangle_{\mathrm{AS}}$? Consider the following matrix element

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

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

$$\langle \alpha_1 \alpha_2 \ldots \alpha_n | a_\alpha = 0 \tag{12}$$

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

$$\langle \alpha_1 \alpha_2 \ldots \alpha_n | a_\alpha = \langle \alpha \alpha_1 \alpha_2 \ldots \alpha_n | \tag{13}$$

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 $\alpha, \alpha_1, \alpha_2, \ldots, \alpha_n$ 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

$$a_\alpha^\dagger a_\alpha \underbrace{|\alpha_1\alpha_2\dots\alpha_n\rangle}_{\neq\alpha} = 0$$
$$a_\alpha a_\alpha^\dagger \underbrace{|\alpha_1\alpha_2\dots\alpha_n\rangle}_{\neq\alpha} = a_\alpha \underbrace{|\alpha\alpha_1\alpha_2\dots\alpha_n\rangle}_{\neq\alpha} = \underbrace{|\alpha_1\alpha_2\dots\alpha_n\rangle}_{\neq\alpha} \qquad (20)$$

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

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

Third case

Finally if the state vector does not contain α and β

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

For all three cases we have

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

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

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