

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. 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_{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

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