Week 35: Ansatzes for fermions and bosons and second quantization

Morten Hjorth-Jensen[1]

Department of Physics and Center for Computing in Science Education,
University of Oslo, Norway[1]

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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. Video of lecture at `https://youtu.be/y6XYhZnRxnc`
    3. Whiteboard notes at `https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/HandwrittenNotes/2024/NotesAugust29.pdf`
    4. Friday: Second quantization
    5. Video of lecture at TBA `https://youtu.be/qOTrTLAy6KU`
    6. Whiteboard notes at `https://github.com/ManyBodyPhysics/FYS4480/blob/master/doc/HandwrittenNotes/2024/NotesAugust30.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

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

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 $\alpha \neq \alpha_1, \alpha_2, \ldots, \alpha_n$. It follows that we can express an antisymmetric state as the product of the creation operators acting on the vacuum state.

$$|\alpha_1 \ldots \alpha_n\rangle_{\mathrm{AS}} = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \ldots a_{\alpha_n}^\dagger |0\rangle \qquad (3)$$

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)

$$|\alpha_1 \ldots \alpha_i \ldots \alpha_k \ldots \alpha_n\rangle_{\mathrm{AS}} = -|\alpha_1 \ldots \alpha_k \ldots \alpha_i \ldots \alpha_n\rangle_{\mathrm{AS}} \qquad (4)$$

we obtain

$$a_{\alpha_i}^\dagger a_{\alpha_k}^\dagger = -a_{\alpha_k}^\dagger a_{\alpha_i}^\dagger \qquad (5)$$

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

$$\langle \alpha_1 \alpha_2 \ldots \alpha_n | a_\alpha | \alpha_1' \alpha_2' \ldots \alpha_m' \rangle \qquad (11)$$

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 $\alpha, \alpha_1, \alpha_2, \dots, \alpha_n$ is identical with the sequence $\alpha'_1, \alpha'_2, \dots, \alpha'_{n+1}$. This results in

$$\langle \alpha_1 \alpha_2 \dots \alpha_n | a_\alpha | \alpha \alpha_1 \alpha_2 \dots \alpha_n \rangle = 1 \qquad (18)$$

and thus

$$a_\alpha | \alpha \alpha_1 \alpha_2 \dots \alpha_n \rangle = | \alpha_1 \alpha_2 \dots \alpha_n \rangle \qquad (19)$$

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.

The action of the anti-commutator $\{a_\alpha^\dagger, a_\alpha\}$ on a given n-particle state is

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

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

if the single-particle state α is not contained in the state.

Anti-commutation rule for Fermions

If it is present we arrive at

$$a_\alpha^\dagger a_\alpha |\alpha_1 \alpha_2 \ldots \alpha_k \alpha \alpha_{k+1} \ldots \alpha_{n-1}\rangle = a_\alpha^\dagger a_\alpha (-1)^k |\alpha \alpha_1 \alpha_2 \ldots \alpha_{n-1}\rangle$$

$$= (-1)^k |\alpha \alpha_1 \alpha_2 \ldots \alpha_{n-1}\rangle = |\alpha_1 \alpha_2 \ldots \alpha_k \alpha \alpha_{k+1} \ldots \alpha_{n-1}\rangle$$

$$a_\alpha a_\alpha^\dagger |\alpha_1 \alpha_2 \ldots \alpha_k \alpha \alpha_{k+1} \ldots \alpha_{n-1}\rangle = 0 \qquad (21)$$

From Eqs. (20) and (21) we arrive at

$$\{a_\alpha^\dagger, a_\alpha\} = a_\alpha^\dagger a_\alpha + a_\alpha a_\alpha^\dagger = 1 \qquad (22)$$

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

$$a_\alpha^\dagger a_\beta |\alpha\beta\alpha_1\alpha_2 \ldots \alpha_{n-2}\rangle = 0$$

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

Second case

The second case gives

$$a_\alpha^\dagger a_\beta |\beta \underbrace{\alpha_1 \alpha_2 \ldots \alpha_{n-1}}_{\neq \alpha}\rangle = |\alpha \underbrace{\alpha_1 \alpha_2 \ldots \alpha_{n-1}}_{\neq \alpha}\rangle$$

$$a_\beta a_\alpha^\dagger |\beta \underbrace{\alpha_1 \alpha_2 \ldots \alpha_{n-1}}_{\neq \alpha}\rangle = a_\beta |\alpha\beta \underbrace{\beta \alpha_1 \alpha_2 \ldots \alpha_{n-1}}_{\neq \alpha}\rangle$$

$$= - |\alpha \underbrace{\alpha_1 \alpha_2 \ldots \alpha_{n-1}}_{\neq \alpha}\rangle \qquad (24)$$

Third case

Finally if the state vector does not contain α and β

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

$$a_\beta a_\alpha^\dagger | \underbrace{\alpha_1 \alpha_2 \ldots \alpha_n}_{\neq \alpha, \beta} \rangle = \qquad a_\beta | \alpha \underbrace{\alpha_1 \alpha_2 \ldots \alpha_n}_{\neq \alpha, \beta} \rangle = 0 \qquad (25)$$

For all three cases we have

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

Summarizing

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

$$\{a_\alpha^\dagger, a_\beta\} = \delta_{\alpha\beta} \qquad (27)$$

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

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

from which follows

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

Hermitian conjugate or just adjoint

The hermitian conjugate has the folowing properties

$$a_\alpha = (a_\alpha^\dagger)^\dagger.$$

Finally we found

$$a_\alpha \underbrace{|\alpha_1'\alpha_2'\ldots\alpha_{n+1}'\rangle}_{\neq\alpha} = 0, \quad \text{in particular } a_\alpha|0\rangle = 0,$$

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

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