

4. SECOND QUANTISATION FORMALISM

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Second quantisation: reformulation of quantum mechanics in terms of creation and annihilation operators

- Does not require an additional quantisation of the fields
- Technique originated from problems where the number of particles is not fixed (useful to describe processes $\mathbb{H}_N \rightarrow \mathbb{H}_{N'}$)
- Allows to represent and manipulate wave functions and operators in a compact way
- Automatically incorporates (anti-)symmetrisation of wave functions

Fock space

Define Fock space \mathcal{F} as the direct sum

$$\begin{aligned}\mathcal{F} &\equiv \mathbb{H}_0 \oplus \mathbb{H}_1 \oplus \dots \oplus \mathbb{H}_N \oplus \dots \\ &= \mathbb{H}_0 \oplus \mathbb{H}_1 \oplus \dots \oplus (\mathbb{H}_1)^{\otimes N} \oplus \dots\end{aligned}$$

of Hilbert spaces having a specific number of particles such that

- 1) \mathbb{H}_0 is the Hilbert space spanned by the normalised vacuum state $|0\rangle$ that contains zero particles (not be confused with null vector!)
- 2) \mathbb{H}_1 is the one-body Hilbert space spanned by $B_1 = \{|d_i\rangle\}$
- 3) \mathbb{H}_N is the N-body Hilbert space spanned by the direct-product basis $B_N = \{|1:d_1 \dots N:d_N\rangle\}$

Then \mathcal{F} is spanned by

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$$\mathcal{B}_{\mathcal{F}} = \mathcal{B}_0 \cup \mathcal{B}_1 \cup \mathcal{B}_2 \cup \dots \cup \mathcal{B}_N \cup \dots$$

If we restrict ourselves to fermions

$$\mathcal{B}_{\mathcal{F}}^{\mp} = \mathcal{B}_0^{\mp} \cup \mathcal{B}_1^{\mp} \cup \dots \cup \mathcal{B}_N^{\mp} \cup \dots$$

(only antisymmetrised bases)

Creation and annihilation operators

Introduce creation a_{μ}^{\dagger} and annihilation a_{μ} operators acting on \mathcal{F} such that

1) They are hermitian conjugate

$$a_{\mu}^{\dagger} = (a_{\mu})^{\dagger}$$

2) a_{μ} annihilates a particle in the single-particle state $|\mu\rangle$, taking the system from N to $N-1$ particles

$$a_{\mu} : \mathcal{H}_N \rightarrow \mathcal{H}_{N-1}$$

if μ unoccupied $|\alpha\beta\dots\rangle \rightarrow a_{\mu} |\alpha\beta\dots\rangle \equiv 0$

if μ occupied $|\mu\beta\dots\rangle \rightarrow a_{\mu} |\mu\beta\dots\rangle = |\beta\dots\rangle$

/
if μ is not on the left one has to perform necessary transpositions

3) a_{μ}^+ creates a particle in the single-particle state $|\mu\rangle$, taking the system from N to $N+1$ particles

$$a_{\mu}^+ : \mathcal{H}_N \rightarrow \mathcal{H}_{N+1}$$

if μ unoccupied $|\alpha\beta\dots\rangle \rightarrow a_{\mu}^+ |\alpha\beta\dots\rangle \equiv |\mu\alpha\beta\dots\rangle$

if μ occupied $|\alpha\dots\mu\dots\rangle \rightarrow a_{\mu}^+ |\alpha\dots\mu\dots\rangle \equiv 0$

ensures Pauli principle

4) annihilation and creation operators obey the anticommutation relationships

$$\{a_{\mu}^+, a_{\nu}^+\} \equiv a_{\mu}^+ a_{\nu}^+ + a_{\nu}^+ a_{\mu}^+ = 0$$

$$\{a_{\mu}, a_{\nu}\} = 0$$

$$\{a_{\mu}, a_{\nu}^+\} = \delta_{\mu\nu}$$

→ Proof (exercise)

Basis transformations

(creation and annihilation operators are in one-to-one correspondence with a given single-particle basis $B_1 = \{|\mu\rangle\}$ of \mathcal{H}_1 (and the particle vacuum $|0\rangle$). In fact one has

$$a_{\mu}^+ |0\rangle = |\mu\rangle$$

If one wants to work with a different basis $B'_1 = \{|\lambda\rangle\}$ the two sets of operators are related by a unitary transformation

Starting from

$$\begin{aligned}
 |\mu\rangle &= \sum_{\lambda} |\lambda\rangle \langle \lambda | \mu \rangle \\
 &= \sum_{\lambda} |\lambda\rangle C_{\lambda\mu}
 \end{aligned}$$

$$\begin{aligned}
 \langle \mu | &= \sum_{\lambda} \langle \mu | \lambda \rangle \langle \lambda | \\
 &= \sum_{\lambda} C_{\lambda\mu}^* \langle \lambda |
 \end{aligned}$$

one deduces the ones valid in \mathcal{F}

$$\begin{cases}
 a_{\mu}^{\dagger} = \sum_{\lambda} b_{\lambda}^{\dagger} C_{\lambda\mu} \\
 a_{\mu} = \sum_{\lambda} b_{\lambda} C_{\lambda\mu}^*
 \end{cases}$$

Slater determinants

(Slater determinants)

Normalised and antisymmetrised product states can be built from the particle vacuum via the repeated application of creation operators

$$|\Phi\rangle = |\alpha\beta \dots\rangle = a_{\alpha}^{\dagger} a_{\beta}^{\dagger} \dots |0\rangle$$

→ The antisymmetry of the Slater determinant is ensured by the anti-commutation relations between a_i and a_i^{\dagger} 's

Recall that the complete set of Slater determinants associated with all $N \in \mathbb{N}$ provides an orthonormalised basis of \mathcal{F}

Let us take here $N=2$ and prove that

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$$\langle \alpha\beta | \mu\nu \rangle = \delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu}$$

Start from

$$|\alpha\beta\rangle = a_\alpha^+ a_\beta^+ |0\rangle$$

Then write

$$\begin{aligned} \langle \alpha\beta | &= |\alpha\beta\rangle^\dagger \\ &= (a_\alpha^+ a_\beta^+ |0\rangle)^\dagger \\ &= \langle 0 | (a_\alpha^+ a_\beta^+)^\dagger \\ &= \langle 0 | (a_\beta^+)^\dagger (a_\alpha^+)^\dagger \\ &= \langle 0 | a_\beta a_\alpha \end{aligned}$$

Then

$$\begin{aligned} \langle \alpha\beta | \mu\nu \rangle &= \langle 0 | a_\beta a_\alpha a_\mu^+ a_\nu^+ |0\rangle \\ &= \langle 0 | a_\beta (\delta_{\alpha\mu} - a_\mu^+ a_\alpha) a_\nu^+ |0\rangle \\ &= \langle 0 | \delta_{\alpha\mu} (\delta_{\beta\nu} - a_\nu^+ a_\beta) |0\rangle \\ &\quad - \langle 0 | (\delta_{\beta\mu} - a_\mu^+ a_\beta) (\delta_{\alpha\nu} - a_\nu^+ a_\alpha) |0\rangle \\ &= \delta_{\alpha\mu} \delta_{\beta\nu} - \delta_{\alpha\nu} \delta_{\beta\mu} \end{aligned}$$

Operators

We had defined operators acting on \mathcal{H}_N : how operators acting on \mathcal{F} .

A one-body operator

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$$F: f \rightarrow F$$

$$|\alpha\beta\dots\rangle \rightarrow F|\alpha\beta\dots\rangle$$

is defined in its second quantised form

$$F = \sum_{\alpha\beta} f_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta}$$

which involve matrix elements of the operator on $\mathcal{H}_1(i)$, written in a compact form

$$f_{\alpha\beta} = \langle i:\alpha | f(i) | i:\beta \rangle \quad (\text{independent of } i)$$

→ While in first quantisation the sum runs over the number of particles N , here it runs over basis states of \mathcal{H}_1 .

→ Trivially $F|0\rangle = 0$

To make the link to first-quantisation operators, let us apply the first-quantised form of F on a basis state $|d_1, d_2, \dots, d_N\rangle$ of \mathcal{H}_N .

$$\begin{aligned} F |d_1, d_2, \dots, d_N\rangle &= \sqrt{N!} A F |1:d_1, \dots, N:d_N\rangle \\ &= \sqrt{N!} \sum_{i=1}^N A f(i) |1:d_1, \dots, N:d_N\rangle \end{aligned}$$

By inserting two completeness relations on $\mathcal{H}_1(i)$, we can rewrite

$$\begin{aligned} f(i) &= \sum_{\alpha\beta} |i:\alpha\rangle \langle i:\alpha | f(i) | i:\beta\rangle \langle i:\beta | \\ &= \sum_{\alpha\beta} f_{\alpha\beta} |i:\alpha\rangle \langle i:\beta | \end{aligned}$$

Then

$$\begin{aligned}
 \bar{F} |d_1, d_2, \dots, d_N\rangle &= \sum_{i=1}^N \sum_{\alpha\beta} f_{\alpha\beta} \sqrt{N!} A |1:d_1\rangle \otimes \dots |i:d\rangle \langle i:\beta| i:d_i\rangle \otimes \dots \otimes |N:d_N\rangle \quad (7) \\
 &= \sum_{i=1}^N \sum_{\alpha\beta} f_{\alpha\beta} f_{\beta\alpha} \sqrt{N!} A |1:d_1 \dots i:d \dots N:d_N\rangle \\
 &= \sum_{i=1}^N \sum_{\alpha} f_{\alpha\alpha} |d_1 \dots d_{i-1} \alpha d_{i+1} \dots d_N\rangle
 \end{aligned}$$

Now, consider second-quantised form of F and compute

$$\begin{aligned}
 [F, a_{\alpha_i}^+] &= \sum_{\alpha\beta} f_{\alpha\beta} [a_{\alpha}^+ a_{\beta}, a_{\alpha_i}^+] \\
 &= \sum_{\alpha\beta} f_{\alpha\beta} (a_{\alpha}^+ a_{\beta} a_{\alpha_i}^+ - a_{\alpha_i}^+ a_{\alpha}^+ a_{\beta}) \\
 &= \sum_{\alpha\beta} f_{\alpha\beta} a_{\alpha}^+ (a_{\beta} a_{\alpha_i}^+ + a_{\alpha_i}^+ a_{\beta}) \\
 &= \sum_{\alpha\beta} f_{\alpha\beta} a_{\alpha}^+ \delta_{\beta\alpha_i} \\
 &= \sum_{\alpha} f_{\alpha\alpha_i} a_{\alpha}^+
 \end{aligned}$$

Let us apply to the product state $|d_1, d_2, \dots, d_N\rangle$

$$\begin{aligned}
 \bar{F} |d_1, d_2, \dots, d_N\rangle &= \bar{F} a_{\alpha_1}^+ a_{\alpha_2}^+ \dots a_{\alpha_N}^+ |0\rangle \\
 &= [F, a_{\alpha_1}^+] a_{\alpha_2}^+ \dots a_{\alpha_N}^+ |0\rangle + a_{\alpha_1}^+ \bar{F} a_{\alpha_2}^+ \dots a_{\alpha_N}^+ |0\rangle \\
 &= [F, a_{\alpha_1}^+] a_{\alpha_2}^+ \dots a_{\alpha_N}^+ |0\rangle \\
 &\quad + a_{\alpha_1}^+ [F, a_{\alpha_2}^+] \dots a_{\alpha_N}^+ |0\rangle \\
 &\quad + \dots \\
 &\quad + a_{\alpha_1}^+ a_{\alpha_2}^+ \dots [F, a_{\alpha_N}^+] |0\rangle
 \end{aligned}$$

$$= \sum_{i=1}^N \sum_{\alpha} f_{\alpha\alpha_i} a_{\alpha_i}^{\dagger} \dots a_{\alpha_{i-1}}^{\dagger} a_{\alpha}^{\dagger} a_{\alpha_{i+1}}^{\dagger} \dots a_{\alpha_N}^{\dagger} |0\rangle$$

$$= \sum_{i=1}^N \sum_{\alpha} f_{\alpha\alpha_i} | \alpha_i \dots \alpha_{i-1} \alpha \alpha_{i+1} \dots \alpha_N | 0 \rangle$$

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→ Note that a one-body operator simplifies in the single-particle basis that diagonalises it, i.e. in which $f_{\alpha\beta} = \sum_{\alpha} \epsilon_{\alpha} \delta_{\alpha\beta}$

$$\Rightarrow F = \sum_{\alpha} \epsilon_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}$$

A two-body operator

$$G: F \rightarrow f$$

$$| \alpha\beta \dots \rangle \rightarrow G | \alpha\beta \dots \rangle$$

has the second-quantised form

$$G = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta}$$

! note the ordering!

where g represent direct-product matrix elements on $\mathbb{A}_2(i, j)$

$$g_{\alpha\beta\gamma\delta} \equiv \langle i: \alpha \ j: \beta | g(i, j) | i: \gamma \ j: \delta \rangle$$

(independent of i, j)

→ Trivially one has $G | 0 \rangle = 0$

→ One also has $G | \mu \rangle = 0$

$$\begin{aligned}
G|\mu\rangle &= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\delta} a_{\mu}^{\dagger} |0\rangle \\
&= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} (\delta_{\delta\mu} - a_{\mu}^{\dagger} a_{\delta}) |0\rangle \\
&= \frac{1}{2} \sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} - \frac{1}{2} \sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta} a_{\alpha}^{\dagger} a_{\beta}^{\dagger} a_{\gamma} a_{\mu}^{\dagger} a_{\delta} |0\rangle \\
&= 0
\end{aligned}$$

Similarly, a k-body operator

$$\begin{aligned}
K : f &\rightarrow \tilde{f} \\
| \alpha \beta \dots \rangle &\rightarrow K | \alpha \beta \dots \rangle
\end{aligned}$$

defined via

$$K = \frac{1}{k!} \sum_{\alpha \dots \beta \gamma \dots \delta} k_{\alpha \dots \beta \gamma \dots \delta} a_{\alpha}^{\dagger} \dots a_{\beta}^{\dagger} a_{\gamma} \dots a_{\delta}$$

involves matrix elements between direct-product states of \mathcal{H}_k

$$\begin{aligned}
k_{\alpha \dots \beta \gamma \dots \delta} &\equiv \langle i : \alpha \dots l : \beta | k(i_1, \dots, l) | i : \gamma \dots l : \delta \rangle \\
&\quad (\text{independent of } i_1, \dots, l)
\end{aligned}$$

→ Action of K on states of \mathcal{H}_N with $N < k$ gives the null vector

Example: particle-number operator

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First-quantised form is given by

$$N = \sum_{i=1}^N n(i) = \sum_{i=1}^N \mathbb{1}_1(i)$$

Given an arbitrary basis, $B_1(i) = \{|i:\mu\rangle\}$ of $\mathcal{H}_1(i)$

$$\begin{aligned} n_{\alpha\beta} &\equiv \langle i:\alpha | n(i) | i:\beta \rangle \\ &= \langle i:\alpha | i:\beta \rangle \\ &= \delta_{\alpha\beta} \end{aligned}$$

Then the second-quantised form reads

$$N = \sum_{\alpha\beta} n_{\alpha\beta} a_{\alpha}^{\dagger} a_{\beta} = \sum_{\alpha} a_{\alpha}^{\dagger} a_{\alpha}$$

(diagonal in any basis of \mathcal{H}_1)

→ States of \mathcal{H}_k are eigenstates of N with eigenvalue k

One has trivially $N|0\rangle = 0$

Then consider $[N, a_{\alpha_1}^{\dagger}] = \sum_{\alpha} n_{\alpha\alpha_1} a_{\alpha}^{\dagger} = a_{\alpha_1}^{\dagger}$

Repeat $[N, a_{\alpha_2}^{\dagger} a_{\alpha_1}^{\dagger}] = a_{\alpha_2}^{\dagger} [N, a_{\alpha_1}^{\dagger}] + [N, a_{\alpha_2}^{\dagger}] a_{\alpha_1}^{\dagger}$

$$= a_{\alpha_2}^{\dagger} a_{\alpha_1}^{\dagger} + a_{\alpha_2}^{\dagger} a_{\alpha_1}^{\dagger}$$

$$= 2 a_{\alpha_2}^{\dagger} a_{\alpha_1}^{\dagger}$$

Again $[N, a_{\alpha_3}^{\dagger} a_{\alpha_2}^{\dagger} a_{\alpha_1}^{\dagger}] = \dots = 3 a_{\alpha_3}^{\dagger} a_{\alpha_2}^{\dagger} a_{\alpha_1}^{\dagger}$

k-times $[N, a_{d_k}^\dagger \dots a_{d_2}^\dagger a_{d_1}^\dagger] = k a_{d_k}^\dagger \dots a_{d_2}^\dagger a_{d_1}^\dagger$

Apply on basis state of \mathcal{H}_k

$$N |d_k \dots d_2 d_1\rangle = N a_{d_k}^\dagger \dots a_{d_2}^\dagger a_{d_1}^\dagger |0\rangle$$

$$= [N, a_{d_k}^\dagger \dots a_{d_2}^\dagger a_{d_1}^\dagger] |0\rangle + a_{d_k}^\dagger \dots a_{d_2}^\dagger a_{d_1}^\dagger N |0\rangle$$

$$= k |d_k \dots d_2 d_1\rangle$$

Example: Nuclear Hamiltonian

In nuclear physics, it is customary to use matrix elements that are

- i) explicitly antisymmetrised on the right
- ii) not normalised

$\bar{g}_{\alpha\beta\gamma\delta} \equiv g_{\alpha\beta\gamma\delta} - g_{\alpha\delta\beta\gamma}$

(Using symmetry Properties one can show that antisymmetrisation of left indices also holds)

Then

$$G = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \bar{g}_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta$$

note the change of prefactor $\frac{1}{2} \rightarrow \frac{1}{4}$

In first quantisation, nuclear Hamiltonian reads

$$H = T + V = \sum_{i=1}^N \frac{p(i)^2}{2m} + \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^N V(i,j) + \frac{1}{3!} \sum_{\substack{i,j,k=1 \\ i \neq j \neq k}}^N W(i,j,k) + \dots$$

Second-quantised form

$$H = \sum_{\alpha\beta} t_{\alpha\beta} a_\alpha^\dagger a_\beta + \left(\frac{1}{2!}\right)^2 \sum_{\alpha\beta\gamma\delta} \bar{V}_{\alpha\beta\gamma\delta} a_\alpha^\dagger a_\beta^\dagger a_\gamma a_\delta + \left(\frac{1}{3!}\right)^2 \sum_{\alpha\beta\gamma\delta\epsilon\zeta} \bar{W}_{\alpha\beta\gamma\delta\epsilon\zeta} a_\alpha^\dagger a_\beta^\dagger a_\gamma^\dagger a_\delta^\dagger a_\epsilon a_\zeta + \dots$$

where antisymmetrised three-body matrix elements are defined as

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$$\overline{W}_{\alpha\beta\gamma\delta\varepsilon\xi} \equiv W_{\alpha\beta\gamma\delta\varepsilon\xi}$$

$$- W_{\alpha\beta\gamma\delta\xi\varepsilon}$$

$$- W_{\alpha\beta\gamma\xi\varepsilon\delta}$$

$$- W_{\alpha\beta\gamma\varepsilon\delta\xi}$$

$$+ W_{\alpha\beta\gamma\xi\varepsilon\delta}$$

$$+ W_{\alpha\beta\gamma\varepsilon\xi\delta}$$

→ One can generalise all above considerations to particle-number-breaking operators, i.e. operators that associate a state of A_N to a state of $A_{N'}$ with $N' \neq N$