4. SECOND QUANTISATION FORMALISM

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 $\mathcal{H}_N \to \mathcal{H}_{N'}$)

→ Allows to represent and manipulate wave functions and operators in a compact way

→ Automatically incorporates (anti-)symmetrisation of wave functions

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3.1 Fock space

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

$$\mathcal{F} \equiv \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \dots \oplus \mathcal{H}_N \oplus \dots$$
$$= \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \dots \oplus (\mathcal{H}_1)^{\otimes N} \oplus \dots$$

of Hilbert spaces having a specif number of particles such that

1) $\mathcal{H}_0$ is the Hilbert space spanned by the normalised vacuum state $|0\rangle$ that contains zero particles (not be confused with null vector!)

2) $\mathcal{H}_1$ is the one-body Hilbert space spanned by $\mathcal{B}_1 = \{|\alpha_i\rangle\}$

3) $\mathcal{H}_N$ is the N-body Hilbert space spanned by the direct-product basis

$$\mathcal{B}_N = \{|1:\alpha_1 \dots N:\alpha_N\rangle\}$$

Then $\mathcal{F}$ is spanned by

$$B_{\mathcal{F}} = B_0 \cup B_1 \cup B_2 \cup \dots \cup B_N \cup \dots$$

If we restrict ourselves to fermions

$$B_{\mathcal{F}}^{\mp} = B_0^{\mp} \cup B_1^{\mp} \cup \dots \cup B_N^{\mp} \cup \dots$$

(only antisymmetrised bases)

3.2 Creation and annihilation operators

Introduce creation a^+_μ and annihilation a_μ operators acting on $\mathcal{F}$ such that

1) They are hermitian conjugate

$$a^+_\mu = (a_\mu)^\dagger$$

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

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

if μ unoccupied $\quad |\alpha\beta\dots\rangle \longrightarrow a_\mu |\alpha\beta\dots\rangle \equiv 0$

if μ occupied $\quad |\mu\beta\dots\rangle \longrightarrow a_\mu |\mu\beta\dots\rangle = |\beta\dots\rangle$

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

$$a^+_\mu : \quad \mathcal{H}_N \longrightarrow \mathcal{H}_{N+1}$$

if μ unoccupied $\quad |\alpha\beta\ldots\rangle \longrightarrow a^+_\mu|\alpha\beta\ldots\rangle \equiv |\mu\alpha\beta\ldots\rangle$

if μ occupied $\quad |\alpha\ldots\mu\ldots\rangle \longrightarrow a^+_\mu|\alpha\ldots\mu\ldots\rangle = 0$

ensures Pauli principle

4) annihilation and creation operators obey the anticommutation relationships

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

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

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

$\rightarrow$ Proof (exercise)

3.3 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

$$|\mu\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\mu\rangle = \sum_\lambda |\lambda\rangle C_{\lambda\mu}$$

$$\langle\mu| = \sum_\lambda \langle\mu|\lambda\rangle\langle\lambda| = \sum_\lambda C^*_{\lambda\mu} \langle\lambda|$$

one deduces the ones valid in $\mathcal{F}$

$$\begin{cases} a^+_\mu = \sum_\lambda b^+_\lambda C_{\lambda\mu} \\ a_\mu = \sum_\lambda b_\lambda C^*_{\lambda\mu} \end{cases}$$

3.4 Slater determinants

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

$$|\Phi\rangle = |\alpha\beta\ldots\rangle = a^+_\alpha a^+_\beta \ldots |0\rangle$$

→ The antisymmetry of the Slater determinant is ensured by the anticommutation relations between a's and a^+'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

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

Start from

$$|\alpha\beta\rangle = a^+_\alpha a^+_\beta |0\rangle$$

Then write

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

Then

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

3.5 Operators

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

A one-body operator

$$F : \mathcal{F} \to \mathcal{F}$$

$$|\alpha\beta\ldots\rangle \to F|\alpha\beta\ldots\rangle$$

is defined in its second quantised form

$$F = \sum_{\alpha\beta} f_{\alpha\beta}\, a^\dagger_\alpha a_\beta$$

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

$$f_{\alpha\beta} \equiv \langle i:\alpha|\, f(i)\, |i:\beta\rangle \qquad \text{(independent of } i\text{)}$$

→ While in first quantisation the sum runs over the number of particles N, here it runs over basis state 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 $|\alpha_1\alpha_2\ldots\alpha_N\rangle$ of $\mathcal{H}_N$

$$F|\alpha_1\alpha_2\ldots\alpha_N\rangle = \sqrt{N!}\,\mathcal{A}\,F\,|1:\alpha_1\ldots N:\alpha_N\rangle$$

$$= \sqrt{N!}\sum_{i=1}^{N}\mathcal{A}\,f(i)\,|1:\alpha_1\ldots N:\alpha_N\rangle$$

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

$$f(i) = \sum_{\alpha\beta} |i:\alpha\rangle\langle i:\alpha|\, f(i)\, |i:\beta\rangle\langle i:\beta|$$

$$= \sum_{\alpha\beta} f_{\alpha\beta}\, |i:\alpha\rangle\langle i:\beta|$$

Then

$$F|\alpha_1 \alpha_2 \ldots \alpha_N\rangle = \sum_{i=1}^{N} \sum_{\alpha\beta} f_{\alpha\beta} \sqrt{N!}\, \mathcal{A}\, |1:\alpha_1\rangle \otimes \ldots |i:\alpha\rangle\langle i:\beta|i:\alpha_i\rangle \otimes \ldots \otimes |N:\alpha_N\rangle$$

$$= \sum_{i=1}^{N} \sum_{\alpha\beta} f_{\alpha\beta}\, \delta_{\beta\alpha_i} \sqrt{N!}\, \mathcal{A}\, |1:\alpha_1 \ldots i:\alpha \ldots N:\alpha_N\rangle$$

$$= \sum_{i=1}^{N} \sum_{\alpha} f_{\alpha\alpha_i} |\alpha_1 \ldots \alpha_{i-1}\, \alpha\, \alpha_{i+1} \ldots \alpha_N\rangle$$

Now, consider second-quantised form of F and compute

$$[F, a^\dagger_{\alpha_i}] = \sum_{\alpha\beta} f_{\alpha\beta} [a^\dagger_\alpha a_\beta, a^\dagger_{\alpha_i}]$$

$$= \sum_{\alpha\beta} f_{\alpha\beta} \left(a^\dagger_\alpha a_\beta a^\dagger_{\alpha_i} - a^\dagger_{\alpha_i} a^\dagger_\alpha a_\beta\right)$$

$$= \sum_{\alpha\beta} f_{\alpha\beta}\, a^\dagger_\alpha \left(a_\beta a^\dagger_{\alpha_i} + a^\dagger_{\alpha_i} a_\beta\right)$$

$$= \sum_{\alpha\beta} f_{\alpha\beta}\, a^\dagger_\alpha\, \delta_{\beta\alpha_i}$$

$$= \sum_{\alpha} f_{\alpha\alpha_i} a^\dagger_\alpha$$

Let us apply to the product state $|\alpha_1 \alpha_2 \ldots \alpha_N\rangle$

$$F|\alpha_1\alpha_2 \ldots \alpha_N\rangle = F a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_N}|0\rangle$$

$$= [F, a^\dagger_{\alpha_1}] a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_N}|0\rangle + a^\dagger_{\alpha_1} F a^\dagger_{\alpha_2} \ldots a^\dagger_{N}|0\rangle$$

$$= [F, a^\dagger_{\alpha_1}] a^\dagger_{\alpha_2} \ldots a^\dagger_{\alpha_N}|0\rangle$$

$$+ a^\dagger_{\alpha_1} [F, a^\dagger_{\alpha_2}] \ldots a^\dagger_{\alpha_N}|0\rangle$$

$$+ \ldots$$

$$+ a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \ldots [F, a^\dagger_{N}]|0\rangle$$

$$= \sum_{i=1}^{N} \sum_{\alpha} f_{\alpha\alpha_i} a^\dagger_{\alpha_1} \cdots a^\dagger_{\alpha_{i-1}} a^\dagger_{\alpha} a^\dagger_{\alpha_{i+1}} \cdots a^\dagger_{\alpha_N} |0\rangle$$

$$= \sum_{i=1}^{N} \sum_{\alpha} f_{\alpha\alpha_i} |\alpha_1 \cdots \alpha_{i-1} \, \alpha \, \alpha_{i+1} \cdots \alpha_N |0\rangle$$

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

$$\Rightarrow \quad F = \sum_{\alpha} \varepsilon_\alpha a^\dagger_\alpha a_\alpha$$

A two-body operator

$$G : \mathcal{F} \to \mathcal{F}$$

$$|\alpha\beta \ldots\rangle \longrightarrow G|\alpha\beta \ldots\rangle$$

has the second-quantised form

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

note the ordering!

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

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

(independent of i, j)

→ Trivially one has $G|0\rangle = 0$

→ One also has $G|\mu\rangle = 0$

$$G|\mu\rangle = \frac{1}{2}\sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta}\, a^+_\alpha a^+_\beta a_\delta a_\gamma a^+_\mu |0\rangle$$

$$= \frac{1}{2}\sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta}\, a^+_\alpha a^+_\beta a_\delta \left(\delta_{\gamma\mu} - a^+_\mu a_\gamma\right)|0\rangle$$

$$= \frac{1}{2}\sum_{\alpha\beta\delta} g_{\alpha\beta\mu\delta}\, a^+_\alpha a^+_\beta a_\delta \;-\; \frac{1}{2}\sum_{\alpha\beta\gamma\delta} g_{\alpha\beta\gamma\delta}\, a^+_\alpha a^+_\beta a_\delta a^+_\mu a_\gamma |0\rangle$$

$$= 0$$

Similarly, a k-body operator

$$K : \mathcal{F} \to \mathcal{F}$$

$$|\alpha\beta\ldots\rangle \longrightarrow K|\alpha\beta\ldots\rangle$$

defined via

$$K = \frac{1}{k!}\sum_{\alpha\ldots\beta\gamma\ldots\delta} k_{\alpha\ldots\beta\gamma\ldots\delta}\, a^+_\alpha \ldots a^+_\beta a_\delta \ldots a_\gamma$$

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

$$k_{\alpha\ldots\beta\gamma\ldots\delta} \equiv \langle i:\alpha \ldots l:\beta|\,k(i,\ldots l)\,|\,i:\gamma \ldots l:\delta\rangle$$

(independent of $i, \ldots l$)

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

Example : particle-number operator

First-quantised form is given by

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

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

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

Then the second-quantised form reads

$$N = \sum_{\alpha\beta} h_{\alpha\beta}\, a^{+}_{\alpha} a_{\beta} = \sum_{\alpha} a^{+}_{\alpha} a_{\alpha}$$

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

→ States of $\mathcal{H}_K$ are eigenstates of N with eigenvalue K

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

Then consider $\quad [N, a^{+}_{\alpha_1}] = \sum_{\alpha} h_{\alpha\alpha_1} a^{+}_{\alpha} = a_{\alpha_1}$

Repeat

$$\begin{aligned} [N, a^{+}_{\alpha_2} a^{+}_{\alpha_1}] &= a^{+}_{\alpha_2}[N, a^{+}_{\alpha_1}] + [N, a^{+}_{\alpha_2}]\, a^{+}_{\alpha_1} \\ &= a^{+}_{\alpha_2} a^{+}_{\alpha_1} + a^{+}_{\alpha_2} a^{+}_{\alpha_1} \\ &= 2\, a^{+}_{\alpha_2} a^{+}_{\alpha_1} \end{aligned}$$

Again $\quad [N, a^{+}_{\alpha_3} a^{+}_{\alpha_2} a^{+}_{\alpha_1}] = \ldots = 3\, a^{+}_{\alpha_3} a^{+}_{\alpha_2} a^{+}_{\alpha_1}$

k-times $\left[N, a^{\dagger}_{\alpha_k} \dots a^{\dagger}_{\alpha_2} a^{\dagger}_{\alpha_1}\right] = k\, a^{\dagger}_{\alpha_k} \dots a^{\dagger}_{\alpha_2} a^{\dagger}_{\alpha_1}$

Apply on basis state of $\mathcal{H}_k$

$$N\,|\alpha_k \dots \alpha_2 \alpha_1\rangle = N\, a^{\dagger}_{\alpha_k} \dots a^{\dagger}_{\alpha_2} a^{\dagger}_{\alpha_1}\,|0\rangle$$

$$= \left[N, a^{\dagger}_{\alpha_k} \dots a^{\dagger}_{\alpha_2} a^{\dagger}_{\alpha_1}\right]|0\rangle + \cancel{a^{\dagger}_{\alpha_k} \dots a^{\dagger}_{\alpha_2} a^{\dagger}_{\alpha_1} N\,|0\rangle}$$

$$= k\,|\alpha_k \dots \alpha_2 \alpha_1\rangle$$

Example : Nuclear Hamiltonian

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

i) explicitly antisymmetrised on the right

ii) not normalised

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

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

Then

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

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

In first quantisation, nuclear Hamiltonian reads

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

Second-quantised form

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

where antisymmetrised three-body matrix elements are defined as

$$
\begin{aligned}
\overline{W}_{\alpha\beta\gamma\delta\varepsilon\zeta} \equiv \; & W_{\alpha\beta\gamma\delta\varepsilon\zeta} \\
& - W_{\alpha\beta\gamma\delta\zeta\varepsilon} \\
& - W_{\alpha\beta\gamma\zeta\varepsilon\delta} \\
& - W_{\alpha\beta\gamma\varepsilon\delta\zeta} \\
& + W_{\alpha\beta\gamma\varepsilon\zeta\delta} \\
& + W_{\alpha\beta\gamma\zeta\delta\varepsilon}
\end{aligned}
$$

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