Second quantisation I

Second quantisation

(Suggested reading: AGD, § 3
Landau – Lifshitz, v.3 § 64–65, „Second quantisation")

One may describe a quantum system of N identical particles by specifying their wavefunction.

Each particle may be in one of states $\psi_1(\vec{r}_1), \psi(\vec{r}_2), \ldots$ (orth., norm) – they form a complete set

Many-particle w.f.

$$\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N, t)$$

$|\Psi(\vec{r}_1, \vec{r}_2, \ldots, \vec{r}_N)|^2 d\vec{r}_1 \ldots d\vec{r}_N$ is the probability to find particle 1 in the element $d\vec{r}_1$ around location $\vec{r}_1$, particle 2 in the element $d\vec{r}_2$ around location $\vec{r}_2$, etc.

The method of second quantisation is a method of describing a system of particles in different variables: the number of particles in each quantum state. In other words, the system is described by a wavefunction $c(n_1, n_2, \dots, n_k, \dots, t)$

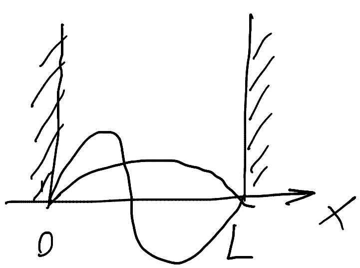
The number of particles in the 1st quantum state

particles in the 2nd state

$|c(n_1, n_2, \dots, n_k, \dots, t)|^2$ – the probability to find n_1 particles in the 1st state, n_2 in the 2nd, ...

Example: a rectangular box:

Single-particle w.f.s



$$\Psi_k = \sqrt{\frac{2}{L}} \sin\left(\frac{k\pi}{L} x\right), \quad k = 1, 2, 3, \dots$$

$$|n_1 n_2 n_3 \dots\rangle$$

Number of particles with $k=1$

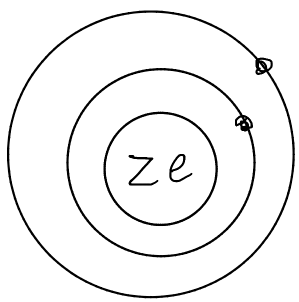
Number of particles with $k=2$

$$\left(\Psi = \sum_{n_1, n_2, \dots} c(n_1, n_2 \dots) |n_1 n_2 \dots\rangle\right)$$

$n_1, n_2, \ldots$

Example:

hydrogen-like atom (a charged core attracting electrons)



n	l	σ_z
1	0	$\pm\frac{1}{2}$
2	0, 1	$\pm\frac{1}{2}$
3	......	

$$|n_1 \; n_2 \; n_3 \ldots\rangle$$

# of electrons in 1S with $\uparrow$

# of electrons in 1S with $\downarrow$

with $\uparrow$

# of electrons in ...

# of electrons in 2S with ↑

As an example, consider a system of <u>bosons</u>

// Reminder $\Psi(\vec{r}_1, \ldots, \vec{r}_i, \ldots, \vec{r}_k, \ldots) = \Psi(\vec{r}_1, \ldots, \vec{r}_k, \ldots, \vec{r}_i, \ldots)$

<u>Non-interacting bosons</u>

$$|n_1, n_2, \ldots, n_k, \ldots\rangle \leftrightarrow \left(\frac{n_1!\, n_2! \ldots n_k! \ldots}{N!}\right)^{\frac{1}{2}} \sum_{\substack{\text{Permutations} \\ \text{of } k_1, k_2, \ldots}} \psi_{k_1}(\vec{r}_1)\, \psi_{k_2}(\vec{r}_2) \ldots$$

<u>Non-interacting fermions</u>

$$|n_1, n_2, \ldots, n_k, \ldots\rangle \leftrightarrow \frac{1}{\sqrt{N!}} \sum_{\text{Permutations}} (-1)^{P\{k\}}\, \psi_{k_1}(\vec{r}_1)\, \psi_{k_2}(\vec{r}_2) \ldots$$

where $P\{k\} = 1$ for $k_1 < k_2 < \ldots$

Because the fermionic wavefunction is antisymmetric with respect to all variables, each occupation number n_i is either 0 or 1

$|0\,0\,0\ldots\rangle$ — <u>Vacuum</u>

Creation and annihilation operators defined both for bosons and for fermions

$$\hat{a}_i\,|n_1,\ldots,n_i,\ldots\rangle = \sqrt{n_i}\,|n_1,\ldots,n_i-1,\ldots\rangle$$

(if the state with n_i-1 particles doesn't exist, i.e. $n_i=0$, then this is 0)

$$\hat{a}_i^+\,|n_1,\ldots,n_i+1,\ldots\rangle = \sqrt{n_i+1}\,|n_1,\ldots,n_i+1,\ldots\rangle$$

(provided this state exists,

otherwise 0)

Consider the fermionic case specifically:

$$\hat{a}_i |\ldots, \underset{\substack{\uparrow \\ i\text{-th}}}{0}, \ldots\rangle = 0$$

$$\hat{a}_i^+ |\ldots, \underset{\substack{\uparrow \\ i\text{-th}}}{1}, \ldots\rangle = 1$$

i-th state is either empty or filled

$$\hat{a}_i |\ldots, 1, \ldots\rangle = |\ldots, 0, \ldots\rangle$$

$$\hat{a}_i^+ |\ldots, 1, \ldots\rangle = 0$$

Operators $\hat{a}_i$ and $\hat{a}_i^+$ are Hermitian-conjugate to each other, as can be seen from finding their matrix elements

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. Matrix elements for bosons

Matrix elements for bosons

$$\langle n_1, \dots, n_i, \dots | \hat{a}_i | n_1, \dots, n_i+1, \dots \rangle = \sqrt{n_i+1}$$

$$\langle n_1, \dots, n_i+1, \dots | \hat{a}_i | n_1, \dots, n_i, \dots \rangle = \sqrt{n_i+1}$$

Indeed, $\hat{a}_i^+ = \hat{a}_i$

Matrix elements for fermions

Consider the operator $\hat{a}_i^+ \hat{a}_k$

$$\langle \dots, \underset{\substack{\uparrow \\ i\text{-th}}}{1}, \dots, \underset{\substack{\uparrow \\ k\text{-th}}}{0}, \dots | \hat{a}_i^+ a_k | \dots, \underset{\substack{\uparrow \\ i\text{-th}}}{0}, \dots, \underset{\substack{\uparrow \\ k\text{-th}}}{1}, \dots \rangle = (-1)^{\sum_{l=i+1}^{l=k-1} n_l}$$

$$\langle \dots, 0, \dots | \hat{a}_i | \dots, 1, \dots \rangle = (-1)^{\sum_{l=1}^{i-1} n_l}$$

$$\rotatebox{-60}{$=$}$$

$$\langle \dots, \underset{\substack{\uparrow \\ i\text{-th}}}{1}, \dots | \hat{a}_i^+ | \dots, 0, \dots \rangle$$

One can also see that $\hat{a}_i^+ = (\hat{a}_i)^+$

Operator of the number of particles

Consider the operator $\hat{a}_i^+ \hat{a}_i$

$$\hat{a}_i^+ \hat{a}_i |n_1, \ldots, n_i, \ldots\rangle = n_i |n_1, \ldots, n_i, \ldots\rangle$$

Do that in detail

So, $\boxed{\hat{n}_i = \hat{a}_i^+ \hat{a}_i}$

One may also consider the operator $\hat{a}_i \hat{a}_i^+$

For bosons, $\hat{a}_i \hat{a}_i^+ |n_1, \ldots, n_i, \ldots\rangle = (n_i + 1) |n_1, \ldots, n_i, \ldots\rangle$

Do that in detail too

So, for bosons, $\hat{n}_i + 1 = \hat{a}_i \hat{a}_i^+$

$$\boxed{\hat{a}_i \hat{a}_i^+ - \hat{a}_i^+ \hat{a}_i = 1} \quad (\text{bosons!})$$

For fermions

$$\begin{cases} \hat{a}_i \hat{a}_i^+ |\ldots, 0, \ldots\rangle = |\ldots, 0, \ldots\rangle \\ \hat{a}_i \hat{a}_i^+ |\ldots, 1, \ldots\rangle = 0 \end{cases} \qquad \begin{cases} \hat{a}_i^+ \hat{a}_i |\ldots, 0, \ldots\rangle = 0 \\ \hat{a}_i^+ \hat{a}_i |\ldots, 1, \ldots\rangle = |\ldots, 1, \ldots\rangle \end{cases}$$

So, for fermions $\hat{a}_i \hat{a}_i^+ = 1 - \hat{n}_i$

$$\boxed{\hat{a}_i \hat{a}_i^+ + \hat{a}_i^+ \hat{a}_i = 1} \quad (\text{fermions!})$$

Generic commutation relations

From the definition of bosonic creation and annihilation operators it follows that

$$\hat{a}_i \hat{a}_k^+ = \hat{a}_k^+ a_i \quad \forall\, i \neq k$$

$$\boxed{[\hat{a}_i, \hat{a}_k^+] \equiv \hat{a}_i \hat{a}_k^+ - \hat{a}_k^+ \hat{a}_i = \delta_{ik}}$$

Similarly, $[\hat{a}_i, \hat{a}_k] = 0$, $[\hat{a}_i^+, \hat{a}_k^+] = 0$

Fermionic operators

$$\hat{a}_i \hat{a}_k^+ = - \hat{a}_k^+ \hat{a}_i$$

$$\boxed{\{\hat{a}_i, \hat{a}_k^+\} \equiv \hat{a}_i \hat{a}_k^+ + \hat{a}_k^+ \hat{a}_i = \delta_{ik}}$$

$$\{\hat{a}_i, \hat{a}_k\} = 0 \quad , \quad \{\hat{a}_i^+, \hat{a}_k^+\} = 0$$

Generically, in physics sets of operators are often called fermionic if $\{\hat{A}, \hat{B}\} = 0$ and bosonic if $[\hat{A}, \hat{B}] = 0$