SECOND QUANTIZATION

Lecture notes with course Quantum Theory

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Second Quantization

1. Introduction and history

Second quantization is the standard formulation of *quantum many-particle theory.* It is important for use both in *Quantum Field Theory* (because a quantized field is a qm operator with *many degrees of freedom*) and in *(Quantum) Condensed Matter Theory* (since matter involves *many particles*).

Identical (= indistinguishable) particles $\longrightarrow$ state of two particles must either be symmetric or anti-symmetric under exchange of the particles.

$$|a \otimes b\rangle_B = \frac{1}{\sqrt{2}}\left(|a_1 \otimes b_2\rangle + |a_2 \otimes b_1\rangle\right) \qquad \text{bosons; symmetric} \tag{1a}$$

$$|a \otimes b\rangle_F = \frac{1}{\sqrt{2}}\left(|a_1 \otimes b_2\rangle - |a_2 \otimes b_1\rangle\right) \qquad \text{fermions; anti-symmetric} \tag{1b}$$

Motivation: why do we need the "second quantization formalism"?

(a) for practical reasons: computing matrix elements between N-particle symmetrized wave functions involves $(N!)^2$ terms (integrals); see the symmetrized states below.

(b) it will be extremely useful to have a formalism that can handle a non-fixed particle number N, as in the grand-canonical ensemble in Statistical Physics; especially if you want to describe processes in which particles are created and annihilated (as in typical high-energy physics accelerator experiments). So: both for Condensed Matter and High-Energy Physics this formalism is crucial!

(c) To describe interactions the formalism to be introduced will be vastly superior to the wave-function- and Hilbert-space-descriptions.

Some historical remarks

1927: Dirac - Field theory of the electromagnetic field using *creation and annihilation operators.*
1927: Jordan & Klein and 1928: Jordan & Wigner - Note that Dirac's description is also useful for many-particle systems in which particles may interact (!).
1932: Fock - Invented *Fock space*
For more history see an article in *Physics Today*, Oct.'99, about Pascual Jordan (1902-1980; who never received a Nobel prize; Dirac received his in 1933, Wigner in 1963).

The spin-statistics theorem: Particles of integer spin $(0, \hbar, 2\hbar, \ldots)$ are bosons, particles of half-integer spin $(\hbar/2, 3\hbar/2, 5\hbar/2, \ldots)$ are fermions.
The proof of this theorem needs the *relativistic theory of quantized field* and is beyond the scope of this course. Also: the proof is very complicated, which is unfortunate for such a fundamental, important result of theoretical physics.

2. The N-boson system

One-boson Hilbert space $\mathcal{E}_1$

complete set of physical properties $\hat{k}$; quantum numbers k;
basis: $\{|k\rangle\}$.

N bosons: product space: $\mathcal{E}_N = \mathcal{E}_1^{(1)} \otimes \mathcal{E}_1^{(2)} \otimes \cdots \otimes \mathcal{E}_1^{(N)}$
basis states: $|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle$
(Note: all k_i can take on all values in $\hat{k}$-spectrum)

Subspace of fully symmetrized states: $\mathcal{E}_N^{(s)}$

$$|k_1 \ldots k_N\rangle \equiv \hat{S}|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle = \frac{1}{N!} \sum_P |k_{P1}^{(1)} k_{P2}^{(2)} \ldots k_{PN}^{(N)}\rangle \tag{2}$$

$\hat{S}$ is the symmetrization operator, working on a general N-particle state.
The set of symmetrized states is complete:

$$\textit{completeness} \qquad \sum_{k_1 \ldots k_N} |k_1 \ldots k_N\rangle\langle k_1 \ldots k_N| = \hat{1} \quad \text{in} \quad \mathcal{E}_N^{(s)} \ , \tag{3}$$

but not normalized(!):

$$\langle k_1 \ldots k_N | k_1' \ldots k_N'\rangle = \frac{1}{N!} \sum_P \delta(k_{P1}, k_1')\delta(k_{P2}, k_2') \ldots \delta(k_{PN}, k_N') \tag{4}$$

Notation: In formula (3) and in the following sums over k should be read as integrals over k in case the spectrum of $\hat{k}$ is continuous. Even though a sum is written the formulae should be understood as covering both the cases of discrete and continuous spectra.

Remark: The symmetrized states are not orthonormal because the RHS (right-hand side) of (4) will in general be smaller than 1, i.e. the basis vectors are *shorter* than 1.

$\hat{k}$-spectrum: $\{a, b, c, \ldots\}$
occupation numbers: $n_a, n_b, n_c, \ldots$ with $\sum_k n_k = N$
Notation for state in **occupation number representation**: $\{n_a, n_b, n_c, \ldots; N\} \equiv \{n_k; N\}$

Orthonormalized, complete set of states:

$$\big|\{n_k; N\}\big\rangle \equiv |n_a, n_b, \ldots; N\rangle = \left(\frac{N!}{\prod_k n_k!}\right)^{\frac{1}{2}} |k_1 \ldots k_N\rangle \tag{5}$$

NB: This only works for a discrete spectrum! (for obvious reasons). One can show orthonormality and completeness for these states:

$$\textit{orthonormality} \qquad \langle \{n_k; N\} | \{n'_k; N\} \rangle \; = \; \prod_k \delta_{n_k n'_k} \tag{6}$$

$$\textit{completeness} \qquad \sum_{\{n_k;N\}} \Big| \{n_k; N\} \rangle \langle \{n_k; N\} \Big| \; = \; \hat{1} \quad \text{in} \quad \mathcal{E}_N^{(s)} \; , \tag{7}$$

For ease of notation and because it works for both discrete **and** continuous spectra, we will work with the (non-orthonormal) symmetrized basis $\{|k_1 \dots k_N\rangle\}$ in the following.
Physical properties for the N-boson system:
one-body operator:

$$\hat{F}_N = \sum_i \hat{f}^{(i)} \; , \tag{8}$$

where $\hat{f}^{(i)}$ is a one-particle operator, e.g. $\hat{p}^2/2m$.
two-body operator:

$$\hat{G}_N = \tfrac{1}{2} \sum_{i \neq j} \hat{g}^{(i,j)} \; , \tag{9}$$

with $\hat{g}^{(i,j)} = \hat{g}^{(j,i)}$ a two-particle operator, e.g. $V\left(|\hat{\vec{r}}_i - \hat{\vec{r}}_j|\right)$.
In the k-representation in $\mathcal{E}_N^{(s)}$ the operators $\hat{F}_N$ and $\hat{G}_N$ take the form:

$$\hat{F}_N = N \sum_{k_1 k'_1} \sum_{k_2 \dots k_N} |k_1 k_2 \dots k_N\rangle f(k_1, k'_1) \langle k'_1 k_2 \dots k_N| \tag{10}$$

with $f(k_1, k'_1) \equiv \langle k_1 | \hat{f}^{(1)} | k'_1 \rangle$. Similarly:

$$\hat{G}_N = \frac{N(N-1)}{2} \sum_{k_1 k'_1 k_2 k'_2} \sum_{k_3 \dots k_N} |k_1 k_2 k_3 \dots k_N\rangle g(k_1, k_2; k'_1, k'_2) \langle k'_1 k'_2 k_3 \dots k_N| \tag{11}$$

with $g(k_1, k_2; k'_1, k'_2) \equiv \langle k_1^{(1)} k_2^{(2)} | \hat{g}^{(1,2)} | k_1'^{(1)} k_2'^{(2)} \rangle$.

Note that because of the use of symmetrized states and the symmetric form of the operators $\hat{F}_N$ and $\hat{G}_N$, these operators can be expressed in terms of matrix elements of one- and two-body operators between one- and two-particle states, respectively.

In this section, we have been concerned with the complication of the requirement of symmetrization, in the next section we will tackle the unifying description for an arbitrary number of particles, which is the actual purpose of the formalism.

3. The many-boson system

a. "The big picture"

a1. Fock space

$$\mathcal{E} = \mathcal{E}_0 \oplus \mathcal{E}_1 \oplus \mathcal{E}_2^{(s)} \oplus \mathcal{E}_3^{(s)} \oplus \cdots \tag{12}$$

The space $\mathcal{E}_0$ consists of only one state: the *vacuum* state: $|0\rangle$.
A linear operator $\hat{A}$ on $\mathcal{E}$ is represented as a *very big* matrix, which can be subdivided into (N, N')-blocks, with N, N' the corresponding fixed-particle-number subspaces of $\mathcal{E}$.

a2. Creation- and annihilation-operators

Creation- and annihilation-operators $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ will be introduced. These will have non-zero matrix elements only in (N, N') blocks which differ by one in particle number.

a3. Many-body operators $\hat{O}$

All many-body operators can be expressed in the fundamental operators, the creation- and annihilation-operators.
Example: The Bose-Hubbard model (or: boson Hubbard model)

$$\hat{H}_{\mathrm{BH}} = -\sum_{\langle i,j\rangle} t_{ij}\left(\hat{b}_i^\dagger \hat{b}_j + \hat{b}_j^\dagger \hat{b}_i\right) + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) \tag{13}$$

where $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$ is the number operator, counting the number of bosons on site i of a lattice. There will be an interaction energy U if there are two bosons on a site. The first term is a *hopping* term for bosons hopping between neighboring sites j and i.

b. "Details" (getting specific)

b1. Creation- and annihilation-operators

Definition of creation operator:

$$\hat{a}^\dagger(k)|0\rangle = |k\rangle \tag{14a}$$

$$\hat{a}^\dagger(k)|k_1 \ldots k_N\rangle = \sqrt{N+1}\,|kk_1 \ldots k_N\rangle \tag{14b}$$

Therefore:

$$|k_1 \ldots k_N\rangle = \frac{1}{\sqrt{N!}}\hat{a}^\dagger(k_1)\ldots\hat{a}^\dagger(k_N)|0\rangle \tag{15}$$

Matrix for $\hat{a}^\dagger(k)$: From this definition for $\hat{a}^\dagger(k)$ one can derive the matrix elements of $\hat{a}^\dagger(k)$ in Fock space: (take $N' = N-1$)

$$\langle k_1 \ldots k_N|\hat{a}^\dagger(k)|k_1' \ldots k_{N-1}'\rangle = \sqrt{N}\langle k_1 \ldots k_N|kk_1' \ldots k_{N-1}'\rangle$$

$$= \frac{\sqrt{N}}{N!}\sum_P \delta(k_{P1}, k)\delta(k_{P2}, k_1')\ldots\delta(k_{PN}, k_{N-1}')$$

$$= \frac{\sqrt{N}}{N!}(N-1)!\left\{\delta(k_1,k)\langle k_2 \ldots k_N|k_1' \ldots k_{N-1}'\rangle + \delta(k_2,k)\langle k_1 k_3 \ldots k_N|k_1' \ldots k_{N-1}'\rangle + \cdots\right\}$$

$$= \frac{1}{\sqrt{N}}\left\{\sum_{i=1}^N \delta(k_i,k)\langle k_1 \ldots k_{i-1}k_{i+1}\ldots k_N|\right\}k_1' \ldots k_{N-1}'\rangle \tag{16}$$

In the first two steps we have used equations (14b) and (4), respectively. In the third step, we split the sum over permutations ($N!$ terms) into N sums with $(N-1)!$ terms each, in which the first sum is over all permutations with $P1 = 1$, the second sum over all permutations with $P1 = 2$, etc. In the second term, $P2$ to PN then take values $1, 3, \ldots N$. In the last step, the expression is written more compactly.

Matrix for $\hat{a}(k)$: Now the matrix elements of $\hat{a}(k)$ are easily derived by making use of: $\langle\omega'|\hat{a}|\omega\rangle = \langle\omega|\hat{a}^\dagger|\omega'\rangle^\star$. For the $(N, N' = N+1)$ block we find:

$$\langle k'_1 \dots k'_{N-1}|\hat{a}(k)|k_1 \dots k_N\rangle = \langle k_1 \dots k_N|\hat{a}^\dagger(k)|k'_1 \dots k'_{N-1}\rangle^\star =$$

$$= \langle k'_1 \dots k'_{N-1}| \left\{ \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \delta(k_i, k)|k_1 \dots k_{i-1}k_{i+1} \dots k_N\rangle \right\} \,, \qquad (17)$$

from which it follows how $\hat{a}(k)$ operates in Fock space :

$$\hat{a}(k)|0\rangle = 0 \qquad (18a)$$

$$\hat{a}(k)|k_1 \dots k_N\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} \delta(k, k_i)|k_1 \dots k_{i-1}k_{i+1} \dots k_N\rangle \qquad (18b)$$

Note that (18b) is more complicated than the lowering operator for the simple harmonic oscillator, $\hat{a}|n\rangle = \sqrt{n}|n-1\rangle$, because there is more choice in what to lower/annihilate. If all k_i equal k, one recovers a similar result as for the simple harmonic oscillator.

It is important to note that (14a) implies:

$$\langle k| = \langle 0|\hat{a}(k) \qquad (19)$$

(therefore the annihilation operator working to the left acts as a creation operator; these names are therefore just a convention!)

b2. Commutation relations

From the results in section b1. the fundamental algebraic relations, i.e. the commutation relations, between the $\hat{a}^\dagger(k)$ and $\hat{a}(k)$ follow directly (work this out for yourself!):

$$\left[\hat{a}^\dagger(k), \hat{a}^\dagger(\ell)\right] = \hat{0} \qquad (20a)$$

$$[\hat{a}(k), \hat{a}(\ell)] = \hat{0} \qquad (20b)$$

$$\left[\hat{a}(k), \hat{a}^\dagger(\ell)\right] = \delta(k, \ell)\, \hat{1} \qquad (20c)$$

NB1: The commutation relation (20c) only takes on this elegant form because of the **factor** $\sqrt{N+1}$ in the definition of $\hat{a}^\dagger(k)$, (14b).

NB2: The commutation relations (20) are now just as we saw them for **phonons** and **independent harmonic oscillators** before.

NB3: The commutation relations are a **consequence of symmetry**! Note that the same in a certain sense is true for the canonical commutation relation $[X, P] = \hbar i \hat{1}$ (see Ch. 8 of Le Bellac).

b3. Many-body operators $\hat{F}$ and $\hat{G}$ in Fock space

$$\hat{F} = \sum_{N=1}^{\infty} \hat{F}_N = \sum_{N=1}^{\infty} \sum_i \hat{f}^{(i)} \tag{21}$$

Now use:

$$|k_1\rangle\langle k_1'| = \hat{a}^\dagger(k_1)|0\rangle\langle 0|\hat{a}(k_1') \tag{22}$$

and:

$$N|k_1 k_2 \dots k_N\rangle\langle k_1' k_2 \dots k_N| = \hat{a}^\dagger(k_1)|k_2 \dots k_N\rangle\langle k_2 \dots k_N|\hat{a}(k_1') \tag{23}$$

Using formula (10), $\hat{F}$ is found to be:

$$\hat{F} = \sum_{k_1,k_1'} \hat{a}^\dagger(k_1) f(k_1,k_1') \left[|0\rangle\langle 0| + \sum_{k_2} |k_2\rangle\langle k_2| + \cdots \right] \hat{a}(k_1') \tag{24}$$

The expression between the large brackets [,] is precisely the identity in $\mathcal{E}$, because of the completeness of the basis of symmetrized states in $\mathcal{E}_N^{(s)}$. The final result for the general form of a many-body operator constructed from one-particle operators in the second quantization formalism therefore is:

$$\hat{F} = \sum_{k_1,k_1'} \hat{a}^\dagger(k_1) f(k_1,k_1') \hat{a}(k_1') \tag{25}$$

Using more ink and formula (11), but completely analogously (*peeling off* two k's) one derives the general form for the many-body operator constructed from two-particle operators:

$$\hat{G} = \tfrac{1}{2} \sum_{k_1,k_2,k_1',k_2'} \hat{a}^\dagger(k_1)\hat{a}^\dagger(k_2) g(k_1,k_2;k_1',k_2') \hat{a}(k_2')\hat{a}(k_1') \tag{26}$$

4. Identical spin-0 particles

Application of the preceding: form of operators in *Second Quantization* for identical particles with mass m and spin 0 (bosons!).

Discrete $\vec{k}$-representation

In $\mathcal{E}_1$: $\hat{\vec{k}}$-basis: $\left\{|\vec{k}\rangle\right\}$

discrete $\Leftrightarrow$ periodicity volume $V = L^3$

$\vec{k} = \frac{2\pi}{L}\vec{n}$ with n_x, n_y, n_z integer numbers.

The creation- and annihilation-operators are written as: $\hat{a}_{\vec{k}}^\dagger$ and $\hat{a}_{\vec{k}}$

a. What is the form of many-body operators $\hat{F}$?

General procedure: (i) determine matrix elements

$$f(\vec{k},\vec{k}') = \langle\vec{k}|\hat{f}^{(1)}|\vec{k}'\rangle \tag{27}$$

(ii) Using (i):

$$\hat{F} = \sum_{\vec{k},\vec{k}'} \hat{a}^{\dagger}_{\vec{k}} f(\vec{k},\vec{k}') \hat{a}_{\vec{k}'} \tag{28}$$

Examples

1. $\hat{f} = |\vec{k}\rangle\langle\vec{k}| \quad \longrightarrow \quad f(\vec{k}',\vec{k}'') = \langle\vec{k}'|\vec{k}\rangle\langle\vec{k}|\vec{k}''\rangle = \delta_{\vec{k}',\vec{k}}\delta_{\vec{k},\vec{k}''} \quad \longrightarrow$

$$\hat{F} = \sum_{\vec{k}',\vec{k}''} \hat{a}^{\dagger}_{\vec{k}'}\, \delta_{\vec{k}',\vec{k}}\, \delta_{\vec{k},\vec{k}''}\, \hat{a}_{\vec{k}''} = \hat{a}^{\dagger}_{\vec{k}}\, \hat{a}_{\vec{k}} \equiv \hat{n}_{\vec{k}} \tag{29}$$

operator: **number of particles with wave vector $\vec{k}$**

2. $\hat{f} = \hat{1} \quad \longrightarrow \quad$ (Use 1. and $\hat{1} = \sum_{\vec{k}} |\vec{k}\rangle\langle\vec{k}|$)

$$\hat{F} = \sum_{\vec{k}} \hat{n}_{\vec{k}} \equiv \hat{N} \tag{30}$$

operator: **total particle number**

3. $\hat{f} = \frac{\hat{\vec{p}}^2}{2m} \quad \longrightarrow \quad f(\vec{k},\vec{k}') = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) \delta_{\vec{k},\vec{k}'}$

$$\hat{F} = \cdots = \sum_{\vec{k}} \varepsilon_k\, \hat{n}_{\vec{k}} \equiv \hat{H}^{(0)} \tag{31}$$

where $\varepsilon_k \equiv \hbar^2 k^2/2m$.
operator: **kinetic energy of many-boson system**

4. (Non-diagonal in $\vec{k}$-representation) external potential $u(\vec{r})$

To compute the necessary $(\vec{k},\vec{k}')$ matrix element it is convenient to switch to the $\vec{r}$-representation (insert two complete sets of states):

$$\langle\vec{k}|u(\vec{r})|\vec{k}'\rangle = \int_V d\vec{r} \int_V d\vec{r}\,'\, \langle\vec{k}\,|\vec{r}\rangle\langle\vec{r}\,|u(\vec{r})|\vec{r}\,'\rangle\langle\vec{r}\,'\,|\vec{k}'\rangle$$

with:

$$\langle\vec{r}\,|\vec{k}\rangle = \frac{1}{\sqrt{V}}\, e^{i\vec{k}\cdot\vec{r}} \qquad (\star)$$

and use that

$$\int_V d\vec{r}\,|\vec{r}\,\rangle\langle\vec{r}\,| = \hat{1}$$

Defining the Fourier components, c.q. transform, as follows:

$$u_{\vec{q}} = \frac{1}{\sqrt{V}} \int_V d\vec{r}\; e^{-i\vec{q}\cdot\vec{r}}\, u(\vec{r}) \tag{32a}$$

(as a result:

$$u(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{\vec{q}} u_{\vec{q}}\; e^{i\vec{q}\cdot\vec{r}} \tag{32b}$$),

one finds (this is one of the problems in Problem Session 6):

$$\hat{F} \longrightarrow \hat{U} = \frac{1}{\sqrt{V}} \sum_{\vec{k},\vec{k}'} \hat{a}^{\dagger}_{\vec{k}}\, u_{\vec{k}-\vec{k}'}\, \hat{a}_{\vec{k}'} = \sum_{\vec{q}} \frac{u_{\vec{q}}}{\sqrt{V}} \sum_{\vec{k}'} \hat{a}^{\dagger}_{\vec{k}'+\vec{q}} \hat{a}_{\vec{k}'} \tag{33}$$

operator: **potential energy of many-boson system**

NB: The Fourier component that appears in the potential energy is the one corresponding to the difference wave vector $\vec{k} - \vec{k}'$ of the two wave vectors of the creation- and annihilation-operators: interaction happens with *conservation of momentum*.

b. Intermezzo: Change of representation and continuous $\vec{k}$-representation

(i) The basic formula for a change of representation is:

$$\hat{a}^{\dagger}(q) = \sum_{k} \hat{a}^{\dagger}(k)\, \langle k|q\rangle \qquad (I.1)$$

It's Hermitian conjugate is:

$$\hat{a}(q) = \sum_{k} \langle q|k\rangle\, \hat{a}(k) \qquad (I.2)$$

Note that we only need the scalar product $\langle k|q\rangle$ of one-particle basis states to switch representation, even for a description of many-body systems.

The above can be shown very elegantly in Dirac notation, as follows. For the q-representation we have:

$$\hat{a}^{\dagger}(q)|0\rangle = |q\rangle \qquad (I.3a)$$

$$\hat{a}^{\dagger}(q)|q_1 \dots q_N\rangle = \sqrt{N+1}|qq_1 \dots q_N\rangle \qquad (I.3b)$$

For one particle we have:

$$|q\rangle = \sum_{k} |k\rangle\langle k|q\rangle \qquad (I.4)$$

Then, symmetrizing state

$$|q_1^{(1)} \dots q_N^{(N)}\rangle = \sum_{k_1 \dots k_N} |k_1^{(1)} \dots k_N^{(N)}\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle$$

gives:

$$|q_1 \dots q_N\rangle = \sum_{k_1 \dots k_N} |k_1 \dots k_N\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle \qquad (I.5)$$

Now the expression of $\hat{a}^{\dagger}(q)$ in terms of the $\hat{a}^{\dagger}(k)$, formula (I.1), follows from:

$$\hat{a}^{\dagger}(q)|q_1 \dots q_N\rangle = \sqrt{N+1}|qq_1 \dots q_N\rangle =$$

$$= \sqrt{N+1} \sum_{kk_1 \dots k_N} |kk_1 \dots k_N\rangle\langle k|q\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle$$

$$= \sum_{kk_1 \ldots k_N} \hat{a}^\dagger(k)|k_1 \ldots k_N\rangle\langle k|q\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle$$

$$= \sum_k \hat{a}^\dagger(k)\langle k|q\rangle \left[\sum_{k_1 \ldots k_N} |k_1 \ldots k_N\rangle\langle k_1|q_1\rangle \cdots \langle k_N|q_N\rangle \right]$$

Because the expression between the big brackets is according to (I.5) precisely $|q_1 \ldots q_N\rangle$ and this holds for a general state $|q_1 \ldots q_N\rangle$ in Fock space, we have proven the change-of-representation formula (I.1).

(ii) continuous $\vec{k}$-representation: to change from the **discrete** $\vec{k}$-representation to the **continuous** $\vec{k}$-representation one just needs to rescale the state vectors:

$$|\vec{k}\rangle_{\text{continuous}} = \left(\frac{L}{2\pi}\right)^{3/2} |\vec{k}\rangle_{\text{discrete}} = \frac{\sqrt{V}}{(2\pi)^{3/2}} |\vec{k}\rangle_{\text{discrete}} \qquad (I.6)$$

This rescaling arises because in the continuum limit, $L \longrightarrow \infty$, sums over discrete $\vec{k}$ turn into integrals over continuous $\vec{k}$ as follows:

$$\frac{1}{L^3} \sum_{\vec{k}} \cdots \qquad \longrightarrow \qquad \int \frac{d\vec{k}}{(2\pi)^3} \cdots \qquad (I.7)$$

(see also section 9.6.2 in Le Bellac). As a result we have:

$$\langle\vec{r}\,|\vec{k}\rangle_{\text{discrete}} = \frac{1}{\sqrt{V}}\, e^{i\vec{k}\cdot\vec{r}} \qquad \text{and} \qquad \langle\vec{r}\,|\vec{k}\rangle_{\text{continuous}} = \frac{1}{(2\pi)^{3/2}}\, e^{i\vec{k}\cdot\vec{r}} \qquad (I.8)$$

(This explains the seeming discrepancy between ($\star$) above and (9.21)-(9.22) in Le Bellac). The completeness relations in the two $\vec{k}$-representations then read as we are used to:

$$\sum_{\vec{k}} |\vec{k}\rangle_{d\ d}\langle\vec{k}| = \hat{1} \qquad \text{and} \qquad \int d\vec{k}\ |\vec{k}\rangle_{c\ c}\langle\vec{k}| = \hat{1} \qquad (I.9)$$

(d: discrete, c: continuous).

c. Quantum fields: the $\vec{r}$-representation

Instead of the discrete (or: continuous) $\vec{k}$-representation, one can also present the whole formalism in the (continuous) $\vec{r}$-representation; it is customary to then call the corresponding creation- and annihilation-operators $\hat{\psi}^\dagger(\vec{r})$ and $\hat{\psi}(\vec{r})$. These operators are what we called *quantized fields* before (Ch.11 of Le Bellac). It is important not to confuse these operators with *wave functions*!

According to (I.2) and (I.8) we have:

$$\hat{\psi}(\vec{r}) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\, \hat{a}_{\vec{k}} \qquad (34a)$$

$$\hat{a}_{\vec{k}} = \frac{1}{\sqrt{V}} \int_V d\vec{r}\; e^{-i\vec{k}\cdot\vec{r}}\, \hat{\psi}(\vec{r}) \qquad (34b)$$

All many-body operators can be expressed in terms of the $\hat{\psi}^\dagger(\vec{r})$ and $\hat{\psi}(\vec{r})$. This can be done in two ways; (i) starting from a definition of $\hat{\psi}^\dagger(\vec{r})$ and $\hat{\psi}(\vec{r})$ in the $\vec{r}$-representation (just as we did for the discrete $\vec{k}$-representation above), or: (ii) starting from the expressions in the discrete $\vec{k}$-representation and using the "Fourier transform" (34a) and (34b). Some examples of the results are:

$$\hat{N} = \int d\vec{r}\; \hat{\psi}^\dagger(\vec{r})\, \hat{\psi}(\vec{r}) \qquad (35)$$

$$\hat{P} = \int d\vec{r}\; \hat{\psi}^\dagger(\vec{r})\, \frac{\hbar}{i}\frac{\partial}{\partial \vec{r}} \hat{\psi}(\vec{r}) \qquad \text{operator: } \textbf{total momentum} \qquad (36)$$

$$\hat{H}^{(0)} = \int d\vec{r}\; \hat{\psi}^\dagger(\vec{r}) \left(-\frac{\hbar^2}{2m}\Delta\right) \hat{\psi}(\vec{r}) \qquad (37)$$

where Δ is the Laplace operator ($= \left(\vec{\nabla}\right)^2$).

<u>Commutation relations</u>: the following commutation relations can be straightforwardly derived from those for the $\hat{a}^\dagger_{\vec{k}}$ and $\hat{a}_{\vec{k}}$:

$$\left[\hat{\psi}(\vec{r}), \hat{\psi}(\vec{r}\,')\right] = 0 \quad , \quad \left[\hat{\psi}^\dagger(\vec{r}), \hat{\psi}^\dagger(\vec{r}\,')\right] = 0 \quad , \quad \left[\hat{\psi}(\vec{r}), \hat{\psi}^\dagger(\vec{r}\,')\right] = \delta(\vec{r} - \vec{r}\,')\, \hat{1} \qquad (38)$$

Since the commutation relations are preserved in the change of representation (34), this change of representation is called a *canonical transformation*.
It is now straightforward to show:

$$\left[\hat{H}^{(0)}, \hat{\psi}(\vec{r})\right] = \frac{\hbar^2}{2m}\Delta\hat{\psi}(\vec{r}) \qquad (39)$$

<u>Dynamics of $\hat{a}^\dagger_{\vec{k}}$ and $\hat{a}_{\vec{k}}$</u>: This is derived in a similar way as in section 11.3.2 of LB (*Quantization of a scalar field in 1D*). For a **free** many-boson system:

$$\frac{d}{dt}\,\hat{a}_{\vec{k}}(t) = \frac{i}{\hbar}\left[\hat{H}^{(0)}, \hat{a}_{\vec{k}}(t)\right] = \frac{i}{\hbar}\sum_{\vec{k}'} \varepsilon_{k'} \left[\hat{n}_{\vec{k}'}, \hat{a}_{\vec{k}}(t)\right] = -\frac{i\varepsilon_k}{\hbar}\,\hat{a}_{\vec{k}}(t) \;\longrightarrow\; \hat{a}_{\vec{k}}(t) = \hat{a}_{\vec{k}}\, e^{-i\omega_k t} \quad (40a)$$

where $\omega_k \equiv \varepsilon_k/\hbar$ (the commutator is evaluated in one of the problems). Analogously:

$$\hat{a}^\dagger_{\vec{k}}(t) = \hat{a}^\dagger_{\vec{k}}\, e^{i\omega_k t} \qquad (40b)$$

Having obtained the above results one can understand how the name "second quantization" came about. Let us recall the time-dependent Schrödinger equation for a free particle:

$$i\hbar\frac{\partial}{\partial t}\,\psi(\vec{r},t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{r},t) \qquad (41)$$

The general solution is a linear combination of plane waves (as substitution will quickly confirm):

$$\psi(\vec{r},t) = \sum_{\vec{k}} a_{\vec{k}} \frac{e^{i(\vec{k}\cdot\vec{r}-\omega_k t)}}{\sqrt{V}} \tag{42}$$

with $\hbar\omega_k = \varepsilon_k = \hbar^2 k^2/2m$ and the $a_{\vec{k}}$ are Fourier**coefficients** (i.e. numbers!).

For the operators $\hat{\psi}(\vec{r},t)$ (Heisenberg picture) we have, in case of free bosons (using the result (39)):

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(\vec{r},t) = -\left[\hat{H}^{(0)}, \hat{\psi}(\vec{r},t)\right] = -\frac{\hbar^2}{2m}\Delta\hat{\psi}(\vec{r},t) \tag{43}$$

Combining (34a) and (40a), we find as a solution:

$$\hat{\psi}(\vec{r},t) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\hat{a}_{\vec{k}}(t) = \sum_{\vec{k}} \hat{a}_{\vec{k}} \frac{e^{i(\vec{k}\cdot\vec{r}-\omega_k t)}}{\sqrt{V}} \tag{44}$$

Comparing (43) and (44) with (41) and (42), we see that we get the *quantum theory of many particles* from the *quantum theory of one particle* by replacing the Fourier-coefficients $a_{\vec{k}}, a^*_{\vec{k}}$ by (annihilation-, creation-) operators $\hat{a}_{\vec{k}}, \hat{a}^\dagger_{\vec{k}}$! This procedure is similar as in the case of *quantizing* the classical electromagnetic field (Fourier-coefficients become operators; see also the other examples in Ch.11 LB). This purely formal resemblance of quantization procedures has led to the unfortunate name of "second quantization", which according to some should be banished, but because of it's widespread use probably never will. It is important to stress that there is no such thing as *quantizing twice*: there is only one Quantum Theory!

5. The N-fermion system

One-fermion Hilbert space $\mathcal{E}_1$

complete set of physical properties $\hat{k}$; quantum numbers k; basis: $\{|k\rangle\}$.

Now what k stands for will at least include a spin quantum number σ: e.g. k stands for: $\vec{k}\sigma$ or $\vec{r}\sigma$
N fermions: product space: $\mathcal{E}_N = \mathcal{E}_1^{(1)} \otimes \mathcal{E}_1^{(2)} \otimes \cdots \otimes \mathcal{E}_1^{(N)}$
basis states: $|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle$
(Note: all k_i can take on all values in $\hat{k}$-spectrum)

Subspace of fully **anti**-symmetrized states: $\mathcal{E}_N^{(a)}$

$$|k_1 \ldots k_N\rangle \equiv \hat{A}|k_1^{(1)} k_2^{(2)} \ldots k_N^{(N)}\rangle = \frac{1}{N!}\sum_P \mathrm{sign}(P)|k_{P1}^{(1)} k_{P2}^{(2)} \ldots k_{PN}^{(N)}\rangle \tag{45}$$

Here the anti-symmetrization operator $\hat{A}$ is defined as:

$$\hat{A} \equiv \frac{1}{N!}\sum_P \mathrm{sign}(P)\,\hat{U}_P \tag{46}$$

where $\hat{U}_P$ is the permutation operator and sign(P) denotes the *sign of the permutation*: sign(P) = +1 or -1, depending on whether the permutation consists of an even or odd number of pair exchanges, respectively (any permutation of N entities can be seen as a product of a number of pair exchanges).

As for the N-boson system, the set of anti-symmetrized states $|k_1 \ldots k_N\rangle$ is overcomplete and non-orthonormal:

$$\langle k_1 \ldots k_N | k'_1 \ldots k'_N \rangle = \frac{1}{N!} \sum_P \text{sign}(P) \delta(k_{P1}, k'_1) \delta(k_{P2}, k'_2) \ldots \delta(k_{PN}, k'_N) \tag{47}$$

Note the extra factor sign(P) compared to the bosonic case; this factor will make it even harder to reach 1, even if $k_1 = k'_1$, etc.; cf. formula (4).

Operators $\hat{F}_N$ and $\hat{G}_N$ are the same as for bosons, formulae (10) and (11).

Occupation-number representation:

$$\Big|\{n_k; N\}\rangle \equiv |n_a, n_b, \ldots; N\rangle \equiv \sqrt{N!}\, |k_1 \ldots k_N\rangle \tag{48}$$

The above formula is the analogon of formula (5) for bosons, where we have taken the *Pauli Exclusion Principle* into account, which demands that the state vector changes sign if two particles are interchanged; therefore n_k cannot be larger than 1: $n_k = 0$ or $n_k = 1$. For fermions the order is important (to determine the overall sign of the state vector); we will typically assume: $k_1 < k_2 < k_3 < \cdots < k_N$. In case k is shorthand for more quantum numbers, one has to agree on a more general convention to order the one-particle states, but this can always be done.

6. The many-fermion system

a. Fock space

$$\mathcal{E} = \mathcal{E}_0 \oplus \mathcal{E}_1 \oplus \mathcal{E}_2^{(a)} \oplus \mathcal{E}_3^{(a)} \oplus \cdots \tag{49}$$

Again the space $\mathcal{E}_0$ consists of only one state: the *vacuum* state: $|0\rangle$.

b. Creation- and annihilation operators

Definition of creation operator:

$$\hat{a}^\dagger(k)|0\rangle = |k\rangle \tag{50a}$$

$$\hat{a}^\dagger(k)|k_1 \ldots k_N\rangle = \sqrt{N+1}\, |k k_1 \ldots k_N\rangle \tag{50b}$$

Using

$$\langle \gamma | \hat{a}^\dagger(k) | \delta \rangle^* = \langle \delta | \hat{a}(k) | \gamma \rangle \tag{51}$$

with $\gamma \equiv |k_1 \dots k_N\rangle$ and $\delta \equiv |k'_1 \dots k'_{N-1}\rangle$, the operation of the annihilation operator for **fermions** turns out to be:

$$\hat{a}(k)|0\rangle = 0 \tag{52a}$$

$$\hat{a}(k)|k_1 \dots k_N\rangle = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (-1)^{i-1}\, \delta(k, k_i)|k_1 \dots k_{i-1}k_{i+1} \dots k_N\rangle \tag{52b}$$

To derive formula (52b) is a rather elaborate exercise, which is sketched below. Note that compared to (18b) for bosons we have an extra factor of $(-1)^{i-1}$ in (52b).

Derivation of (52b): Starting from (51) we consider:

$$\langle k_1 \dots k_N|\hat{a}^\dagger(k)|k'_1 \dots k'_{N-1}\rangle = \sqrt{N}\langle k_1 \dots k_N|kk'_1 \dots k'_{N-1}\rangle$$

$$= \frac{\sqrt{N}}{N!} \sum_P \operatorname{sign}(P)\delta(k_{P1}, k)\delta(k_{P2}, k'_1) \dots \delta(k_{PN}, k'_{N-1})$$

$$= \frac{\sqrt{N}}{N!}\delta(k_1, k) \sum_{P'} \operatorname{sign}(P')\delta(k_{P'2}, k'_1) \dots \delta(k_{P'N}, k'_{N-1})$$

$$+ \frac{\sqrt{N}}{N!}\,(-\delta(k_2, k)) \sum_{P''} \operatorname{sign}(P'')\delta(k_{P''1}, k'_1)\delta(k_{P''3}, k'_2) \dots \delta(k_{P''N}, k'_{N-1})$$

$$+ \quad \text{etc.},$$

where in the first step we used the definition of $\hat{a}^\dagger(k)$, in the second step formula (47); in the third step, we have split the sum over permutations P into N sums over permutations that leave 1 invariant ($P1 = 1$), take it to 2 ($P1 = 2$), etc. Since in the second term of the last step 1 and 2 have been interchanged we get an extra minus sign (we have taken: $P = P''P_{12}$, where P_{12} interchanges 1 and 2). Using (47) it is now easy to see that the sum over P' above can be written as:

$$\sum_{P'} \operatorname{sign}(P')\delta(k_{P'2}, k'_1) \dots \delta(k_{P'N}, k'_{N-1}) = (N-1)!\langle k_2 \dots k_N|k'_1 \dots k'_{N-1}\rangle\ ,$$

and the sum over P'' as:

$$\sum_{P''} \operatorname{sign}(P'')\delta(k_{P''1}, k'_1)\delta(k_{P''3}, k'_2) \dots \delta(k_{P''N}, k'_{N-1}) = (N-1)!\langle k_1 k_3 \dots k_N|k'_1 \dots k'_{N-1}\rangle\ ,$$

and similarly for the other sums over permutations. Now we can sum the terms again to:

$$\frac{1}{\sqrt{N}} \sum_{i=1}^{N} (-1)^{i-1}\, \delta(k_i, k)\langle k_1 \dots k_{i-1}k_{i+1} \dots k_N|k'_1 \dots k'_{N-1}\rangle$$

Taking the complex conjugate of this expression should, according to (51), equal:
$\langle k'_1 \dots k'_{N-1}|\hat{a}(k)|k_1 \dots k_N\rangle$, so that (52b) can be read off.

c. Anti-commutation relations

From the definition of $\hat{a}^\dagger(k)$ and the derived result for $\hat{a}(k)$ it follows:

$$\left\{\hat{a}^\dagger(k), \hat{a}^\dagger(\ell)\right\} = \hat{0} \qquad (53a)$$

$$\{\hat{a}(k), \hat{a}(\ell)\} = \hat{0} \qquad (53b)$$

$$\left\{\hat{a}(k), \hat{a}^\dagger(\ell)\right\} = \delta(k,\ell)\,\hat{1} \qquad (53c)$$

where $\left\{\hat{A}, \hat{B}\right\} \equiv \hat{A}\hat{B} + \hat{B}\hat{A}$ is the **anti-commutator** of two operators $\hat{A}$ and $\hat{B}$. Note that $\left\{\hat{A}, \hat{B}\right\} = \left\{\hat{B}, \hat{A}\right\}$.

Proof of (53c): First:

$$\hat{a}(k)\,\hat{a}^\dagger(\ell)|k_1 \ldots k_N\rangle = \hat{a}(k)\,\sqrt{N+1}|\ell\; k_1 \ldots k_N\rangle =$$

$$\frac{\sqrt{N+1}}{\sqrt{N+1}}\left[\delta(k,\ell)\,|k_1 \ldots k_N\rangle + \sum_{i=1}^{N}(-1)^i\,\delta(k,k_i)|\ell\; k_1 \ldots k_{i-1}k_{i+1} \ldots k_N\rangle\right] ,$$

where in the first step we have used (50b) and in the second step (52b), taking into account that the "ℓ-term" is the first term and the k_1-term is the second term, which therefore gets an extra minus-sign. Now we change the order of the operators and use (52b) first and (50b) second:

$$\hat{a}^\dagger(\ell)\,\hat{a}(k)|k_1 \ldots k_N\rangle = \hat{a}^\dagger(\ell)\,\frac{1}{\sqrt{N}}\sum_{i=1}^{N}(-1)^{i-1}\,\delta(k,k_i)|k_1 \ldots k_{i-1}k_{i+1} \ldots k_N\rangle =$$

$$\frac{\sqrt{N}}{\sqrt{N}}(-)\sum_{i=1}^{N}(-1)^i\,\delta(k,k_i)|\ell\; k_1 \ldots k_{i-1}k_{i+1} \ldots k_N\rangle$$

Adding the two results gives:

$$\left\{\hat{a}(k), \hat{a}^\dagger(\ell)\right\}|k_1 \ldots k_N\rangle = \delta(k,\ell)|k_1 \ldots k_N\rangle$$

Since the last result is for an arbitrary state vector in $\mathcal{E}$, we have shown (53c).

d. Many-body operators for fermions

This works analogously as for bosons: see formulae (25) and (26) for $\hat{F}$ and $\hat{G}$. It is important to note that for fermions (because of the anti-commutation relations) the order in which the creation- and annihilation operators appear is of significance.

e. Change of representation

This works exactly as for bosons: formulae (I.1) and (I.2).

7. Identical spin-$\frac{1}{2}$ particles

Application of the preceding: form of operators in *Second Quantization* for identical particles with mass m and spin $\frac{1}{2}$ (fermions!).

The one-fermion theory is often called "Schrödinger-Pauli theory". It's Hilbert space is again called $\mathcal{E}_1$.

Basis in discrete $\vec{k}$-representation in $\mathcal{E}_1$: $\left\{|\vec{k}\sigma\rangle\right\}$
$\vec{k} = \frac{2\pi}{L}\,\vec{n}$ with n_x, n_y, n_z integer numbers; $\sigma = +1$ or -1 (spin $\frac{1}{2}$).
In (continuous) $\vec{r}$-representation: $\{|\vec{r}\sigma\rangle\}$

The connection between the $\vec{k}\sigma$- and $\vec{r}\sigma$-representations is (cf. (I.8)):

$$\langle\vec{r}\sigma\,|\vec{k}\sigma'\rangle = \frac{1}{\sqrt{V}}\,e^{i\vec{k}\cdot\vec{r}}\,\delta_{\sigma,\sigma'} \tag{54}$$

a. The $\vec{k}\sigma$-representation

The form of operators for many-fermion systems is derived quite analogously to that for the bosonic case; one has to drag along an extra spin index σ, compared to the spin 0 case.

<u>Many-body operators</u>

$$\hat{n}_{\vec{k}\sigma} = \hat{a}^{\dagger}_{\vec{k}\sigma}\,\hat{a}_{\vec{k}\sigma} \tag{55}$$

$$\hat{n}_{\vec{k}} = \sum_{\sigma}\hat{n}_{\vec{k}\sigma} \tag{56}$$

$$\hat{N} = \sum_{\vec{k}\sigma}\hat{n}_{\vec{k}\sigma} \qquad \textbf{total particle number} \tag{57}$$

$$\hat{H^{(0)}} = \sum_{\vec{k}\sigma}\varepsilon_k\hat{n}_{\vec{k}\sigma} = \sum_{\vec{k}\sigma}\varepsilon_k\,\hat{a}^{\dagger}_{\vec{k}\sigma}\,\hat{a}_{\vec{k}\sigma} \qquad \text{with} \qquad \varepsilon_k = \frac{\hbar^2k^2}{2m} \tag{58}$$

We need to use our knowledge of the Hilbert space for spin-$\frac{1}{2}$ objects to find many-body operators that involve spin in a less trivial manner.

General procedure [cf. (27)-(28)]: (i) determine matrix elements

$$f_{\vec{k}\sigma,\vec{k}'\sigma'} = \langle\vec{k}\sigma|\hat{f}^{(1)}|\vec{k}'\sigma'\rangle \tag{59}$$

(ii) Using (i):

$$\hat{F} = \sum_{\vec{k}\sigma}\sum_{\vec{k}'\sigma'}\hat{a}^{\dagger}_{\vec{k}\sigma}f_{\vec{k}\sigma,\vec{k}'\sigma'}\hat{a}_{\vec{k}'\sigma'} \tag{60}$$

For instance, the operator $\hat{\Sigma}_x$, x-component of spin of the many-fermion system (in units of $\hbar/2$), is derived from the (one-particle) operator $\hat{\sigma}_x$ as follows (using the appropriate Pauli matrix):

$$\langle\vec{k}\sigma|\hat{\sigma}_x|\vec{k}'\sigma'\rangle = \delta_{\vec{k},\vec{k}'}\,[\delta_{\sigma,1}\,\delta_{\sigma',-1} + \delta_{\sigma,-1}\,\delta_{\sigma',1}] \qquad \longrightarrow$$

$$\hat{\Sigma}_x = \sum_{\vec{k}} \left[\hat{a}^{\dagger}_{\vec{k},1}\, \hat{a}_{\vec{k},-1} + \hat{a}^{\dagger}_{\vec{k},-1}\, \hat{a}_{\vec{k},1} \right] \tag{61a}$$

The other components of spin are (check for yourself):

$$\hat{\Sigma}_y = \sum_{\vec{k}} \left[-i\, \hat{a}^{\dagger}_{\vec{k},1}\, \hat{a}_{\vec{k},-1} + i\, \hat{a}^{\dagger}_{\vec{k},-1}\, \hat{a}_{\vec{k},1} \right] \tag{61b}$$

$$\hat{\Sigma}_z = \sum_{\vec{k}} \left[\hat{a}^{\dagger}_{\vec{k},1}\, \hat{a}_{\vec{k},1} - \hat{a}^{\dagger}_{\vec{k},-1}\, \hat{a}_{\vec{k},-1} \right] = \sum_{\vec{k}} \left(\hat{n}_{\vec{k},1} - \hat{n}_{\vec{k},-1} \right) \tag{61c}$$

It is important to note that not all commutators have to be replaced by anti-commutators in going from bosons to fermions. For instance, the dynamics of operators (Heisenberg picture) is still governed by the Heisenberg equations and these contain commutators. As an example we compute the time-dependence of the annihilation operator (in the $\vec{k}\sigma$-representation):

$$\frac{d}{dt} \left(\hat{a}_{\vec{k}\sigma}(t) \right) = \frac{i}{\hbar} \left[\hat{H}^{(0)}, \hat{a}_{\vec{k}\sigma}(t) \right] = \frac{i}{\hbar} \sum_{\vec{k}'\sigma'} \varepsilon_{k'} \left[\hat{a}^{\dagger}_{\vec{k}'\sigma'}\, \hat{a}_{\vec{k}'\sigma'}, \hat{a}_{\vec{k}\sigma} \right] (t) \tag{62}$$

To compute the commutator we use the general operator formula:

$$\left[\hat{A}\hat{B}, \hat{C} \right] = \hat{A} \left\{ \hat{B}, \hat{C} \right\} - \left\{ \hat{A}, \hat{C} \right\} \hat{B} \tag{63}$$

(which is easily proved by writing out the (anti-)commutators). Using the anti-commutation relations we then find:

$$\left[\hat{a}^{\dagger}_{\vec{k}'\sigma'}\, \hat{a}_{\vec{k}'\sigma'}, \hat{a}_{\vec{k}\sigma} \right] = \hat{a}^{\dagger}_{\vec{k}'\sigma'} \cdot 0 \; - \; \delta_{\vec{k},\vec{k}'}\, \delta_{\sigma,\sigma'}\, \hat{a}_{\vec{k}'\sigma'}$$

Substituting in (62), we have:

$$\frac{d}{dt} \left(\hat{a}_{\vec{k}\sigma}(t) \right) = -\frac{i\varepsilon_k}{\hbar}\, \hat{a}_{\vec{k}\sigma}(t) \quad \longrightarrow \quad \hat{a}_{\vec{k}\sigma}(t) = \hat{a}_{\vec{k}\sigma}\, e^{-i\omega_k t} \;, \tag{64}$$

where $\omega_k = \varepsilon_k/\hbar$. Note that this is the same result as for bosons in (40), but that the calculation is quite different!

b. The $\vec{r}\sigma$-representation

The change of representation is now easily made using formulae (I.2) and (54):

$$\hat{a}_{\vec{k}\sigma} \qquad \longrightarrow \qquad \hat{\psi}(\vec{r}\sigma)$$

Mostly it is just a matter of replacing $\int d\vec{r} \ldots$ by $\sum_\sigma \int d\vec{r} \ldots$, but for spin operators there are some differences.

Examples

$$\begin{aligned}
\hat{n}(\vec{r}\sigma) &= \hat{\psi}^\dagger(\vec{r}\sigma)\,\hat{\psi}(\vec{r}\sigma) && (65)\\
\hat{n}(\vec{r}) &= \sum_\sigma \hat{n}(\vec{r}\sigma) && (66)\\
\hat{N} &= \sum_\sigma \int d\vec{r}\ \hat{n}(\vec{r}\sigma) && (67)\\
\hat{\Sigma}_x &= \int d\vec{r}\,\Big(\hat{\psi}^\dagger(\vec{r},1)\,\hat{\psi}(\vec{r},-1) + \hat{\psi}^\dagger(\vec{r},-1)\,\hat{\psi}(\vec{r},1)\Big) && (68)
\end{aligned}$$

where the latter formula is an example of an operator which is non-diagonal in spin space. The above examples can all be obtained from the $\vec{k}\sigma$-representation forms by using the change-of-representation formula (cf. (34) for bosons):

$$\hat{\psi}(\vec{r}\sigma) = \sum_{\vec{k}} \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{V}}\,\hat{a}_{\vec{k}\sigma} \qquad (69)$$

One could again view the many-fermion formalism as a "quantization" of the Schrödinger-Pauli wavefunction;

$$\psi(\vec{r}\sigma,t) \qquad \longrightarrow \qquad \hat{\psi}(\vec{r}\sigma,t)$$

("second quantization").

In summary, the second quantization formalism allows to express many-body operators for systems of identical, interacting particles with fluctuating particle number in terms of creation- and annihilation operators, which obey commutation relations (20) for bosons and anti-commutation relations (53) for fermions.

8. Bose-Einstein and Fermi-Dirac distributions

After the hard work of introducing the second quantization formalism and the experience with operator calculus in the earlier part of the course, it is now relatively easy to derive the important Bose-Einstein- and Fermi-Dirac distributions of quantum statistical physics.

$$\begin{aligned}
\langle n_k\rangle &= \frac{1}{e^{\beta(\varepsilon_k-\mu)}-1} \quad \text{BE distribution} && (70)\\
\langle n_k\rangle &= \frac{1}{e^{\beta(\varepsilon_k-\mu)}+1} \quad \text{FD distribution}\ , && (71)
\end{aligned}$$

where $\beta = 1/k_\mathrm{B}T$, k_B: Boltzmann's constant, T: absolute temperature, μ: chemical potential (= energy of adding a particle to the system: $\mu = \frac{\partial F}{\partial N}$, F: (Helmholtz) free energy).

Generally we have for an expectation value:

$$\langle A\rangle = \mathrm{Tr}\,(\hat{\rho}\,\hat{A})\ , \qquad (72)$$

where the trace Tr is taken in Fock space and the (grand-canonical) state operator (or: density operator) is given by:

$$\hat{\rho} = \frac{e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}}{\mathrm{Tr}\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}} = \frac{1}{\Xi}\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} \tag{73}$$

$\hat{H}$ and $\hat{N}$ are taken as given in previous sections: $\hat{H}^{(0)}$ and $\hat{N}$. Ξ is the grand-canonical partition function. Our derivation will therefore be for free particles, but the results also hold for interacting particles if we can somehow define one-particle energies ε_k and occupation numbers n_k.

$$\langle n_k \rangle = \mathrm{Tr}\left(\hat{\rho}\, \hat{n}_k\right) = \frac{1}{\Xi}\, \mathrm{Tr}\, \left(e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\, \hat{a}_k^\dagger\, \hat{a}_k\right) \tag{74}$$

To compute the trace we need an operator identity that was derived in Exercise 2.4.11 in Le Bellac (see Problem Session 1):

$$e^{t\hat{A}}\, \hat{B}\, e^{-t\hat{A}} = \hat{B} + t\, \left[\hat{A}, \hat{B}\right] + \frac{t^2}{2!}\, \left[\hat{A}, \left[\hat{A}, \hat{B}\right]\right] + \cdots$$

For the special case that: $\left[\hat{A}, \hat{B}\right] = \gamma\, \hat{B}$, we have (put $t = 1$):

$$e^{\hat{A}}\, \hat{B}\, e^{-\hat{A}} = e^{\gamma}\, \hat{B} \tag{75}$$

We furthermore need the following commutator, which holds for both bosons and fermions (!), as we calculated in previous sections:

$$\left[\hat{n}_k, \hat{a}_k^\dagger\right] = \hat{a}_k^\dagger \tag{76}$$

Then:

$$\left[\hat{H} - \mu\hat{N}, \hat{a}_k^\dagger\right] = (\varepsilon_k - \mu)\, \hat{a}_k^\dagger \longrightarrow e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\, \hat{a}_k^\dagger\, e^{\beta\left(\hat{H}-\mu\hat{N}\right)}\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\, \hat{a}_k = e^{-\beta(\varepsilon_k-\mu)}\, \hat{a}_k^\dagger\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}\, \hat{a}_k\ ,$$

where we have used (75) in the last step (in the first step, convince yourself that the equality sign also holds for fermions!). From (74) it then follows;

$$\langle n_k \rangle = \frac{1}{\Xi}\, e^{-\beta(\varepsilon_k-\mu)}\, \mathrm{Tr}\, \left(\hat{a}_k^\dagger\, e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} \hat{a}_k\right) = e^{-\beta(\varepsilon_k-\mu)}\, \langle \hat{a}_k\, \hat{a}_k^\dagger \rangle\ , \tag{77}$$

where in the first step we have used the previous formula and in the last step we performed a rotation of operators in the trace (which leaves it unchanged). Now the expectation value in formula (77) equals $\langle n_k \rangle + 1$ for **bosons** (commutation relation (20c)) and equals $-\langle n_k \rangle + 1$ for **fermions** (anti-commutation relation (53c)). Inserting this back into (77) one readily recovers the BE- and FD-distributions (70) and (71), respectively.