Theoretical Physics V

Advanced Quantum Mechanics

Lecture Script SS 2021

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Contents

Chapter 1

Second quantization

In this first part, we shall consider nonrelativistic systems consisting of a large number of identical particles. In order to treat these, we will introduce a particularly efficient formalism, namely, the method of second quantization.

Nature has given us two types of particle, bosons and fermions. These have states that are, respectively, completely symmetric and completely antisymmetric. Fermions possess half-integer spin values, whereas boson spins have integer values. This connection between spin and symmetry (statistics) is proved within relativistic quantum field theory (the spin-statistics theorem). An important consequence in many-particle physics is the existence of Fermi-Dirac statistics and Bose-Einstein statistics.

We start with some preliminary remarks.

1.1 Identical particles and many particle states

Consider N "identical" particles (e.g. electrons, π-mesons, ...).

Hamilton-Operator:	$\hat{H} = \hat{H}(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \cdots, \mathbf{r}_N\sigma_N)$	abbreviated as: $\hat{H}(1, 2, \cdots, N)$
Wave function:	$\psi = \psi(\mathbf{r}_1\sigma_1, \mathbf{r}_2\sigma_2, \cdots, \mathbf{r}_N\sigma_N)$	abbreviated as: $\psi(1, 2, \cdots, N)$.

Definition: **permutation operator** P_{ij}:

$$P_{ij}\psi(\cdots, i, \cdots, j, \cdots, N) = \psi(\cdots, j, \cdots, i, \cdots, N)$$

Since $P_{ij}^2 = 1$ the eigenvalues of P_{ij} are ± 1. Due to the symmetry of the Hamiltonian $\hat{H}$ under particle exchange, one has for every element P of the permutation group:

$$\forall ij : \qquad P_{ij}\hat{H} = \hat{H}P_{ij}$$

e.g. an ordinary many-particle Hamiltonian has the form:

$$\hat{H}(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_N) = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + \sum_{i=1}^{N} U(\mathbf{r}_i) + \sum_{\{i,j\}} W(|\mathbf{r}_i - \mathbf{r}_j|)$$

$$\Rightarrow \qquad \hat{H}(\ldots, \mathbf{r}_i, \ldots, \mathbf{r}_j, \ldots) = \hat{H}(\ldots, \mathbf{r}_j, \ldots, \mathbf{r}_i, \ldots)$$

$S_N :=$ Group of all permutations of N objects. $\#S_N = N!$.

Each $P \in S_N$ can be represented as a product of transpositions P_{ij}. P is said to be even (odd) when the number of transpositions P_{ij} composing it is even (odd).

Properties:

(i) $\psi(1, \cdots, N)$ is an eigenfunction of $\hat{H}$ with eigenvalue E
$\Longrightarrow \quad P\psi(1, \cdots, N)$ also eigenfunction with eigenvalue E

(ii) $\forall P \in S_N, \quad \langle \phi \,|\, \psi \rangle = \langle P\phi \,|\, P\psi \rangle$

(iii) P is unitary ($P^\dagger P = PP^\dagger$)

(iv) For every symmetric operator $S(1, \cdots, N)$ we have $[P, S] = 0$, $\forall P \in S_N$ and $\langle P\psi_i \,|\, S \,|\, P\psi_j \rangle = \langle \psi_i \,|\, S \,|\psi_j \rangle$. The converse is also true.

Since identical particles are all influenced identically by any physical process (e.g. repulsion/attraction of a particle by a potential), all physical operators must be symmetric. Hence, the states ψ and $P\psi$ are experimentally indistinguishable. The question arises as to whether all these $N!$ states are realized in nature.

In fact, the totally symmetric and totally antisymmetric states (ψ_S) and (ψ_A) do play a special role. These states are defined by

$$\forall ij, \qquad P_{ij}\psi_S = +\psi_S; \quad P_{ij}\psi_A = -\psi_A$$

Experimentally: It is an experimental fact that there are two types of particle, bosons and fermions, whose states are totally symmetric and totally antisymmetric, respectively. As mentioned at the outset, bosons have integer, and fermions half-integer spin.

Bosons	**Fermions**
totally symmetric	totally antisymmetric
integer spin	half-integer spin

Remarks:

(i) The symmetry character of a state does not change in the course of time:

$$\psi(t) = e^{-i\hat{H}t/\hbar}\psi(0) \quad \Longrightarrow \quad P\psi(t) = e^{-i\hat{H}t/\hbar}P\psi(0)$$

(ii) $\forall P \in S_N$:

$$P\psi_S = \psi_S$$
$$P\psi_A = (-1)^{\mathrm{sgn}(P)}\psi_A \qquad \text{with} (-1)^{\mathrm{sgn}(P)} = \begin{cases} +1 & \text{for even permutations } P \\ -1 & \text{for odd permutations } P \end{cases}$$

Thus, the states ψ_S and ψ_A form the basis of two one-dimensional representations of the permutation group S_N.

Example:

$$N = 2: \qquad \psi_S(1,2) = \psi(1,2) + \psi(2,1)$$
$$\psi_A(1,2) = \psi(1,2) - \psi(2,1)$$

$$
\begin{aligned}
N=3: \quad & \psi_S(1,2,3) = \psi(1,2,3)+\psi(2,1,3)+\psi(1,3,2)+\psi(3,2,1)+\psi(3,1,2)+\psi(2,3,1) \\
& \psi_A(1,2,3) = \psi(1,2,3)-\psi(2,1,3)-\psi(1,3,2)-\psi(3,2,1)+\psi(3,1,2)+\psi(2,3,1)
\end{aligned}
$$

Remark: The minus sign in the fermionic case implicates that no two fermions can occupy the same state, because the wave function then vanishes (can easily be seen in the examples above). This fact is known as *Pauli principle*.

The permutations become necessary, because a state like $\psi(1,2,3)$ contains too much information. It is possible to assign a position to a specific particle, which isn't possible in nature for indistinguishable particles. On the other hand, the expressions become really confusing with increasing N, so we are looking for a formalism to condense the information. This will lead to the introduction of *Fock states*.

1.2 Totally symmetric and anti-symmetric states

Now let $\{|\,i\,\rangle\} = \{|\,1\,\rangle, |\,2\,\rangle, ...\}$ be a complete orthonormal system basis of one-particle states. We denote a one-particle state of particle α as $|\,i\,\rangle_\alpha$.
$\rightsquigarrow$ basis states of the N-particle system:

$$
|i_1, \cdots, i_\alpha, \cdots, i_N\rangle = |i_1\rangle_1 \cdots |i_\alpha\rangle_\alpha \cdots |i_N\rangle_N
$$

where $|i_\alpha\rangle_\alpha$ means that particle α is in state i_α.

$\{|i_1, \cdots, i_N\rangle\}$ is a complete orthogonal basis of the N-particle Hilbert space $\mathcal{H}^N$ $(= \mathcal{H}^N_S \oplus \mathcal{H}^N_A \oplus$ Rest)

The symmetrized and antisymmetrized basis states (i.e. the basis of $\mathcal{H}^N_S$ and $\mathcal{H}^N_A$) are defined by

$$
\boxed{S_\pm |i_1, \cdots, i_N\rangle = \frac{1}{\sqrt{N!}} \sum_{P \in S_N} (\pm 1)^{\mathrm{sgn}(P)} P\, |i_1, \cdots, i_N\rangle}
$$

If $|i_1, \cdots, i_N\rangle$ contains single-particle states occurring more than once, then $S_+ |i_1, \cdots, i_N\rangle$ is no longer normalized to unity. Let us assume that the first state occurs n_1 times, the second n_2 times, etc. Then $S_+ |i_1, \cdots, i_N\rangle$ contains only $N!/n_1!n_2!\cdots$ different terms and each of them appears with multiplicity $n_1! \cdot n_2! \cdots$.

$$
\Longrightarrow \langle i_1, \cdots, i_N|\, S_+^\dagger S_+ \,|i_1, \cdots, i_N\rangle = \frac{1}{N!}(n_1!n_2!\cdots)^2 \frac{N!}{n_1!n_2!\cdots} = n_1!n_2!\cdots
$$

$\rightsquigarrow$ The normalized Boson basis functions are

$$
\frac{S_+}{\sqrt{n_1!n_2!\cdots}}\,|i_1, \cdots, i_N\rangle = \frac{1}{\sqrt{N!n_1!n_2!\cdots}} \sum_{P \in S_N} P\,|i_1, \cdots, i_N\rangle \qquad (*)
$$

[n.b. It is $S_- |i_1, \cdots, i_N\rangle = 0$ if in $|i_1, \cdots, i_N\rangle$ one-particle states occur more than once.]

1.3 Bosons

The state $(*)$ is fully characterized by specifying the occupation numbers $\{n_i\}$:

$$|n_1, n_2, \cdots\rangle = \frac{S_+}{\sqrt{n_1! n_2! \cdots}} |i_1, \cdots, i_N\rangle$$

Here, n_1 is the number of times that the state 1 occurs, n_2 the number of times that state 2 occurs, etc. Alternatively: n_1 is the number of particles in state 1, n_2 is the number of particles in state 2, ... The sum of all occupation numbers n_i must be equal to the total number of particles:

$$N = \sum_{i=1}^{\infty} n_i$$

Apart from this constraint the n_i can take any of the values $0, 1, 2, ...$ These states form a complete orthonormal system of completely symmetric N-particle states. By linear superposition, one can construct from these any desired symmetric N-particle state.
We now combine the states for $N = 0, 1, 2, ...$ and obtain a complete orthonormal system of states for arbitrary particle number, which form the basis of the Fock-space:

$$\text{Fock-space} := \mathcal{H}^0 \oplus \mathcal{H}_S \oplus \cdots \oplus \mathcal{H}_S^N \oplus \cdots$$

$\mathcal{H}^0 = \{|0\rangle\}$ or vacuum (zero particles)
Complete orthonormal system: $\{|n_1, n_2, \cdots\rangle\}_{n_i=0,1,\cdots}$
- •Orthogonality relation $\langle n_1, n_2, \cdots | n_1', n_2', \cdots\rangle = \delta_{n_1 n_1'} \delta_{n_2 n_2'} \cdots$
- •Completeness relation: $\sum_{n_1, n_2, \cdots} |n_1, n_2, \cdots\rangle \langle n_1, n_2, \cdots| = \mathbf{1}$

The operators we have considered so far act only within a subspace of fixed particle number. On applying $\mathbf{p}$, $\mathbf{x}$ etc. to an N-particle state, we obtain again an N-particle state. We now define *creation* and *annihilation* operators, which lead from the space of N-particle states to the spaces of $N \pm 1$-particle states:

$$\begin{aligned} \hat{a}_i^\dagger |\cdots, n_i, \cdots\rangle &= \sqrt{n_i + 1} |\cdots, n_i + 1, \cdots\rangle \\ \hat{a}_i |\cdots, n_i, \cdots\rangle &= \sqrt{n_i} |\cdots, n_i - 1, \cdots\rangle \end{aligned} \qquad (**)$$

The operators $\hat{a}_i^\dagger$ and $\hat{a}_i$ respectively increases and decreases the occupation number of the state $|i\rangle$ by 1. One shows straightforwardly that $\hat{a}_i^\dagger$ is indeed the adjoined operator of $\hat{a}_i$:

$$\begin{aligned} (**) \implies & \langle n_i | \hat{a}_i = \sqrt{n_i + 1} \langle n_i + 1| \\ \implies & \langle n_i | \hat{a}_i | n_i' \rangle = \sqrt{n_i + 1} \langle n_i + 1 | n_i' \rangle = \sqrt{n_i + 1} \delta_{n_i + 1, n_i'} \end{aligned}$$

The above relations and the completeness of the states yield the *Bose commutation relations*

$$[\hat{a}_i, \hat{a}_j] = 0\,; \quad \left[\hat{a}_i^\dagger, \hat{a}_j^+\right] = 0\,; \quad \left[\hat{a}_i, \hat{a}_j^\dagger\right] = \delta_{ij}$$

$$\left(\hat{a}_i^\dagger \hat{a}_i \left| n_i \right\rangle = \hat{a}_i^\dagger \sqrt{n_i} \left| n_i - 1 \right\rangle = n_i \left| n_i \right\rangle ; \quad \hat{a}_i \hat{a}_i^\dagger \left| n_i \right\rangle = \sqrt{n_i + 1}\, \hat{a}_i \left| n_i + 1 \right\rangle = (n_i + 1) \left| n_i \right\rangle \right)$$

Starting from the *ground state* $\equiv$ *vacuum state* $|\, 0\, \rangle \equiv |\, 0, 0, \cdots \rangle$ which contains no particles at all, we can construct all states: single-particle states

$$\begin{aligned} \hat{a}_i^\dagger \left| 0 \right\rangle &= \left| 0, \cdots, n_i = 1, \cdots \right\rangle \\ \hat{a}_i^\dagger \hat{a}_j^\dagger \left| 0 \right\rangle &= \left| 0, \cdots, n_i = 1, \cdots, n_j = 1, \cdots \right\rangle \quad i \neq j \end{aligned}$$

Generally:

$$\boxed{\left| n_1, n_2, \cdots \right\rangle = \prod_{i=1}^{\infty} \frac{(\hat{a}_i^\dagger)^{n_i}}{\sqrt{n_i!}} \,|\, 0\, \rangle}$$

Definition:

$\boxed{\hat{n}_i := \hat{a}_i^\dagger \hat{a}_i}$ is the **particle number operator** (occupation number operator for the state $|\, i\, \rangle$)

$$\hat{n}_i \left| \cdots, n_i, \cdots \right\rangle = n_i \left| \cdots, n_i, \cdots \right\rangle$$

$\boxed{\hat{N} := \sum_i \hat{n}_i}$ is the **operator for the total number of particles**

$$\hat{N} \left| n_1, n_2, \cdots \right\rangle = \left(\sum_i n_i \right) \left| n_1, n_2, \cdots \right\rangle = N \left| n_1, n_2, \cdots \right\rangle$$

Let us consider an operator for the N-particle system which is a sum of single-particle operators

$$T = \sum_{\alpha=1}^{N} t_\alpha$$

where t_α is a one-particle operator (e.g. $t_\alpha = p_\alpha^2/2m$ or $V(x_\alpha)$). Let $t_{ij} := \langle\, i \,|\, t \,|\, j\, \rangle$ be the matrix elements of the one-particle operator t. Then $t = \sum_{i,j} t_{ij} |\, i\, \rangle\langle\, j\, |$ and $T = \sum_{i,j} t_{ij} \sum_\alpha |\, i\, \rangle_\alpha \langle\, j\, |_\alpha$.

Our aim is to represent this operator in terms of creation and annihilation operators $\boxed{T = \sum_{i,j} t_{ij} \hat{a}_i^\dagger \hat{a}_j}$

Proof:

Consider first the effect of $\hat{A}_{ij} := \sum_\alpha |\, i\, \rangle_\alpha \langle\, j\, |_\alpha$ on $\left| n_1, n_2, \cdots \right\rangle = \frac{S_+}{\sqrt{n_1! n_2! \cdots}} \left| k_1, k_2, \cdots, k_N \right\rangle$ If $n_j = 0$, then $\forall \alpha \in \{1, \cdots, N\}$ $k_\alpha \neq j$ $|\, i\, \rangle_\alpha \langle\, j\, |_\alpha\, n_1, n_2, ... \rangle = 0$

$$\begin{aligned} n_j = 1, \text{ wlog} \quad & k_1 = j \rightsquigarrow & |\, i\, \rangle_1 \langle\, j\, |_1\, k_1, k_2, \cdots, k_N \rangle &= \left| i, k_2, \cdots, k_N \right\rangle \\ n_j = 2, \text{ wlog} \quad & k_1 = k_2 = j \rightsquigarrow & |\, i\, \rangle_1 \langle\, j\, |_1\, k_1, k_2, \cdots, k_N \rangle &= \left| i, k_2, k_3, \cdots, k_N \right\rangle \\ & & |\, i\, \rangle_2 \langle\, j\, |_2\, k_1, k_2, \cdots, k_N \rangle &= \left| k_1, i, k_3, \cdots, k_N \right\rangle \end{aligned}$$

etc.

This means $\hat{A}_{ij}$ decreases n_j by 1 and increases n_i by 1, in n_j summands.

$$
\begin{aligned}
\rightsquigarrow \quad \hat{A}_{ij}\left|n_1, n_2, \cdots\right\rangle &= \hat{A}_{ij}\frac{S_+}{\sqrt{n_1! n_2! \cdots}}\left|k_1, k_2, \cdots, k_N\right\rangle \\
&= \frac{S_+}{\sqrt{n_1! n_2! \cdots}}\hat{A}_{ij}\left|k_1, k_2, \cdots, k_N\right\rangle \\
&= \frac{S_+}{\sqrt{n_1! n_2! \cdots}}\underbrace{\left(\left|i, k_2, \cdots, k_N\right\rangle + \left|k_1, i, k_3, \cdots\right\rangle + \cdots + \left|\cdots, k_{j-1}, i, k_{j+1}, \cdots\right\rangle\right)}_{n_j \text{ times}} \\
&= n_j \cdot \frac{S_+}{\sqrt{\cdots(n_i+1)!/(n_i+1)\cdots(n_j-1)! n_j \cdots}}\left|i, k_2, \cdots, k_N\right\rangle \\
&= n_j \cdot \sqrt{\frac{n_i+1}{n_j}}\left|\cdots, n_i+1, \cdots, n_j-1, \cdots\right\rangle \\
&= \sqrt{n_j\left(n_i+1\right)}\left|\cdots, n_i+1, \cdots, n_j-1, \cdots\right\rangle \\
&= \hat{a}_i^\dagger \hat{a}_j\left|\cdots, n_i, \cdots, n_j, \cdots\right\rangle
\end{aligned}
$$

For the special case that t is diagonal: $t_{ij} = \varepsilon_i \delta_{ij} \quad \rightsquigarrow \quad H_0 = \sum_i \varepsilon_i \hat{a}_i^\dagger \hat{a}_i$ ■

Analogously, one shows for the two-particle operators

$$
F = \frac{1}{2}\sum_{\alpha \neq \beta} f^{(2)}\left(\mathbf{r}_\alpha, \mathbf{r}_\beta\right) \tag{+}
$$

that they can be written as

$$
F = \frac{1}{2}\sum_{i,j,k,m} f_{ijkm}\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k
$$

with

$$
f_{ijkm} = \langle\, i, j \,|\; f^{(2)} \;|\, k, m \,\rangle = \int d\mathbf{r} \int d\mathbf{r}'\, \phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}) f^{(2)}(\mathbf{r}, \mathbf{r}')\, \phi_k(\mathbf{r}')\phi_m(\mathbf{r}')
$$

Proof:

(+) means in the N-particle space

$$
F = \frac{1}{2}\sum_{\alpha \neq \beta}\sum_{i,j,k,m}\langle\, i, j \,|\, f^{(2)} \,|\, k, m \,\rangle \,|\, i \,\rangle_\alpha \,|\, j \,\rangle_\beta \,\langle\, k \,|_\alpha \,\langle\, m \,|_\beta
$$

Now it is

$$
\begin{aligned}
\sum_{\alpha \neq \beta} |\, i \,\rangle_\alpha \,|\, j \,\rangle_\beta \,\langle\, k \,|_\alpha \,\langle\, m \,|_\beta &= \sum_{\alpha \neq \beta} |\, i \,\rangle_\alpha \,\langle\, k \,|_\alpha \,|\, j \,\rangle_\beta \,\langle\, m \,|_\beta \\
&= \sum_{\alpha, \beta} |\, i \,\rangle_\alpha \,\langle\, k \,|_\alpha \,|\, j \,\rangle_\beta \,\langle\, m \,|_\beta - \underbrace{\langle\, k \,|\, j \,\rangle}_{\delta_{kj}} \sum_\alpha |\, i \,\rangle_\alpha \,\langle\, m \,|_\alpha \\
&= \hat{a}_i^\dagger \hat{a}_k \,\hat{a}_j^\dagger \hat{a}_m - \hat{a}_i^\dagger \left[\hat{a}_k, \hat{a}_j^\dagger\right] \hat{a}_m \\
&= \hat{a}_i^\dagger \hat{a}_j^\dagger \,\hat{a}_m \hat{a}_k
\end{aligned}
$$

■

1.4 Fermions

The symmetrized basis states for an N particle system of fermions are

$$S_- |i_1 i_2 \cdots i_N\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} |i_1\rangle_1 & |i_1\rangle_2 & \cdots & |i_1\rangle_N \\ \vdots & \vdots & \vdots & \vdots \\ |i_N\rangle_1 & |i_N\rangle_2 & \cdots & |i_N\rangle_N \end{vmatrix} \qquad \text{(Slater determinant)}$$

(n.b.: exchange of two particles $\hat{=}$ exchange of two columns $\hat{=}$ change of sign)

Here, too, we shall characterize the states by specifying their occupation numbers, which now can take the values 0 and 1. The state with n_1 particles in state 1, n_2 particles in state 2, etc is $\{|n_1 n_2 \cdots\rangle\}$, which forms the basis of the Fock space. $\underbrace{\mathcal{H}^0}_{\{|0\rangle\}} \oplus \mathcal{H}^1 \oplus \cdots \oplus \mathcal{H}^N \oplus \cdots$. Scalar product and completeness relation as for Bosons.

Here, we wish to introduce creation operators $\hat{a}_i^\dagger$ once again. These must be defined such that the result of applying them twice is zero. Furthermore, the order in which they are applied must play a role. We thus define the creation operators $\hat{a}_i^\dagger$ by

Definition:

$$\begin{aligned} S_- |i_1, i_2, \cdots, i_N\rangle &= \hat{a}_{i_1}^\dagger \hat{a}_{i_2}^\dagger \cdots \hat{a}_{i_N}^\dagger |0\rangle \\ S_- |i_2, i_1, \cdots, i_N\rangle &= \hat{a}_{i_2}^\dagger \hat{a}_{i_1}^\dagger \cdots \hat{a}_{i_N}^\dagger |0\rangle \end{aligned}$$

Since $S_- |i_1 i_2 \cdots\rangle = -S_- |i_2 i_1 \cdots\rangle$, it follows

$$\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} := \hat{a}_i^\dagger \hat{a}_j^\dagger + \hat{a}_j^\dagger \hat{a}_i + = 0$$

and therefore also

$$\left(\hat{a}_i^\dagger\right)^2 = 0$$

In occupation number representation $|n_1 n_2 \cdots\rangle = \left(\hat{a}_1^\dagger\right)^{n_1} \left(\hat{a}_2^\dagger\right)^{n_2} \cdots |0\rangle$ with $n_i \in \{0, 1\}$.

Then the effect of $\hat{a}_i^\dagger$ is:

$$\boxed{\hat{a}_i^\dagger |\cdots, n_i, \cdots\rangle = \underbrace{(1 - n_i)}_{=0 \text{ for } n_i = 1} (-1)^{\sum_{j<i} n_j} |\cdots, n_i + 1, \cdots\rangle}$$

$\sum_{j<i} n_j$: number of anti-commutations to bring bring $\hat{a}_i^\dagger$ to position i.

The adjoined relation is

$$\begin{aligned} &\langle \cdots, n_i, \cdots | \hat{a}_i = (1 - n_i)(-1)^{\sum_{j<i} n_j} \langle \cdots, n_i + 1, \cdots | \\ \Longrightarrow &\langle \cdots, n_i, \cdots | \hat{a}_i | \cdots, n_i', \cdots\rangle = (1 - n_i)(-1)^{\sum_{j<i} n_j} \delta_{n_i + 1, n_i'} \end{aligned}$$

With this we compute

$$\begin{aligned} \hat{a}_i |\cdots, n_i', \cdots\rangle &= \sum_{n_i} |n_i\rangle \underbrace{\langle n_i| \hat{a}_i |n_i'\rangle}_{= \begin{cases} 0 & \text{for } n_i' = 0 \\ (-1)^{\sum_{j<i} n_j} \delta_{n_i 0} & \text{for } n_i' = 1 \end{cases}} \\ &= \begin{cases} 0 & \text{for } n_i' = 0 \\ (-1)^{\sum_{j<i} n_j} |\cdots, n_i' - 1, \cdots\rangle & \text{for } n_i' = 1 \end{cases} \end{aligned}$$

therefore

$$\hat{a}_i \left|\cdots, n_i, \cdots\right\rangle = n_i (-1)^{\sum_{j<i} n_j} \left|\cdots, n_i - 1, \cdots\right\rangle$$

It follows

$$\begin{aligned} \hat{a}_i \hat{a}_i^\dagger \left|\cdots, n_i, \cdots\right\rangle &= (1-n_i)\,(-1)^{2\sum_{j<i} n_j}\,(n_i+1) \left|\cdots, n_i, \cdots\right\rangle \\ &= (1-n_i) \left|\cdots, n_i, \cdots\right\rangle \end{aligned}$$

$$\begin{aligned} \hat{a}_i^\dagger \hat{a}_i \left|\cdots, n_i, \cdots\right\rangle &= n_i\,(-1)^{2\sum_{j<i} n_j}\,(1-n_i+1) \left|\cdots, n_i, \cdots\right\rangle \\ &= n_i \left|\cdots, n_i, \cdots\right\rangle \end{aligned}$$

$\hat{a}_i^\dagger \hat{a}_i$ is obviously the occupation number operator for the state $|\, i \,\rangle$. Moreover, by adding both equations one gets $\{\hat{a}_i,\, \hat{a}_i^\dagger\} = 1$. For $\{\hat{a}_i,\, \hat{a}_j^\dagger\}$ with $i \neq j$ the phase factor in both summands is different: $\{\hat{a}_i,\, \hat{a}_j^\dagger\} \propto (1-n_j) n_i (1-1) = 0$.
So, $\{\hat{a}_i,\, \hat{a}_j\}$ has for $i \neq j$ a different phase factor, and since $\hat{a}_i \hat{a}_i = \hat{a}_i^2 = 0$ one obtains the

anti-commutation rules for for fermions

$$\{\hat{a}_i,\, \hat{a}_j\} = 0; \quad \{\hat{a}_i^\dagger,\, \hat{a}_j^\dagger\} = 0; \quad \{\hat{a}_i,\, \hat{a}_j^\dagger\} = \delta_{ij}$$

One shows the relation $\sum_\alpha |\, i \,\rangle_\alpha \langle\, j \,|_\alpha = \hat{a}_i^\dagger \hat{a}_j$ as follows: (wlog $i_1 < i_2 < \cdots < i_N$)

$$\begin{aligned} \sum_\alpha |\, i \,\rangle_\alpha \langle\, j \,|_\alpha S_- \left|i_1, i_2, \cdots, i_N\right\rangle &= S_- \left(\sum_\alpha |\, i \,\rangle_\alpha \langle\, j \,|_\alpha \right) \left|i_1, i_2, \cdots, i_N\right\rangle \\ &= n_j\,(1-n_i)\,S_- \left|i_1, i_2, \cdots, i_N\right\rangle |_{j \to i} \end{aligned}$$

$|_{j\to i}$ means that the state $|\, j \,\rangle$ is replaced by $|\, i \,\rangle$. To get i to the right position one has to perform for $i \leq j : \sum_{k<j} n_k + \sum_{k<i} n_k$ line exchanges and for $i > j : \sum_{k<j} n_k + \sum_{k<i} n_k - 1$ line exchanges. This yields the same phase factor as by applying $\hat{a}_i^\dagger \hat{a}_j$.

$$\begin{aligned} \hat{a}_i^\dagger \hat{a}_j \left|\cdots, n_i, \cdots, n_j, \cdots\right\rangle &= n_j\,(-1)^{\sum_{k<j} n_k}\,\hat{a}_i^\dagger \left|\cdots, n_i, \cdots, n_j - 1\right\rangle \\ &= n_i\,(1-n_i)\,(-1)^{\sum_{k<i} n_k + \sum_{k<j} n_k - \delta_{i>j}} \left|\cdots, n_i + 1, \cdots, n_j - 1\right\rangle \end{aligned}$$

Thus one has for one-particle and two-particle operators – for fermions and for bosons

$$\begin{aligned} T &= \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j \\ F &= \frac{1}{2} \sum_{ijkm} \langle\, i, j \,|\; f^{(2)} \;|\, k, m \,\rangle\, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k \end{aligned}$$

e.g.

$$\hat{H} = \sum_{ij} (\underbrace{b_{ij}}_{\mathrm{E_{kin}}} + \underbrace{U_{ij}}_{\mathrm{E_{pot}}})\, \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{ijkm} \underbrace{f_{ijkm}}_{\mathrm{E_{int}}} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k$$

1.5 Field operators

Let $\{|i\rangle\}$ and $\{|\xi\rangle\}$ be two complete orthogonal bases of one-particle states. Then one has $|\xi\rangle = \sum_i |i\rangle \langle i|\xi\rangle$.

$$\Longleftrightarrow \quad \hat{a}_\xi^\dagger = \sum_i \hat{a}_i^\dagger \langle i|\xi\rangle \qquad \text{b.c. } \hat{a}_i^\dagger \ (\hat{a}_\xi^\dagger) \text{ creates a particle in } |i\rangle \ \ (|\xi\rangle)$$

$$\hat{a}_\xi = \sum_i \hat{a}_i \langle \xi \,|i\rangle \qquad \text{follows from the adjugated relation}$$

Important special case: Eigenstates of the position operator $|\mathbf{r}\rangle$:

$$\langle \mathbf{r}|i\rangle = \phi_i(\mathbf{r}) \qquad \text{one-particle wave function in position representation}$$

Definition: **Field operators**

$$\boxed{\begin{aligned} \hat{\psi}(\mathbf{r}) &= \sum_i \phi_i(\mathbf{r})\,\hat{a}_i \\ \hat{\psi}^\dagger(\mathbf{r}) &= \sum_i \phi_i^*(\mathbf{r})\,\hat{a}_i^\dagger \end{aligned}}$$

$\hat{\psi}^\dagger(\mathbf{r})$ generates a particle in the eigenstate $|\mathbf{r}\rangle$, i.e. at position $\mathbf{r}$. It is:

$$\begin{aligned} \left[\hat{\psi}(\mathbf{r}),\ \hat{\psi}(\mathbf{r}')\right]_\pm &= 0 \\ \left[\hat{\psi}^\dagger(\mathbf{r}),\ \hat{\psi}^\dagger(\mathbf{r}')\right]_\pm &= 0 \\ \left[\hat{\psi}(\mathbf{r}),\ \hat{\psi}^\dagger(\mathbf{r}')\right]_\pm &= \sum_{i,j} \phi_i(\mathbf{r})\,\phi_j^*(\mathbf{r}')\,\underbrace{\left[\hat{a}_i,\ \hat{a}_j^\dagger\right]_\pm}_{\delta_{ij}} = \delta(\mathbf{r}-\mathbf{r}')\,, \end{aligned}$$

where

$$\begin{aligned} [\bullet,\bullet]_+ &= [\bullet,\bullet] && \text{commutator} \\ [\bullet,\bullet]_- &= \{\bullet,\bullet\} && \text{anti-commutator} \end{aligned}$$

Operator can be expressed via field operators:

Kinetic energy:

$$\begin{aligned} \sum_{i,j} \hat{a}_i^\dagger T_{ij} \hat{a}_j &= \sum_{i,j} \int d\mathbf{r}\ \hat{a}_i^\dagger \phi_i^*(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\Delta\right) \phi_j(\mathbf{r}) \hat{a}_j \\ &\underset{\hat{\psi}(\mathbf{r}\to\infty)\to 0}{=} \frac{\hbar^2}{2m} \int d\mathbf{r}\ \nabla\hat{\psi}^\dagger(\mathbf{r}) \cdot \nabla\hat{\psi}(\mathbf{r}) \end{aligned}$$

One-particle potential:

$$\begin{aligned} \sum_{i,j} \hat{a}_i^\dagger U_{ij} \hat{a}_j &= \sum_{i,j} \int d\mathbf{r}\ \hat{a}_i^\dagger \phi_i^*(\mathbf{r}) U(\mathbf{r}) \phi_j(\mathbf{r}) \hat{a}_j \\ &= \int d\mathbf{r}\ U(\mathbf{r}) \hat{\psi}^\dagger(\mathbf{r}) \hat{\psi}(\mathbf{r}) \end{aligned}$$

Two-particle interaction:

$$\frac{1}{2}\sum_{i,j,k,m}\int d\mathbf{r}\, d\mathbf{r}'\; \phi_i^*(\mathbf{r})\phi_j^*(\mathbf{r}')\, V(\mathbf{r},\mathbf{r}')\, \phi_k(\mathbf{r})\phi_m(\mathbf{r}')\, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k$$
$$=\frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\; V(\mathbf{r},\mathbf{r}')\, \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})$$

Hamiltonian:

$$\hat{H} = \int d\mathbf{r}\; \left(\frac{\hbar^2}{2m}\nabla\hat{\psi}^\dagger(\mathbf{r})\nabla\hat{\psi}(\mathbf{r}) + U\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})\right) + \frac{1}{2}\int d\mathbf{r}\, d\mathbf{r}'\; \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\, V(\mathbf{r},\mathbf{r}')\, \hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})$$

Particle density:

$$\begin{aligned}\hat{n}(\mathbf{r}) &= \sum_\alpha \delta\left(\mathbf{r}-\mathbf{r}_\alpha\right)\\ &= \sum_\alpha\sum_{i,j} |i\rangle_\alpha \underbrace{{}_\alpha\langle i|\delta(\mathbf{r}-\mathbf{r}_\alpha)|j\rangle_\alpha}_{\substack{=\int d\mathbf{r}'\; \phi_i^*(\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}')\phi_j(\mathbf{r}')\\ =\phi_i^*(\mathbf{r})\phi_j(\mathbf{r})}} \langle j|_\alpha\\ &= \sum_{i,j}\underbrace{\sum_\alpha |i\rangle_\alpha\langle j|_\alpha}_{=\hat{a}_i^\dagger\hat{a}_j}\phi_i^*(\mathbf{r})\phi_j(\mathbf{r})\end{aligned}$$

$$\Rightarrow \hat{n}(\mathbf{r}) = \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$$

Particle number operator:

$$\hat{N} = \int d\mathbf{r}\; \hat{n}(\mathbf{r}) = \int d\mathbf{r}\; \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})$$

$\rightsquigarrow$ e.g. current density operator $\boxed{\hat{\jmath}(\mathbf{r}) = \frac{\hbar}{2\imath m}\left\{\hat{\psi}^\dagger(\mathbf{r})\left(\nabla\hat{\psi}(\mathbf{r})\right) - \left(\nabla\hat{\psi}^\dagger(\mathbf{r})\right)\hat{\psi}(\mathbf{r})\right\}}$

Field equation: Heisenberg picture for operators $\quad\hat{\psi}(\mathbf{r},t) = e^{\imath\hat{H}t/\hbar}\,\hat{\psi}(\mathbf{r},0)\,e^{-\imath\hat{H}t/\hbar}$

$$\boxed{\imath\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{r},t) = \left(-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r})\right)\hat{\psi}(\mathbf{r},t) + \int d\mathbf{r}'\; \hat{\psi}^\dagger(\mathbf{r}',t)\, V(\mathbf{r},\mathbf{r}')\, \hat{\psi}(\mathbf{r}',t)\hat{\psi}(\mathbf{r},t)}$$

Proof (*see exercise*): using Heisenberg equation of motion $\imath\hbar\frac{\partial}{\partial t}\hat{\psi}(\mathbf{r},t) = -\left[\hat{H},\hat{\psi}(\mathbf{r},t)\right]$
analogous for $\hat{\psi}^\dagger(\mathbf{r},t)$ (yields a minus sign on the right hand side)
From this follows the equation of motion of the density operator:

$$\frac{\partial}{\partial t}\hat{n}(\mathbf{r},t) = \hat{\psi}^\dagger\dot{\hat{\psi}} + \dot{\hat{\psi}}^\dagger\hat{\psi} = \frac{1}{\imath\hbar}\left(-\frac{\hbar^2}{2m}\right)\left\{\hat{\psi}^\dagger\left(\Delta\hat{\psi}\right) - \left(\Delta\hat{\psi}^\dagger\right)\hat{\psi}\right\}$$

i.e. $\boxed{\frac{\partial}{\partial t}\hat{n}(\mathbf{r},t) = -\nabla\hat{\jmath}(\mathbf{r},t)}$

1.6 Momentum representation

We consider a cuboidal volume $V = L_x L_y L_z$ and periodic boundary conditions $\phi(\mathbf{r} + L_x \hat{e}_x) = \phi(\mathbf{r})$ (analogous for the remaining spatial directions). Normalized momentum eigenfunctions: $\psi_{\mathbf{k}} = e^{\imath \mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$, where $\mathbf{k} = 2\pi \left(\frac{n_x}{L_x}, \frac{n_y}{L_y}, \frac{n_z}{L_z}\right)$, $n_x, n_y, n_z \in \mathbb{Z}$

$$\rightsquigarrow \quad \int d\mathbf{r}\; \phi^*_{\mathbf{k}}(\mathbf{r})\phi_{\mathbf{k}'}(\mathbf{r}) = \delta_{\mathbf{k}\mathbf{k}'} \qquad \text{(orthogonality)}$$

Representation of the Hamiltonian in second quantization:

The matrix elements read

$$E_{\text{kin}}: \quad \int d\mathbf{r}\; \phi^*_{\mathbf{k}'}(\mathbf{r})(-\Delta)\phi_{\mathbf{k}}(\mathbf{r}) = \mathbf{k}^2\, \delta_{\mathbf{k},\mathbf{k}'}$$

$$E_{\text{pot}}: \quad \int d\mathbf{r}\; \phi^*_{\mathbf{k}'}(\mathbf{r})U(\mathbf{r})\phi_{\mathbf{k}}(\mathbf{r}) = \frac{1}{V} \quad \underbrace{U_{\mathbf{k}',-\mathbf{k}}}_{\substack{\text{Fourier transfo}\\ \text{of } U(\mathbf{r})}}$$

E_{int}: Consider two-particle potentials $V(\mathbf{r}, \mathbf{r}')$ which only depend on the distance $\mathbf{r} - \mathbf{r}'$
Define: $V_{\mathbf{q}} := \int d\mathbf{r}\; e^{-\imath\mathbf{q}\cdot\mathbf{r}}\, V(\mathbf{r}) \quad \left(\rightsquigarrow V(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{q}} V_{\mathbf{q}} e^{\imath\mathbf{q}\cdot\mathbf{r}}\right)$
The two-particle matrix element then reads

$$\begin{aligned}
\langle \mathbf{p}', \mathbf{k}' | V(\mathbf{r} - \mathbf{r}') | \mathbf{p}, \mathbf{k} \rangle &= \frac{1}{V^2} \int d\mathbf{r}\, d\mathbf{r}'\; e^{-\imath\mathbf{p}'\cdot\mathbf{r}} e^{-\imath\mathbf{k}'\cdot\mathbf{r}'}\; V(\mathbf{r} - \mathbf{r}') e^{\imath\mathbf{k}'\cdot\mathbf{r}'} e^{\imath\mathbf{p}\cdot\mathbf{r}} \\
&= \frac{1}{V^3} \sum_{\mathbf{q}} V_{\mathbf{q}} \int d\mathbf{r}\, d\mathbf{r}'\; e^{-\imath\mathbf{p}'\cdot\mathbf{r} - \mathbf{k}'\cdot\mathbf{r}' + \imath\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}') + \imath\mathbf{k}\cdot\mathbf{r}' + \imath\mathbf{p}\cdot\mathbf{r}} \\
&= \frac{1}{V^3} \sum_{\mathbf{q}} V_{\mathbf{q}} V \underbrace{\delta_{-\mathbf{p}'+\mathbf{q}+\mathbf{p},0}}_{\mathbf{p}'=\mathbf{p}+\mathbf{q}}\, V \underbrace{\delta_{-\mathbf{k}'-\mathbf{q}+\mathbf{k},0}}_{\mathbf{k}'=\mathbf{k}-\mathbf{q}}
\end{aligned}$$

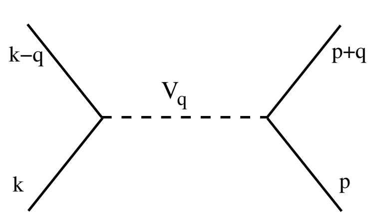
Combining the above results leads to:

$$\boxed{\hat{H} = \sum_{\mathbf{k}} \frac{(\hbar\mathbf{k})^2}{2m} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}} + \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}'} U_{\mathbf{k}'-\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}'} \hat{a}_{\mathbf{k}} + \underbrace{\frac{1}{2V} \sum_{\mathbf{q},\mathbf{p},\mathbf{k}} V_{\mathbf{q}} \hat{a}^\dagger_{\mathbf{p}+\mathbf{q}} \hat{a}^\dagger_{\mathbf{k}-\mathbf{q}} \hat{a}_{\mathbf{k}} \hat{a}_{\mathbf{p}}}_{\text{interaction term}}}$$

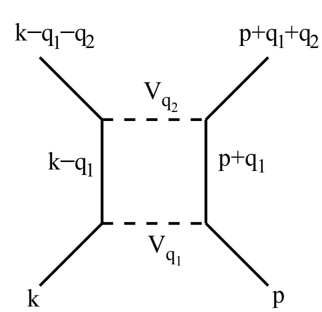
$\hat{a}^\dagger_{\mathbf{k}}$ ($\hat{a}_{\mathbf{k}}$) creates (annihilates) a particle with wave number $\mathbf{k}$, where the following commutation relations apply:

$$[\hat{a}_{\mathbf{k}},\, \hat{a}_{\mathbf{k}'}]_\pm = 0, \quad \left[\hat{a}^\dagger_{\mathbf{k}},\, \hat{a}^\dagger_{\mathbf{k}'}\right]_\pm = 0, \quad \left[\hat{a}_{\mathbf{k}},\, \hat{a}^\dagger_{\mathbf{k}'}\right] = \delta_{\mathbf{k}\mathbf{k}'}$$

Visualization of the interaction term:



2nd order perturbation theory: (double dispersion of two particles)



Fourier transformation of the density:

$$\hat{n}_{\mathbf{q}} = \int d\mathbf{r}\ \hat{n}(\mathbf{r})e^{-\imath\mathbf{q}\cdot\mathbf{r}} = \int d\mathbf{r}\ \hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})e^{-\imath\mathbf{q}\cdot\mathbf{r}}$$

Using the expressions $\hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} e^{\imath\mathbf{p}\cdot\mathbf{r}}\hat{a}_{\mathbf{p}}$ and $\hat{\psi}^\dagger(\mathbf{r}) = \frac{1}{\sqrt{V}}\sum_{\mathbf{p}} e^{-\imath\mathbf{p}\cdot\mathbf{r}}\hat{a}^\dagger_{\mathbf{p}}$ gives

$$\boxed{\hat{n}_{\mathbf{q}} = \sum_{\mathbf{p}} \hat{a}^\dagger_{\mathbf{p}}\hat{a}_{\mathbf{p}+\mathbf{q}}}$$

Consideration of spin:

$$\left.\begin{array}{ccc} \hat{\psi}(\mathbf{r}) & \rightarrow & \hat{\psi}_\sigma(\mathbf{r}) \\ \hat{a}_{\mathbf{p}} & \rightarrow & \hat{a}_{\mathbf{p},\sigma} \end{array}\right\} \quad \longrightarrow \quad \begin{array}{ccc} n(\mathbf{r}) & = & \sum_\sigma \hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r}) \\ n_{\mathbf{q}} & = & \sum_{\mathbf{p},\sigma} \hat{a}^\dagger_{\mathbf{p},\sigma}\hat{a}_{\mathbf{p}+\mathbf{q},\sigma} \end{array}$$

In the case of spin-$\frac{1}{2}$ fermions $\sigma = \pm\frac{1}{2}$.
Spin density operator:

$$\hat{\mathbf{S}}(\mathbf{r}) = \sum_i \delta(\mathbf{r}-\mathbf{r}')\hat{\mathbf{S}}_i = \frac{\hbar}{2}\sum_{\sigma,\sigma'} \hat{\psi}^\dagger_\sigma(\mathbf{r})\boldsymbol{\sigma}_{\sigma\sigma'}\hat{\psi}_{\sigma'}(\mathbf{r})\,,$$

where $\boldsymbol{\sigma}_{\sigma\sigma'}$ are the matrix elements of the Pauli matrices. Otherwise everything remains the same with spin index σ.

1.7 Summary of second quantization

The most important facts about second quantization are summarized in the Table 1.1. Some of the relations are identical for bosons and fermions: in those cases we use the generic notation $\hat{a}$ for the annihilation operator. Otherwise we denote it $\hat{b}$ for bosons and $\hat{c}$ for fermions.
Let us end this chapter with a few practical tips concerning the creation-annihilation permutations (CAPs). In all applications of the second quantization, you run into expressions consisting of a long product of CAPs, stacked between two basis vectors of the Fock-space. In order to derive any useful result, you must be able to manipulate those products of CAPs, i.e. you must master the definition and commutation relations of the CAPs at an operational level. You can handle the following simple rules:

a) Do not panic. You can do this, it is a routine calculation.

b) Try to reduce the number of operators by converting them to occupation number operators $\hat{a}^\dagger_i\hat{a}_i\,|\{n_k\}\rangle = n_i\,|\{n_k\}\rangle$.

c) In order to achieve this, permute the operators using the commutation rules.

d) Do not calculate parts which reduce obviously to zero. Use common sense and the definition of CAPs to guess whether an expression is zero before evaluating it.

Let us illustrate this by evaluating the following expression involving fermionic operators:

$$\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_3}\hat{c}_{i_4}\,|\{n_k\}\rangle$$

The last rule comes first. The bra and ket states are identical, and this allows us to establish relations between the level indices i_1, i_2, i_3, and i_4. The two annihilation operators in the expression kill particles in the ket state in the levels i_3 and i_4. In order to end up in $|\{n_k\}\rangle$ again and thus have a non-zero result, the particles in these levels have to be re-created by the creation operators. So we have to concentrate on two possibilities only:

$$\begin{aligned} & i_1 = i_3, \quad i_2 = i_4, \quad i_1 \neq i_2, \\ \text{or} \qquad & i_1 = i_4, \quad i_2 = i_3, \quad i_1 \neq i_2. \end{aligned}$$

The case $i_1 = i_2 = i_3 = i_4$ gives zero since all levels can only be occupied once. The term $\hat{c}_{i_3}\hat{c}_{i_3}$ then always produce zero.

We now focus on the first probability, and try to reduce the CAPs to occupation number operators,

$$\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_1}\hat{c}_{i_2}\,|\{n_k\}\rangle = -\,\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_2}\,|\{n_k\}\rangle$$

permuting the first and the third terms. We now use the reduction rule twice:

$$\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_1}\hat{c}_{i_2}\,|\{n_k\}\rangle = -n_{i_2}\,\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}_{i_1}\,|\{n_k\}\rangle = -n_{i_1}n_{i_2}.$$

Treating the second possibility in the same way, we find

$$\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_2}\hat{c}_{i_1}\,|\{n_k\}\rangle = -\,\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_1}\hat{c}_{i_2}\,|\{n_k\}\rangle = \langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_2}\,|\{n_k\}\rangle$$

where we permute (i) the third and the fourth terms, and (ii) the second and the third terms. We now use the reduction rule twice:

$$\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_2}\hat{c}_{i_1}\,|\{n_k\}\rangle = n_{i_2}\,\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}_{i_1}\,|\{n_k\}\rangle = n_{i_1}n_{i_2}$$

We finally obtain:

$$\langle\{n_k\}|\,\hat{c}^\dagger_{i_1}\hat{c}^\dagger_{i_2}\hat{c}_{i_3}\hat{c}_{i_4}\,|\{n_k\}\rangle = -n_{i_1}n_{i_2}\delta_{i_1,i_3}\delta_{i_2,i_4} + n_{i_1}n_{i_2}\delta_{i_1,i_4}\delta_{i_2,i_3}.$$

	Bosons	Fermions
Many-particle wave function $\Psi(\|\mathbf{r}_i\rangle, t)$	fully symmetric	fully antisymmetric
Fock-space, where the basis states are labeled by the sets $\{n_{\mathbf{k}}\}$ of occupations numbers	non-negative integers	0 or 1
Creation and annihilation operators	commute $[\hat{b}_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}] = 0$ $[\hat{b}^\dagger_{\mathbf{k}}, \hat{b}^\dagger_{\mathbf{k}'}] = 0$ $[\hat{b}^\dagger_{\mathbf{k}}, \hat{b}_{\mathbf{k}'}] = \delta_{\mathbf{kk}'}$	anticommute $\{\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}\} = 0$ $\{\hat{c}^\dagger_{\mathbf{k}}, \hat{c}^\dagger_{\mathbf{k}'}\} = 0$ $\{\hat{c}^\dagger_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}\} = \delta_{\mathbf{kk}'}$
Occupation number operator number of particles in same level **k**: total number of particles:	$\hat{n}_{\mathbf{k}} = \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}}$ $\hat{N} = \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}} = \sum_{\mathbf{k}} \hat{a}^\dagger_{\mathbf{k}} \hat{a}_{\mathbf{k}}$	
Hamiltonian with particle-particle interactions	$\hat{H} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}} +$ $\frac{1}{2V} \sum\limits_{\mathbf{k},\mathbf{k}',\mathbf{q}} V_{\mathbf{q}} \hat{b}^\dagger_{\mathbf{k}+\mathbf{q}} \hat{b}^\dagger_{\mathbf{k}'-\mathbf{q}} \hat{b}_{\mathbf{k}} \hat{b}_{\mathbf{k}'}$	the same, with spins
Field operators: dynamics (without interactions): Heisenberg equation:	$\hat{\Psi}(\mathbf{r}) = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}} \phi_{\mathbf{k}}(\mathbf{r})$ Schrödinger equation for the wave function $i\hbar\partial_t \hat{\Psi}(\mathbf{r}, t) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right] \hat{\Psi}(\mathbf{r}, t)$	

Table 1.1: Summary of second quantization

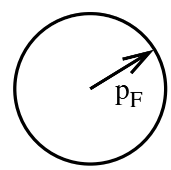
Chapter 2

Application of second quantization

2.1 Spin-$\frac{1}{2}$ fermions

Non-interacting fermions, particle number N. For the ground state $|\phi_0\rangle$, all single-particle states up to the wave number $|\mathbf{p}| < p_F$ are occupied, where p_F is called the *Fermi wave number*, $|\mathbf{p}| < p_F$ represents the *Fermi sphere*. The ground state is given by

$$|\phi_0\rangle = \prod_{\substack{\mathbf{p} \\ |\mathbf{p}|<p_F}} \prod_{\sigma} \hat{c}^\dagger_{\mathbf{p},\sigma} |0\rangle \qquad \sigma = \pm\frac{\hbar}{2}$$



Expectation value of particle number operator in momentum space:

$$\hat{n}_{\mathbf{p},\sigma} = \langle\phi_0|\hat{c}^\dagger_{\mathbf{p},\sigma}\hat{c}_{\mathbf{p},\sigma}|\phi_0\rangle = \begin{cases} 1 & |\mathbf{p}| \leq p_F \\ 0 & |\mathbf{p}| > p_F \end{cases}$$

For $|\mathbf{q}| > p_F$ one has

$$\hat{c}_{\mathbf{q},\sigma} |\phi_0\rangle = \prod_{\substack{\mathbf{p} \\ |\mathbf{p}|<p_F}} \prod_{\sigma} \hat{c}^\dagger_{\mathbf{p},\sigma}\hat{c}_{\mathbf{q},\sigma} |0\rangle = 0$$

The total particle number is connected to the Fermi momentum by

$$N = \sum_{\mathbf{p},\sigma} n_{\mathbf{p},\sigma} = 2 \sum_{|\mathbf{p}|<p_F} 1 \overset{(*)}{=} 2V \int_0^{p_F} \frac{d\mathbf{p}}{(2\pi)^3} = \frac{V\,p_F^3}{3\pi^2}$$

$$\left((*)\text{: } \sum_{\mathbf{k}} f(\mathbf{k}) = \sum_{\mathbf{k}} \frac{\Delta k}{\left(\frac{2\pi}{L}\right)^3} f(\mathbf{k}) = \left(\frac{L}{2\pi}\right)^3 \int d\mathbf{k} f(\mathbf{k}) \right)$$

With this it follows

$$p_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3} = (3\pi^2 n)^{1/3} \qquad \text{with} \quad n = \frac{N}{V} \text{ mean particle density.}$$

$\hbar p_F$: the Fermi momentum, and $\varepsilon_F = (\hbar p_F)^2/2m$: the Fermi energy.

The total energy is

$$\frac{E}{V} = \frac{1}{V}\sum_{\mathbf{p},\sigma}\varepsilon_{\mathbf{p},\sigma} = \frac{2}{V}\sum_{|\mathbf{p}|<p_F}\frac{\hbar^2\mathbf{p}^2}{2m} = 2\int_0^{p_F}\frac{d\mathbf{p}}{(2\pi)^3}\frac{\hbar^2\mathbf{p}^2}{2m} = \frac{\hbar^2}{2\pi^2 m}\int_0^{p_F} dp\, p^4 = \frac{\hbar^2 p_F^5}{10\pi^2 m}.$$

The relation with the Fermi energy is then:

$$\frac{E}{V} = \varepsilon_F\frac{p_F^3}{5\pi^2} = \frac{3}{5}n\varepsilon_F \qquad \text{and} \qquad \frac{E}{N} = \frac{3}{5}\varepsilon_F,$$

and the relation with the density n is:

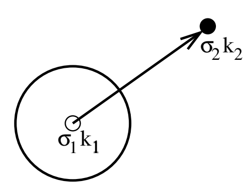
$$\frac{E}{V} = \frac{3\hbar^2}{10\pi^2 m}(3\pi^2 n)^{5/3}.$$

Expectation value of particle density:

$$\begin{aligned}
\langle\hat{n}\rangle &= \sum_\sigma \langle\phi_0|\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})|\phi_0\rangle \\
&= \sum_\sigma\sum_{\mathbf{p},\mathbf{p}'}\frac{e^{-\imath\mathbf{p}\cdot\mathbf{r}}e^{\imath\mathbf{p}'\cdot\mathbf{r}}}{V}\underbrace{\langle\phi_0|\hat{c}^\dagger_{\mathbf{p},\sigma}\hat{c}_{\mathbf{p}',\sigma}|\phi_0\rangle}_{=\delta_{\mathbf{p},\mathbf{p}'}n_{\mathbf{p},\sigma}} \\
&= \frac{1}{V}\sum_{\mathbf{p},\sigma}n_{\mathbf{p},\sigma} = \frac{N}{V} = n.
\end{aligned}$$

Excitation of a Fermi gas:

$\vert\phi\rangle = \hat{c}^\dagger_{\mathbf{k}_2,\sigma_2}\hat{c}_{\mathbf{k}_1,\sigma_1}\vert\phi_0\rangle$	$\equiv$	particle hole pair
$\hat{b}_{\mathbf{k},\sigma} = \hat{c}^\dagger_{-\mathbf{k},-\sigma}$		hole annihilator
$\hat{b}^\dagger_{\mathbf{k},\sigma} = \hat{c}_{-\mathbf{k},-\sigma}$		hole creator

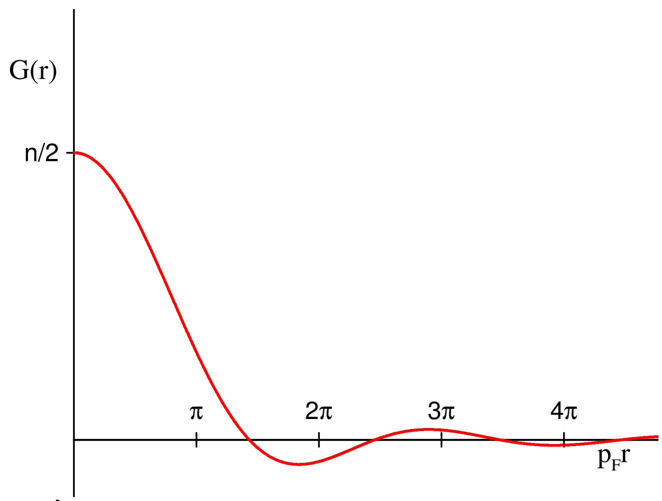


Correlation function of the field operators (for the ground state):

$$\begin{aligned}
G_\sigma(\mathbf{r}-\mathbf{r}') = &\quad \langle\phi_0|\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r}')|\phi_0\rangle \\
\equiv &\quad \frac{n}{2}\times\text{prob. amp. for}\quad \underbrace{\hat{\psi}_\sigma(\mathbf{r}')\,|\phi_0\rangle}_{\text{particle missing at pos. }\mathbf{r}'} \quad\to\quad \underbrace{\hat{\psi}_\sigma(\mathbf{r})\,|\phi_0\rangle}_{\text{particle missing at pos. }\mathbf{r}} \\
&\quad \Uparrow \\
\text{b.c.} &\quad \left(\langle\phi_0|\hat{\psi}^\dagger_\sigma(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r}')|\phi_0\rangle = \frac{n}{2}\right)
\end{aligned}$$

$$
\begin{aligned}
G_\sigma(\mathbf{r}-\mathbf{r}') &= \sum_{\mathbf{p},\mathbf{p}'} \frac{1}{V} e^{-\imath\mathbf{p}\cdot\mathbf{r}+\imath\mathbf{p}'\cdot\mathbf{r}'} \underbrace{\langle\phi_0|\hat{c}^\dagger_{\mathbf{p},\sigma}\hat{c}_{\mathbf{p}',\sigma}|\phi_0\rangle}_{=\delta_{\mathbf{p},\mathbf{p}'}n_{\mathbf{p},\sigma}=\delta_{\mathbf{p},\mathbf{p}'}\Theta(p_F-|\mathbf{p}|)} \\
&= \frac{1}{V}\sum_{|\mathbf{p}|<p_F} e^{-\imath\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} = \int_{|\mathbf{p}|<p_F} \frac{d\mathbf{p}}{(2\pi)^3} e^{-\imath\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} \\
&= \frac{1}{(2\pi)^2}\int_0^{p_F} dp\, p^2 \underbrace{\int_{-1}^{1} d\eta\, e^{\imath p|r-r'|\eta}}_{=\frac{e^{\imath pr}-e^{-\imath pr}}{\imath pr},\ r=|\mathbf{r}-\mathbf{r}'|} , \qquad (\eta=\cos(\theta)) \\
&= \frac{1}{2\pi^2 r} \underbrace{\int_0^{p_F} dp\, p\sin(pr)}_{\substack{= -\frac{\partial}{\partial r}\int_0^{p_F} dp\,\cos(pr) \\ = -\frac{\partial}{\partial r}\frac{\sin(p_F r)}{r} \\ = \frac{\sin(p_F r)}{r^2} - \frac{p_F\cos(p_F r)}{r}}} \\
&= \frac{\sin(p_F r) - p_F r\,\cos(p_F r)}{2\pi^2 r^3}
\end{aligned}
$$

$$
\text{i.e.} \quad G_\sigma(\mathbf{r}) = \frac{3n}{2}\,\frac{\sin(p_F r) - p_F r\,\cos(p_F r)}{(p_F r)^3}
$$



Pair distribution function:
Consider a $(N-1)$-particle state $|\phi'(\mathbf{r},\sigma)\rangle = \hat{\psi}_\sigma(\mathbf{r})\,|\phi_0\rangle$. The density distribution of this state reads

$$
\begin{aligned}
\langle\phi'(\mathbf{r},\sigma)|\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')|\phi'(\mathbf{r},\sigma)\rangle &= \langle\phi_0|\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')\hat{\psi}_\sigma(\mathbf{r})|\phi_0\rangle \\
&= \left(\frac{n}{2}\right)^2 \underbrace{g_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}')}_{\text{pair distribution function}}
\end{aligned}
$$

It is

$$
\begin{aligned}
\left(\frac{n}{2}\right)^2 g_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') &= \langle\phi_0|\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_\sigma(\mathbf{r})\hat{\psi}^\dagger_{\sigma'}(\mathbf{r}')\hat{\psi}_{\sigma'}(\mathbf{r}')|\phi_0\rangle - \delta_{\sigma,\sigma'}\delta(\mathbf{r}-\mathbf{r}')\,\langle\phi_0|\hat{\psi}^\dagger_\sigma(\mathbf{r})\hat{\psi}_{\sigma'}(\mathbf{r}')|\phi_0\rangle \\
&= \langle\phi_0|\hat{n}_\sigma(\mathbf{r})\hat{n}_{\sigma'}(\mathbf{r}')|\phi_0\rangle - \delta_{\sigma,\sigma'}\delta(\mathbf{r}-\mathbf{r}')\,\langle\phi_0|\hat{n}_\sigma(\mathbf{r})|\phi_0\rangle
\end{aligned}
$$

In the Fourier-space we have

$$\left(\frac{n}{2}\right)^2 g_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') = \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{k}'\mathbf{p}\mathbf{p}'} e^{-\imath\mathbf{k}\cdot\mathbf{r}} e^{-\imath\mathbf{p}\cdot\mathbf{r}'} e^{\imath\mathbf{p}'\cdot\mathbf{r}'} e^{\imath\mathbf{k}'\cdot\mathbf{r}} \langle\phi_0|\, \hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}^\dagger_{\mathbf{p},\sigma'}\hat{c}_{\mathbf{p}',\sigma'}\hat{c}_{\mathbf{k}',\sigma}\,|\phi_0\rangle\,.$$

It is non zero only if $\mathbf{p}=\mathbf{p}'$, $\mathbf{k}=\mathbf{k}'$ or $\mathbf{p}=\mathbf{k}'$, $\mathbf{k}=\mathbf{p}'$. These conditions give

$$\begin{aligned}
\left(\frac{n}{2}\right)^2 g_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}') =& \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{p}} \underbrace{\langle\phi_0|\, \hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}^\dagger_{\mathbf{p},\sigma'}\hat{c}_{\mathbf{p},\sigma'}\hat{c}_{\mathbf{k},\sigma}\,|\phi_0\rangle}_{=\langle\phi_0|\hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma}\hat{c}^\dagger_{\mathbf{p},\sigma'}\hat{c}_{\mathbf{p},\sigma'}|\phi_0\rangle-\delta_{\sigma\sigma'}\delta_{\mathbf{p}\mathbf{k}}\langle\phi_0|\hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}_{\mathbf{p},\sigma'}|\phi_0\rangle} \\
&+ \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{p}} e^{-\imath\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} e^{-\imath\mathbf{p}\cdot(\mathbf{r}'-\mathbf{r})} \underbrace{\langle\phi_0|\, \hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}^\dagger_{\mathbf{p},\sigma'}\hat{c}_{\mathbf{k},\sigma'}\hat{c}_{\mathbf{p},\sigma}\,|\phi_0\rangle}_{=-\langle\phi_0|\hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}_{\mathbf{k},\sigma'}\hat{c}^\dagger_{\mathbf{p},\sigma'}\hat{c}_{\mathbf{p},\sigma}|\phi_0\rangle+\delta_{\sigma\sigma'}\delta_{\mathbf{p}\mathbf{k}}\langle\phi_0|\hat{c}^\dagger_{\mathbf{k},\sigma}\hat{c}_{\mathbf{p},\sigma}|\phi_0\rangle} \\
=& \frac{1}{V^2}\sum_{\mathbf{k}\mathbf{p}} \langle\phi_0|\, \hat{n}_{\mathbf{k},\sigma}\hat{n}_{\mathbf{p},\sigma'}\,|\phi_0\rangle - \delta_{\sigma\sigma'}\frac{1}{V^2}\sum_{\mathbf{k}\mathbf{p}} e^{-\imath\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')} e^{-\imath\mathbf{p}\cdot(\mathbf{r}'-\mathbf{r})} \langle\phi_0|\, \hat{n}_{\mathbf{k},\sigma}\hat{n}_{\mathbf{p},\sigma}\,|\phi_0\rangle
\end{aligned}$$

For $\sigma \neq \sigma'$, we find

$$\left(\frac{n}{2}\right)^2 g_{\sigma\sigma'}\left(\mathbf{r}-\mathbf{r}'\right) = \frac{1}{V^2}\langle\phi_0|\underbrace{\sum_{\mathbf{k}}\hat{n}_{\mathbf{k},\sigma}}_{\rightsquigarrow N/2}\underbrace{\sum_{\mathbf{p}}\hat{n}_{\mathbf{p},\sigma'}}_{\rightsquigarrow N/2}|\phi_0\rangle = \frac{1}{V^2}\cdot\frac{N}{2}\cdot\frac{N}{2} = \frac{n^2}{4},$$

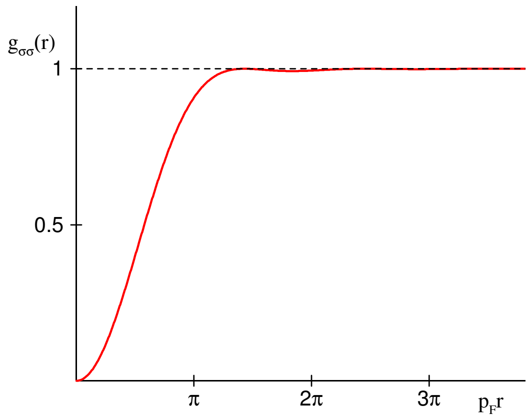
which gives $g_{\sigma\sigma'}\left(\mathbf{r}-\mathbf{r}'\right) = 1$.

For $\sigma = \sigma'$, we find

$$\begin{aligned}
\left(\frac{n}{2}\right)^2 g_{\sigma\sigma}(\mathbf{r}-\mathbf{r}') &= \left(\frac{n}{2}\right)^2 - \langle\phi_0|\underbrace{\frac{1}{V}\sum_{\mathbf{k}} e^{-\imath\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')}\hat{n}_{\mathbf{k},\sigma}}_{\rightsquigarrow G_\sigma(\mathbf{r}-\mathbf{r}')}\underbrace{\frac{1}{V}\sum_{\mathbf{p}} e^{-\imath\mathbf{p}\cdot(\mathbf{r}'-\mathbf{r})}\hat{n}_{\mathbf{p},\sigma}}_{\rightsquigarrow G^*_\sigma(\mathbf{r}-\mathbf{r}')}|\phi_0\rangle \\
&= \left(\frac{n}{2}\right)^2 - \left[G_\sigma(\mathbf{r}-\mathbf{r}')\right]^2.
\end{aligned}$$

Combining these results leads to

$$\Rightarrow g_{\sigma\sigma'}\left(\mathbf{r}-\mathbf{r}'\right) = 1 - \frac{9}{(p_F r)^6}\Big(\sin(p_F r) - p_F r\,\cos(p_F r)\Big)^2\delta_{\sigma\sigma'}\,, \qquad r = |\mathbf{r}-\mathbf{r}'|$$



$$g(\mathbf{r}) = \frac{V}{N(N-1)} \left\langle \sum_{\alpha\neq\beta} \delta\left(\mathbf{r} - \mathbf{r}_\alpha + \mathbf{r}_\beta\right) \right\rangle$$

Because of the above relation, the pair distribution function represents the probability density for pair of particles to be at a distance $\mathbf{r}$! The reduction of $g(\mathbf{r})$ for distances $\lesssim p_F^{-1}$ is called the correlation or exchange hole. It is an effect of the antisymmetry of the N-particle state.

Density correlation function:

$$\begin{aligned}
\tilde{G}(\mathbf{r}) = \langle \hat{n}(\mathbf{r})\hat{n}(0)\rangle &= \frac{1}{V}\int d\mathbf{r}' \, \langle \hat{n}(\mathbf{r}+\mathbf{r}')\hat{n}(\mathbf{r}')\rangle \\
&= \frac{1}{V}\sum_{\alpha,\beta}\int d\mathbf{r}' \, \langle \delta(\mathbf{r}+\mathbf{r}'-\mathbf{r}_\alpha)\delta(\mathbf{r}'-\mathbf{r}_\beta)\rangle = \frac{1}{V}\sum_{\alpha,\beta}\langle \delta(\mathbf{r}-\mathbf{r}_\alpha+\mathbf{r}_\beta)\rangle \\
&= \frac{1}{V}\left(\sum_\alpha \delta(\mathbf{r}) + \frac{N(N-1)}{V} g(\mathbf{r})\right) = n\delta(\mathbf{r}) + \frac{N(N-1)}{V^2} g(\mathbf{r})
\end{aligned}$$

$$\begin{aligned}
\sum_{\alpha\neq\beta} \delta(\mathbf{r}-\mathbf{r}_\alpha+\mathbf{r}_\beta) \quad \longrightarrow \quad & \int d\mathbf{r}' \, d\mathbf{r}'' \, \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}'')\delta(\mathbf{r}-\mathbf{r}'+\mathbf{r}'')\hat{\psi}(\mathbf{r}'')\hat{\psi}(\mathbf{r}') \\
&= \int d\mathbf{r}' \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}'-\mathbf{r})\hat{\psi}(\mathbf{r}'-\mathbf{r})\hat{\psi}(\mathbf{r}')
\end{aligned}$$

$$\left\langle \sum_{\alpha\neq\beta} \delta(\mathbf{r}-\mathbf{r}_\alpha+\mathbf{r}_\beta) \right\rangle = V \left\langle \hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}^\dagger(\mathbf{r}'-\mathbf{r})\hat{\psi}(\mathbf{r}'-\mathbf{r})\hat{\psi}(\mathbf{r}') \right\rangle$$

Static structure factor:

$$\begin{aligned}
S(\mathbf{q}) := \frac{1}{N}\left\langle \sum_{\alpha,\beta} e^{-\imath\mathbf{q}\cdot(\mathbf{r}_\alpha-\mathbf{r}_\beta)} \right\rangle - N\delta_{\mathbf{q},\mathbf{0}} &= \frac{1}{N}\langle \hat{n}_\mathbf{q}\hat{n}_{-\mathbf{q}}\rangle - N\delta_{\mathbf{q},\mathbf{0}} \\
&= \frac{N}{V}\int d\mathbf{r} \, e^{-\imath\mathbf{q}\cdot\mathbf{r}} g(\mathbf{r}) + 1 - N\delta_{\mathbf{q},\mathbf{0}},
\end{aligned}$$

i.e.

$$S(\mathbf{q}) - 1 = n\int d\mathbf{r} \, e^{-\imath\mathbf{q}\cdot\mathbf{r}} \left(g(\mathbf{r}) - 1\right),$$

and

$$g(\mathbf{r}) - 1 = \frac{1}{n}\int \frac{d\mathbf{q}}{(2\pi)^3} e^{\imath\mathbf{q}\cdot\mathbf{r}} \left(S(\mathbf{q}) - 1\right).$$

2.2 Magnetic (polarized) ground state of interacting Fermi gas

The ground-state of interacting Fermi gas is polarized. The Hamiltonian writes $\hat{H} = \hat{H}_{\text{kin}} + \hat{H}_{\text{int}}$ with

$$\hat{H}_{\text{kin}} = \sum_{\mathbf{k},\sigma} \frac{\hbar^2 \mathbf{k}^2}{2m} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} \qquad \text{and} \qquad \hat{H}_{\text{int}} = \frac{1}{2V} \sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \sum_{\sigma,\sigma'} U_{\mathbf{q}} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma}.$$

The polarization is defined by

$$P = \frac{N_\uparrow + N_\downarrow}{N}$$

where $N_\uparrow$ and $N_\downarrow$ are the number of particles in the spin states $\sigma = \uparrow$ and $\sigma = \downarrow$, respectively. Note that $N = N_\uparrow + N_\downarrow$. Then we have the populations

$$N_{\uparrow,\downarrow} = \frac{N}{2}(1 \pm P).$$

The ground-state is supposed polarized, i.e. with a polarization $P \neq 0$. We will prove it with a variational calculation with a polarized trial wave function:

$$|g_P\rangle = \left(\prod_{|\mathbf{k}|<k_{F,\uparrow}} c^\dagger_{\mathbf{k},\uparrow} \right) \left(\prod_{|\mathbf{k}|<k_{F,\downarrow}} c^\dagger_{\mathbf{k},\downarrow} \right) |0\rangle ,$$

where $N_\uparrow$ are created in the state $\uparrow$ and $N_\downarrow$ in the state $\downarrow$. Note that if $N_\uparrow = N_\downarrow = N/2$ for a zero-polarization, the Fermi momemtum are equal to $k_{F,\uparrow} = k_{F,\downarrow} = (3\pi^2 n)^{1/3}$ and the ground-state is $|g_P\rangle = |\phi_0\rangle$. We use the variational calculus based on the determination of the minimal energy:

$$E_{\text{GS}} = \min_{\Psi} \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

where $|\Psi\rangle = |g_P\rangle$ for an infinitely many polarizations. We will then compute the expression for the energy and calculate the polarization of its minimum.

Kinetic energy:

$$E_{\text{kin}}(P) = \langle g_P | \hat{H}_{\text{kin}} | g_P \rangle = \sum_{\mathbf{k},\sigma} \frac{\hbar^2 \mathbf{k}^2}{2m} n_{\mathbf{k},\sigma}$$

where $n_{\mathbf{k},\sigma} = \Theta(k_{F,\sigma} - |\mathbf{k}|)$. It gives:

$$\frac{E_{\text{kin}}(P)}{V} = 1 \cdot \int_{|\mathbf{k}|<k_{F,\uparrow}} \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\hbar^2 \mathbf{k}^2}{2m} + 1 \cdot \int_{|\mathbf{k}|<k_{F,\downarrow}} \frac{d^3\mathbf{k}}{(2\pi)^3} \frac{\hbar^2 \mathbf{k}^2}{2m} = \frac{1}{2} \left\{ \frac{\hbar^2 k^5_{F,\uparrow}}{10\pi^2 m} + \frac{\hbar^2 k^5_{F,\downarrow}}{10\pi^2 m} \right\}.$$

and we have

$$n_\uparrow = \frac{N_\uparrow}{V} = 1 \cdot \int_{|\mathbf{k}|<k_{F,\uparrow}} \frac{d^3\mathbf{k}}{(2\pi)^3} = \frac{1}{2} \frac{k^3_{F,\uparrow}}{3\pi^2}, \qquad n_\downarrow = \frac{1}{2} \frac{k^3_{F,\downarrow}}{3\pi^2},$$

which give the Fermi momenta:

$$k_{F,\uparrow\downarrow} = (2 \cdot 3\pi^2 n_{\uparrow\downarrow})^{1/3}.$$

Remember we have

$$\frac{E_K}{V} \equiv \frac{E(P=0)}{V} = \underbrace{(3\pi^2)^{2/3}\frac{3\hbar^2}{10m}}_{\equiv C}\left(\frac{N}{V}\right)^{5/3} \quad \Rightarrow \quad C = \frac{E_K}{V}\left(\frac{V}{N}\right)^{5/3}.$$

$$\begin{aligned} \frac{E_{\text{kin}}(P)}{V} &= \frac{C}{2}\left[(2n_\uparrow)^{5/3} + (2n_\downarrow)^{5/3}\right] \\ &= \frac{E_K}{2V}\left(\frac{V}{N}\right)^{5/3}\left[\left(2\frac{N_\uparrow}{V}\right)^{5/3} + \left(2\frac{N_\downarrow}{V}\right)^{5/3}\right] \\ &= \frac{E_K}{2V}\left[\left(2\frac{N_\uparrow}{N}\right)^{5/3} + \left(2\frac{N_\downarrow}{N}\right)^{5/3}\right] \end{aligned}$$

Hence the kinetic energy is

$$E_{\text{kin}}(P) = \frac{E_K}{2}\left[(1+P)^{5/3} + (1-P)^{5/3}\right],$$

which is minimum for $P = 0$ with the value $E(P=0) = E_K$.

Potential energy:
The Coulomb potential is

$$U(\mathbf{r}) = \frac{e^2}{4\pi r} \Rightarrow U(\mathbf{q}) = \frac{e^2}{\mathbf{q}^2}.$$

Since electron-electron interaction is screened (Yukawa potential):

$$U(\mathbf{r}) = \frac{e^2}{4\pi r}\exp(-r/r_c) \Rightarrow U(\mathbf{q}) = \frac{e^2}{\mathbf{q}^2 + r_c^{-2}}.$$

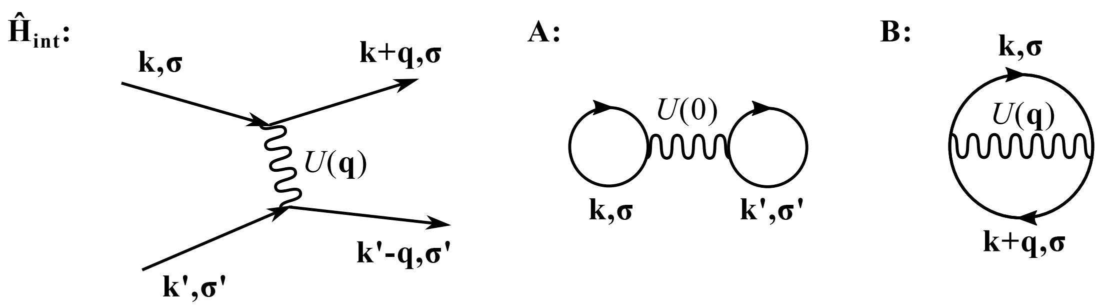
We use here a simpler model (very strongly screened $|\mathbf{q}|r_c \ll 1$:

$$U(\mathbf{r}) = U\delta(r) \Rightarrow U(\mathbf{q}) = U.$$

The potential energy is then

$$\langle g_P|\,\hat{H}_{\text{int}}\,|g_P\rangle = \frac{U}{2V}\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\sum_{\sigma,\sigma'} \underbrace{\langle g_P|\, c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma}\,|g_P\rangle}_{\neq 0 \text{ only for } \begin{array}{l}(\text{A})\ \mathbf{k}'-\mathbf{q}=\mathbf{k}',\ \mathbf{k}+\mathbf{q}=\mathbf{k}\ \Rightarrow\ \mathbf{q}=0 \\ (\text{B})\ \mathbf{k}'-\mathbf{q}=\mathbf{k},\ \mathbf{k}+\mathbf{q}=\mathbf{k}',\ \sigma=\sigma'\end{array}}.$$

Diagrams of corresponding interactions:



(A) Hartree term:

$$E_H = \frac{U}{2V}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\sigma,\sigma'} \underbrace{\langle g_P| c^\dagger_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k}',\sigma'} c_{\mathbf{k},\sigma} |g_P\rangle}_{\begin{subarray}{l} = \langle g_P| c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} c^\dagger_{\mathbf{k}',\sigma'} c_{\mathbf{k}',\sigma'} |g_P\rangle - \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'} \langle g_P| c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} |g_P\rangle \\ = n_{\mathbf{k}',\sigma'} n_{\mathbf{k},\sigma} - \delta_{\mathbf{k},\mathbf{k}'}\delta_{\sigma,\sigma'} n_{\mathbf{k},\sigma} \end{subarray}}$$

$$= \frac{U}{2V}\left[\left(\sum_{\mathbf{k}}\sum_{\sigma} n_{\mathbf{k},\sigma}\right)^2 - \sum_{\mathbf{k}}\sum_{\sigma} n_{\mathbf{k},\sigma}\right] = \frac{U}{2V}(N^2 - N) \simeq \frac{UV}{2}n^2$$

for a large number of particles $N \gg 1$. E_H is independent of the polarization P.

(B) Fock term:

$$E_{\text{Fock}} = \frac{U}{2V}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\sigma} \underbrace{\langle g_P| c^\dagger_{\mathbf{k}',\sigma} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma} |g_P\rangle}_{\begin{subarray}{l} = -\langle g_P| c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k}',\sigma} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} |g_P\rangle + \delta_{\mathbf{k},\mathbf{k}'} \langle g_P| c^\dagger_{\mathbf{k}',\sigma} c_{\mathbf{k},\sigma} |g_P\rangle \\ = -n_{\mathbf{k}',\sigma'} n_{\mathbf{k},\sigma} + \delta_{\mathbf{k},\mathbf{k}'} n_{\mathbf{k},\sigma} \end{subarray}}$$

$$= -\frac{U}{2V}\left[\sum_{\sigma}\left(\sum_{\mathbf{k}} n_{\mathbf{k},\sigma}\right)^2 - \sum_{\mathbf{k}}\sum_{\sigma} n_{\mathbf{k},\sigma}\right] = -\frac{U}{2V}(N_\uparrow^2 + N_\downarrow^2 - N)$$

$$\simeq -E_H\left(\frac{N_\uparrow^2}{N^2} + \frac{N_\downarrow^2}{N^2}\right) = -E_H\left(\frac{(1+P)^2}{4} + \frac{(1-P)^2}{4}\right) = -E_H\frac{1+P^2}{2}.$$

E_{Fock} is minimal for $|P| = 1$. It comes from the Pauli principle.

Total energy:

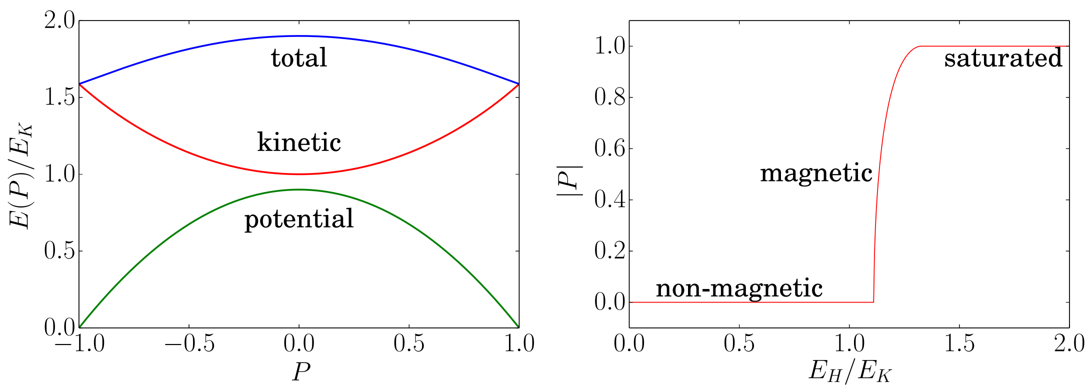
$$E(P) = \frac{E_K}{2}\left[(1+P)^{5/3} + (1-P)^{5/3}\right] + \frac{E_H}{2}(1-P^2).$$

For E_H/E_K the optimal polarization can be determined as being the state with minimal total energy:

$$\frac{\partial E}{\partial P}(P) = \frac{5E_K}{6}\left[(1+P)^{2/3} - (1-P)^{2/3}\right] - E_H P = 0$$

$$\Rightarrow \frac{E_H}{E_K} = \frac{5}{6P}\left[(1+P)^{2/3} - (1-P)^{2/3}\right].$$

Although it is impossible to solve this equation analytically with respect to P, it suffices to plot the optimal polarization versus E_H/E_K, as in the figure below.



From the plot we understand the following:

a) If the interaction is weak, $E_H/E_K < 10/9$, the ground state is non-magnetic.

b) A transition to a magnetic state occurs at $E_H/E_K = 10/9$. The polarization is still vanishing at the transition point and gradually increases above it.

c) At $E_H/E_K > 5/6 \cdot 2^{2/3}$ the ground state is completely polarized.

Of course our model is too simplistic to account for all details of ferromagnetism in metals. However, we manage to capture several qualitative features of the phenomenon.

2.3 Free bosons

Pair distribution function for free bosons. We assume non-interacting bosons with spin zero. $\rightsquigarrow$ Only quantum number is the momentum.
Consider the N-particle state

$$|\phi\rangle = |n_{\mathbf{p}_0}, n_{\mathbf{p}_1}, \dots\rangle \qquad n_{\mathbf{p}_i} \in \{0, 1, 2, \dots\}$$

Particle density:

$$\langle\phi|\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}(\mathbf{r})|\phi\rangle = \frac{1}{V}\sum_{\mathbf{k},\mathbf{k}'} e^{-\imath\mathbf{k}\cdot\mathbf{r}+\imath\mathbf{k}'\cdot\mathbf{r}} \langle\phi|\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}'}|\phi\rangle = \frac{1}{V}\sum_{\mathbf{k}} n_{\mathbf{k}} = \frac{N}{V} = n.$$

$\rightsquigarrow$ No position dependency of the density for the state $|\phi\rangle$.

Pair distribution function:

$$n^2 g(\mathbf{r}-\mathbf{r}') = \langle\phi|\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})|\phi\rangle = \frac{1}{V^2}\sum_{\substack{\mathbf{k},\mathbf{k}',\\ \mathbf{q},\mathbf{q}'}} e^{-\imath\mathbf{k}\mathbf{r}-\imath\mathbf{q}\mathbf{r}'+\imath\mathbf{q}'\mathbf{r}'+\imath\mathbf{k}'\mathbf{r}} \langle\phi|\hat{b}^\dagger_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{q}}\hat{b}_{\mathbf{q}'}\hat{b}_{\mathbf{k}'}|\phi\rangle\,.$$

$\langle\phi|\hat{b}^\dagger_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{q}}\hat{b}_{\mathbf{q}'}\hat{b}_{\mathbf{k}'}|\phi\rangle$: This term is only different form 0 when $\mathbf{k}=\mathbf{k}'$ and $\mathbf{q}=\mathbf{q}'$ or $\mathbf{k}=\mathbf{q}'$ and $\mathbf{q}=\mathbf{k}'$. Consider case $\mathbf{k}=\mathbf{q}$ separately

$$\begin{aligned}\langle\phi|\hat{b}^\dagger_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{q}}\hat{b}_{\mathbf{q}'}\hat{b}_{\mathbf{k}'}|\phi\rangle &= (1-\delta_{\mathbf{k}\mathbf{q}})\left(\delta_{\mathbf{k}\mathbf{k}'}\delta_{\mathbf{q}\mathbf{q}'}\langle\phi|\hat{b}^\dagger_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{q}}\hat{b}_{\mathbf{q}}\hat{b}_{\mathbf{k}}|\phi\rangle + \delta_{\mathbf{k}\mathbf{q}'}\delta_{\mathbf{q}\mathbf{k}'}\langle\phi|\hat{b}^\dagger_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{q}}\hat{b}_{\mathbf{k}}\hat{b}_{\mathbf{q}}|\phi\rangle\right)\\ &\quad + \delta_{\mathbf{k}\mathbf{q}}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\mathbf{q}\mathbf{q}'}\langle\phi|\hat{b}^\dagger_{\mathbf{k}}\hat{b}^\dagger_{\mathbf{k}}\hat{b}_{\mathbf{k}}\hat{b}_{\mathbf{k}}|\phi\rangle\\ &= (1-\delta_{\mathbf{k}\mathbf{q}})\left(\delta_{\mathbf{k}\mathbf{k}'}\delta_{\mathbf{q}\mathbf{q}'} + \delta_{\mathbf{k}\mathbf{q}'}\delta_{\mathbf{q}\mathbf{k}'}\right) n_{\mathbf{k}} n_{\mathbf{q}} + \delta_{\mathbf{k}\mathbf{q}}\delta_{\mathbf{k}\mathbf{k}'}\delta_{\mathbf{q}\mathbf{q}'} n_{\mathbf{k}}\,(n_{\mathbf{k}}-1)\end{aligned}$$

With this it follows

$$\begin{aligned}\langle\phi|\hat{\psi}^\dagger(\mathbf{r})\hat{\psi}^\dagger(\mathbf{r}')\hat{\psi}(\mathbf{r}')\hat{\psi}(\mathbf{r})|\phi\rangle =& \frac{1}{V^2}\left[\sum_{\mathbf{k}\mathbf{q}}(1-\delta_{\mathbf{k},\mathbf{q}})\left(1+e^{-\imath(\mathbf{k}-\mathbf{q})(\mathbf{r}-\mathbf{r}')}\right)n_{\mathbf{k}}n_{\mathbf{q}} + \sum_{\mathbf{k}} n_{\mathbf{k}}\,(n_{\mathbf{k}}-1)\right]\\ =& \frac{1}{V^2}\left[\sum_{\mathbf{k},\mathbf{q}} n_{\mathbf{k}}n_{\mathbf{q}} - \sum_{\mathbf{k}} n_{\mathbf{k}}^2 + \left|\sum_{\mathbf{k}} e^{-\imath\mathbf{k}(\mathbf{r}-\mathbf{r}')}n_{\mathbf{k}}\right|^2 - \sum_{\mathbf{k}} n_{\mathbf{k}}^2 + \sum_{\mathbf{k}} n_{\mathbf{k}}^2 - \sum_{\mathbf{k}} n_{\mathbf{k}}\right]\\ =& n^2 + \left|\frac{1}{V}\sum_{\mathbf{k}} e^{-\imath\mathbf{k}(\mathbf{r}-\mathbf{r}')}n_{\mathbf{k}}\right|^2 - \frac{1}{V^2}\sum_{\mathbf{k}} n_{\mathbf{k}}\,(n_{\mathbf{k}}+1) \qquad (*)\end{aligned}$$

In contrast to fermions the second term is positive, the last term is completely missing for fermions.

Looking at two examples:
1) <u>All bosons occupying the same state $\mathbf{p}_0$.</u> Then

$$n^2 g(\mathbf{r}-\mathbf{r}') = n^2 + n^2 - \frac{1}{V^2}N(N+1) = \frac{N(N-1)}{V^2}$$

i.e. the pair distribution function is independent of the position. The amplitude of detecting the first particle is N/V, for the second particle it is $(N-1)/V$.

2) Particle distributed over many momentum states. Distribution given by a Gaussian.

$$n_{\mathbf{k}} = \frac{(2\pi)^3 n}{(\sqrt{\pi}\Delta)^3} e^{-(\mathbf{k}-\mathbf{k}_0)^2/\Delta^2} \qquad \text{with} \qquad \int \frac{d\mathbf{p}}{(2\pi)^3} n_{\mathbf{p}} = n \qquad \text{(normalization)}$$

as for instance for the ground state of free Bosons in a harmonic external potential (remember harmonic oscillator, TP3). One then finds

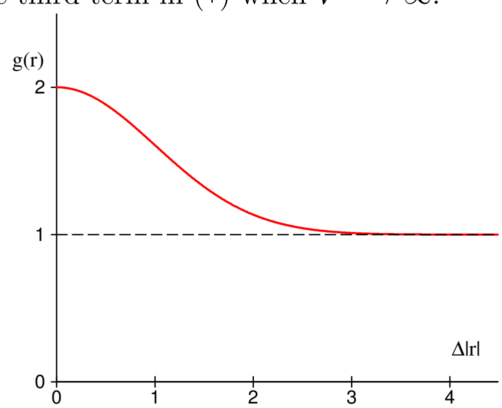
$$\int \frac{d\mathbf{k}}{(2\pi)^3} e^{-\imath\mathbf{k}(\mathbf{r}-\mathbf{r}')} n_{\mathbf{k}} = n\, e^{-\frac{\Delta^2}{4}(\mathbf{r}-\mathbf{r}')^2} e^{-\imath\mathbf{k}_0(\mathbf{r}-\mathbf{r}')}$$

and

$$\frac{1}{V}\int \frac{d\mathbf{k}}{(2\pi)^3} n_{\mathbf{k}}^2 = \frac{1}{V}\left[\frac{(2\pi)^3 n}{(\sqrt{\pi}\Delta)^3}\right]^2 \int \frac{d\mathbf{k}}{(2\pi)^3} e^{-2(\mathbf{k}-\mathbf{k}_0)^2/\Delta^2} \sim \frac{n^2\Delta^3}{V\Delta^6} \sim \frac{n^2}{V\Delta^3}$$

For $n \equiv$ const. and $\Delta \equiv$ const. disappears the third term in $(*)$ when $V \longrightarrow \infty$.

$$\boxed{n^2 g(\mathbf{r}-\mathbf{r}') = n^2\left(1 + e^{-\frac{\Delta^2}{2}(\mathbf{r}-\mathbf{r}')^2}\right)}$$



When $r < \Delta^{-1}$, the probability of finding two particles is increased. Because of the symmetry of the wave function bosons tend to cluster.

2.4 Weakly interacting Bosons

Non-interacting Bose gas

The Hamiltonian for non-interacting bosons (NIB) is

$$\hat{H}^{(1)} = \sum_{\mathbf{k}} E(\mathbf{k}) \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}}; \qquad E(\mathbf{k}) = \frac{\hbar^2 \mathbf{k}^2}{2m}.$$

Ground state: all particles are in $\mathbf{k} = 0$-level:

$$|N\rangle = \frac{\left(\hat{b}_0\right)^N}{\sqrt{N!}} |0\rangle = |N, 0, 0, 0, \cdots\rangle .$$

Note: states with different particle number N have the same energy, namely zero. Hence any superposition also has zero energy, e.g.

$$|\phi\rangle = \sum_N |N\rangle .$$

The model of the NIB is too idealized to decide upon the <u>real</u> ground state. Hence we take into account the interactions.

Weakly interacting Bosons

Hamiltonian:

$$\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \frac{1}{2V} \sum_{\mathbf{k},\mathbf{p},\mathbf{q}} U_{\mathbf{q}} \hat{b}^{\dagger}_{\mathbf{k}+\mathbf{q}} \hat{b}^{\dagger}_{\mathbf{p}-\mathbf{q}} \hat{b}_{\mathbf{p}} \hat{b}_{\mathbf{k}} \, , \tag{2.1}$$

where $\hat{b}_{\mathbf{k}}$ and $\hat{b}^{\dagger}_{\mathbf{k}}$ are bosonic annihilator/creator.
Low temperatures: Bose-Einstein-condensation in the ($\mathbf{k} = 0$)-mode, i.e. even with a weak interaction $U(\mathbf{r})$ is present, we assume that in the ground state $|N\rangle$ the single-particle state with $\mathbf{k} = 0$ is *macroscopically* occupied.

$$N_0 = \langle N | \hat{b}^{\dagger}_0 \hat{b}_0 | N \rangle \lesssim N,$$

i.e. the number of excited particles is small:

$$N - N_0 \ll N_0 \lesssim N.$$

Neglecting the interaction among excited particles, we restrict ourself to the interaction of excited particles with particles of the condensate

$$\begin{aligned}
\hat{H} = \sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} + \frac{1}{2V} U_0 \hat{b}^{\dagger}_0 \hat{b}^{\dagger}_0 \hat{b}_0 \hat{b}_0 \qquad & (\mathbf{k} = \mathbf{p} = \mathbf{q} = 0 \text{ in } (2.1)) \\
+ \frac{1}{V} \sum_{\mathbf{k} \neq 0} \left(U_0 + U_{\mathbf{k}}\right) \hat{b}^{\dagger}_0 \hat{b}_0 \hat{b}^{\dagger}_{\mathbf{k}} \hat{b}_{\mathbf{k}} \qquad & \left(\begin{array}{ll} & \mathbf{p} = \mathbf{q} = 0, \\ \text{resp.} & \mathbf{p} = \mathbf{q}, \mathbf{k} = 0 \text{ in } (2.1) \end{array} \right) \\
+ \frac{1}{2V} \sum_{\mathbf{k} \neq 0} U_{\mathbf{k}} \left(\hat{b}^{\dagger}_{\mathbf{k}} \hat{b}^{\dagger}_{-\mathbf{k}} \hat{b}_0 \hat{b}_0 + \hat{b}^{\dagger}_0 \hat{b}^{\dagger}_0 \hat{b}_{\mathbf{k}} \hat{b}_{-\mathbf{k}} \right) \qquad & \left(\begin{array}{lll} & \mathbf{k} = 0, & \mathbf{p} = 0 \\ \text{resp.} & \mathbf{k} = -\mathbf{q}, & \mathbf{p} = \mathbf{q} \text{ in } (2.1) \end{array} \right) \\
+ \mathcal{O}(\hat{b}^3_{\mathbf{k}}) \qquad &
\end{aligned}$$

Because

$$\begin{aligned}\hat{b}_0 \left|\ldots, N_0, \ldots\right\rangle &= \sqrt{N_0}\left|\ldots, N_0 - 1, \ldots\right\rangle \\ \hat{b}_0^\dagger \left|\ldots, N_0, \ldots\right\rangle &= \sqrt{N_0 + 1}\left|\ldots, N_0 + 1, \ldots\right\rangle \\ \hat{b}_0\hat{b}_0^\dagger - \hat{b}_0^\dagger\hat{b}_0 &= 1\end{aligned}$$

and $N_0 \propto 10^{23} \gg 1$, we neglect the operator properties of $\hat{b}_0^\dagger$ and $\hat{b}_0$ and treat them as complex numbers:

$$\hat{b}_0^\dagger \approx \hat{b}_0 \approx \sqrt{N_0}.$$

$$\implies \hat{H} = \sum_{\mathbf{k}\neq 0} \frac{\hbar^2\mathbf{k}^2}{2m}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + \frac{1}{2V}N_0^2 U_0 + \frac{N_0}{V}\sum_{\mathbf{k}\neq 0}\left[(U_0 + U_\mathbf{k})\,\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + \frac{1}{2}U_\mathbf{k}\left(\hat{b}_\mathbf{k}^\dagger\hat{b}_{-\mathbf{k}}^\dagger + \hat{b}_\mathbf{k}\hat{b}_{-\mathbf{k}}\right)\right] + \ldots$$

N_0 is currently unknown, but we know that must hold:

$$\hat{N} = N_0 + \sum_{\mathbf{k}\neq 0}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k}$$

$$\Big(\text{total particle number} = \#(\text{condensated bosons}) + \#(\text{excited particles})\Big)$$

It is for example

$$\frac{U_0}{2V}N_0^2 = \frac{U_0}{2V}N^2 - \frac{NU_0}{V}\sum_{\mathbf{k}\neq 0}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + \frac{U_0}{2V}\sum_{\mathbf{k},\mathbf{k}'\neq 0}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k}\hat{b}_{\mathbf{k}'}^\dagger\hat{b}_{\mathbf{k}'}$$

and

$$\begin{aligned}\hat{H} &= \sum_{\mathbf{k}\neq 0}\frac{\hbar^2\mathbf{k}^2}{2m}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + \underbrace{\frac{U_0}{2V}N_0^2 + \frac{N_0}{V}\sum_{\mathbf{k}}U_0\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k}}_{\approx\frac{N^2U_0}{2V}} + \frac{N_0}{V}\sum_{\mathbf{k}\neq 0}U_\mathbf{k}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + \frac{N_0}{V}\sum_{\mathbf{k}\neq 0}U_\mathbf{k}\left(\hat{b}_\mathbf{k}^\dagger\hat{b}_{-\mathbf{k}}^\dagger + \hat{b}_\mathbf{k}\hat{b}_{-\mathbf{k}}\right) \\ &\approx \sum_{\mathbf{k}\neq 0}\frac{\hbar^2\mathbf{k}^2}{2m}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + \frac{N^2}{2V}U_0 + \frac{N}{V}\sum_{\mathbf{k}\neq 0}U_\mathbf{k}\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k} + \frac{N}{2V}\sum_{\mathbf{k}\neq 0}U_\mathbf{k}\left(\hat{b}_\mathbf{k}^\dagger\hat{b}_{-\mathbf{k}}^\dagger + \hat{b}_\mathbf{k}\hat{b}_{-\mathbf{k}}\right) + \hat{H}'\end{aligned}$$

$\hat{H}'$ contains terms with 4 creation and annihilation operators ($\mathbf{k} \neq 0$) and these are in the order of $(n')^2 = (N - N_0)^2/V^2$. The **Bogolivbov approximation** (neglecting $\hat{H}'$) is a good approximation when $n' \ll n$. We will see that this condition is fulfilled for a dilute, weakly interacting Bose gas. Note that

$$\frac{N}{V} = n.$$

$\hat{H}$ is a quadric form (in $\hat{b}_\mathbf{k}^\dagger\hat{b}_\mathbf{k}$), which still has to be diagonalized ($\rightsquigarrow$ Bogolivbov transformation).

Ansatz:

$$\begin{aligned}\hat{b}_\mathbf{k} &= U_\mathbf{k}\hat{\alpha}_\mathbf{k} + v_\mathbf{k}\hat{\alpha}_{-\mathbf{k}}^\dagger \\ \hat{b}_\mathbf{k}^\dagger &= U_\mathbf{k}\hat{\alpha}_\mathbf{k}^\dagger + v_\mathbf{k}\hat{\alpha}_{-\mathbf{k}}\end{aligned}$$

If $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$ fulfilled, then $\hat{\alpha}_{\mathbf{k}}$ and $\hat{\alpha}_{\mathbf{k}}^\dagger$ are again bosonic operators:

$$
\begin{aligned}
[\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}_{\mathbf{k}'}] &= \left[\hat{\alpha}_{\mathbf{k}}^\dagger, \hat{\alpha}_{\mathbf{k}'}^\dagger\right] = 0 \\
\left[\hat{\alpha}_{\mathbf{k}}, \hat{\alpha}_{\mathbf{k}'}^\dagger\right] &= \delta_{\mathbf{k},\mathbf{k}'}
\end{aligned}
$$

(Proof: see exercise)
The inverse transformation reads

$$
\begin{aligned}
\hat{\alpha}_{\mathbf{k}} &= U_{\mathbf{k}} \hat{b}_{\mathbf{k}} - v_{\mathbf{k}} \hat{b}_{-\mathbf{k}}^\dagger \\
\hat{\alpha}_{\mathbf{k}}^\dagger &= U_{\mathbf{k}} \hat{b}_{\mathbf{k}}^\dagger - v_{\mathbf{k}} \hat{b}_{-\mathbf{k}}
\end{aligned}
$$

A longer calculation (see exercise) leads to

$$
\begin{aligned}
\hat{H} = \frac{1}{2V} N^2 U_0 &+ \sum_{\mathbf{k}\neq 0} \left(\frac{\hbar^2 \mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right) \left[u_{\mathbf{k}}^2 \hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + v_{\mathbf{k}}^2 \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^\dagger + \underline{u_{\mathbf{k}} v_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{-\mathbf{k}}^\dagger + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}\right)}\right] \\
&+ \frac{N}{2V} \sum_{\mathbf{k}\neq 0} U_{\mathbf{k}} \left[\underline{\left(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2\right) \left(\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{-\mathbf{k}}^\dagger + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{-\mathbf{k}}\right)} + 2u_{\mathbf{k}} v_{\mathbf{k}} \left(\hat{\alpha}_{\mathbf{k}}^\dagger \hat{\alpha}_{\mathbf{k}} + \hat{\alpha}_{\mathbf{k}} \hat{\alpha}_{\mathbf{k}}^\dagger\right)\right]
\end{aligned}
$$

For the non-diagonal term (underlined) to disappear, one needs

$$
\left(\frac{\hbar^2 \mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right) u_{\mathbf{k}} v_{\mathbf{k}} + \frac{n}{2} U_{\mathbf{k}} \left(u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2\right) = 0
$$

With the condition $u_{\mathbf{k}}^2 - v_{\mathbf{k}}^2 = 1$ one calculates

$$
\begin{aligned}
u_{\mathbf{k}}^2 &= \frac{\omega_{\mathbf{k}} + \left(\frac{\hbar^2 \mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)}{2\omega_{\mathbf{k}}} \\
v_{\mathbf{k}}^2 &= \frac{-\omega_{\mathbf{k}} + \left(\frac{\hbar^2 \mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)}{2\omega_{\mathbf{k}}} ,
\end{aligned}
$$

where

$$
\omega_{\mathbf{k}} = \left[\left(\frac{\hbar^2 \mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)^2 - (nU_{\mathbf{k}})^2\right]^{1/2} = \left[\left(\frac{\hbar^2 \mathbf{k}^2}{2m}\right)^2 + \frac{n\hbar^2 \mathbf{k}^2 U_{\mathbf{k}}}{m}\right]^{1/2}
$$

It follows

$$
u_{\mathbf{k}} U_{\mathbf{k}} = \frac{\left[\left(\frac{\hbar^2 \mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)^2 - \omega_{\mathbf{k}}^2\right]^{1/2}}{2\omega_{\mathbf{k}}} = -\frac{nU_{\mathbf{k}}}{2\omega_{\mathbf{k}}}
$$

We can now further calculate $\hat{H}$

$$\begin{aligned}
\hat{H} &= \frac{N^2U_0}{2V} + \sum_{\mathbf{k}\neq 0}\left(\frac{\hbar^2\mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)\left(u_{\mathbf{k}}^2\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}} + v_{\mathbf{k}}^2\underbrace{\left(1+\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}}\right)}_{\hat{\alpha}_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}^\dagger}\right) \\
&\quad + \frac{n}{2}U_{\mathbf{k}}\,2\left(-\frac{nU_{\mathbf{k}}}{2\omega_{\mathbf{k}}}\left(\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}} + \underbrace{1+\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}}}_{\hat{\alpha}_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}^\dagger}\right)\right) \\
&= \frac{N^2U_0}{2V} + \sum_{\mathbf{k}\neq 0}\left(u_{\mathbf{k}}^2+v_{\mathbf{k}}^2\right)\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}} + \left(\frac{\hbar^2\mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)v_{\mathbf{k}}^2 - \frac{n^2V_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}} - \frac{n^2V_{\mathbf{k}}^2}{2\omega_{\mathbf{k}}} \\
&= \frac{N^2U_0}{2V} + \sum_{\mathbf{k}\neq 0}\frac{1}{\omega_{\mathbf{k}}}\left[\underbrace{\left(\frac{\hbar^2\mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)^2 - (nU_{\mathbf{k}})^2}_{=\omega_{\mathbf{k}}^2}\right]\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}} - \frac{1}{2}\left(\frac{\hbar^2\mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right) \\
&\quad + \frac{1}{2\omega_{\mathbf{k}}}\left[\underbrace{\left(\frac{\hbar^2\mathbf{k}^2}{2m} + nU_{\mathbf{k}}\right)^2 - \frac{n^2V_{\mathbf{k}}^2}{\omega_{\mathbf{k}}}}_{=\omega_{\mathbf{k}}^2}\right]
\end{aligned}$$

$$\Longrightarrow \hat{H} = \underbrace{\frac{N^2U_0}{2V} - \frac{1}{2}\sum_{\mathbf{k}\neq 0}\left(\frac{\hbar^2\mathbf{k}^2}{2m} + nU_{\mathbf{k}} - \omega_{\mathbf{k}}\right)}_{\text{ground state energy } E_0} + \underbrace{\sum_{\mathbf{k}\neq 0}\omega_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}^\dagger\hat{\alpha}_{\mathbf{k}}}_{\substack{\text{excitation of}\\ \text{“quasiparticles”}}}$$

The ground state $|N\rangle$ of the system is fixed by the condition $\hat{\alpha}_{\mathbf{k}}|N\rangle = 0$, i.e. no quasiparticles are excited. It is now possible to calculate the number of *real* particles outside of the condensate

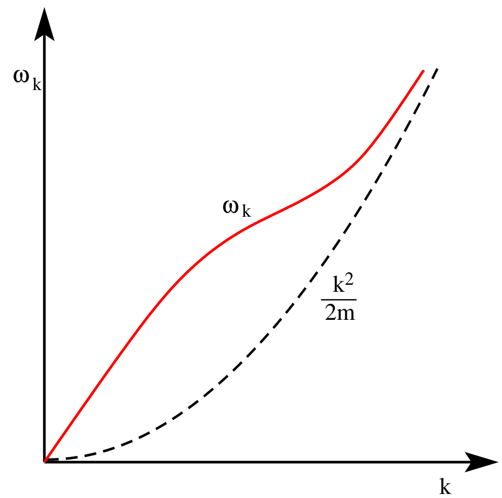
$$N' = \langle N|\sum_{\mathbf{k}\neq 0}\hat{b}_{\mathbf{k}}^\dagger\hat{b}_{\mathbf{k}}|N\rangle = \langle N|\sum_{\mathbf{k}\neq 0}v_{\mathbf{k}}^2\hat{\alpha}_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}^\dagger|N\rangle = \sum_{\mathbf{k}\neq 0}v_{\mathbf{k}}^2$$

Choosing as example a contact potential $U(\mathbf{r}) = U\delta(\mathbf{r})$, one finds $n' = N'/V = \frac{m^{3/2}}{3\pi^2}(nU)^{3/2}$ (see exercise). n' is small, when the expansion parameter $nU \equiv$ (density $\times$ interacting strength) is small, consistent with our assumption of a dilute, weakly interacting gas.

Remark: The dependence of n' on nU is nonanalytic, i.e. it cannot be derived by perturbation theory (starting from $U = 0$).

Exited states are generated by $\hat{\alpha}_{\mathbf{k}}^\dagger|N\rangle$. Their energy is $\hbar\omega_{\mathbf{k}}$. One finds the dispersion relation

$$\omega_{\mathbf{k}} = \left[\left(\frac{\hbar^2 \mathbf{k}^2}{2m} \right)^2 + \frac{n\hbar^2 \mathbf{k}^2 U_{\mathbf{k}}}{m} \right]^{1/2}$$
$$= \begin{cases} ck & \text{for } k \to 0 \text{ where } c = \sqrt{\frac{nU_0}{m}} \\ \frac{\hbar^2 \mathbf{k}^2}{2m} + nU_{\mathbf{k}} & \text{for } k \to \infty \end{cases}$$



Notes: $U_{\mathbf{k}=0} = U_0$ must be positive for the ground state to be stable without quasiparticles, i.e. there is a *repulsive* interaction of the bosons.
$U_{\mathbf{k}} \to 0$ for a *short range* interaction potential of the bosons, i.e. for $k \to \infty$, $\omega_{\mathbf{k}}$ is identical to E_{kin} of free bosons.

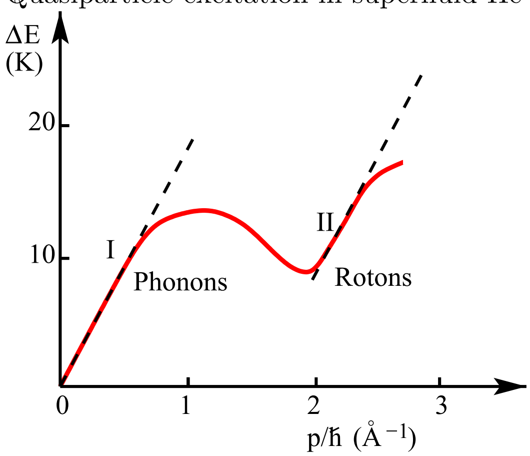
Distinctive feature: $\min\left\{\frac{\omega_{\mathbf{k}}}{k}\right\} =: v_{\text{crit}} \neq 0$ leads to *superfluidity*.

Chapter 3

Superfluidity

3.1 Landau's model Helium 4 superfluid

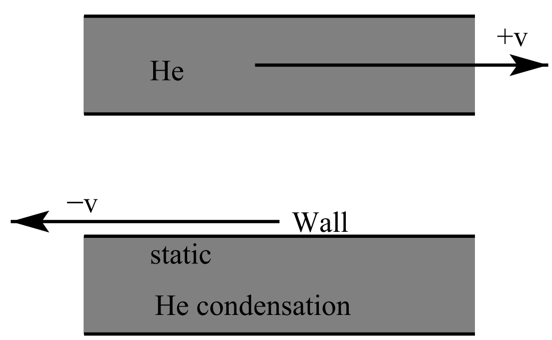
Quasiparticle excitation in superfluid He^4



Area I:
Excitations: phonons
$\varepsilon_p = cp, \quad c = 238\,\mathrm{m/s}$

Area II:
Minimum at $p_0 = 1.91\,\AA^{-1}\hbar$
Excitations: rotons
$\varepsilon_p = \Delta + \frac{(|p|-p_0)^2}{2\mu}, \quad \mu = 0.16\,\mathrm{m_{He}}, \;\; \Delta/k = 8.6\,\mathrm{K}$

Consequences for the dynamical behaviour: Two-fluid model, superfluidity (Landau). Consider $T = 0$, fluid in ground state (condensate), no excitations present. The condensate moves through a pipe as an unit with drift velocity v:



Assertion:
There is no friction if $v < v_{\mathrm{crit}}$. Consider Galilei-Transformation: condensate is at rest, walls are moving. If the fluid would be viscous, the pipe would be decelerated, in which case energy and momentum in the form of excitations (quasiparticles) would be transmitted in the fluid.

If there is no excitation present, then:

Rest frame (of fluid):

$$\mathbf{P}_0 = 0, \quad E = E_{\text{gs}}$$

Lab frame (fluid moving, vel. $\mathbf{v}$):

$$\mathbf{P} = M\mathbf{v}, \quad E = E_{\text{gs}} + \frac{M\mathbf{v}^2}{2}$$

Assuming now there exist excitations with (total) momentum $\mathbf{p}$ and energy $\varepsilon(\mathbf{p})$.
Rest frame:

$$\mathbf{P}_0 = \mathbf{p}, \quad E = E_{\text{gs}} + \varepsilon(\mathbf{p})$$

Lab frame:

$$\mathbf{P} = M\mathbf{v} + \mathbf{p}, \quad E = \frac{M\mathbf{v}^2}{2} + \mathbf{v}\cdot\mathbf{p} + E_{\text{gs}} + \varepsilon(\mathbf{p})$$

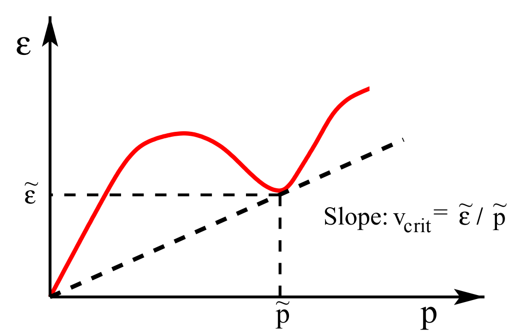
$$\Rightarrow \Delta E = \varepsilon(\mathbf{p}) + \mathbf{v}\cdot\mathbf{p}$$

Is it energetically beneficial to excite quasiparticles, i.e. $\Delta E < 0$?
Because $\varepsilon(\mathbf{p}) > 0$, the energy difference assumes it smallest value when $\mathbf{p}$ and $\mathbf{v}$ are antiparallel. For an excitation to have an energetic benefit the following inequality must be satisfied:

$$\varepsilon(\mathbf{p}) - |\mathbf{v}||\mathbf{p}| < 0 \quad \Leftrightarrow \quad v > \frac{\varepsilon(\mathbf{p})}{|\mathbf{p}|}$$

The critical velocity is therefore given by

$$v_{\text{crit}} = \min_{\mathbf{p}} \left\{ \frac{\varepsilon(\mathbf{p})}{|\mathbf{p}|} \right\}$$



Implication: For $|\mathbf{v}| < v_{\text{crit}}$ there is no excitation possible and the fluid flows frictionless $\rightsquigarrow$ superfluidity.
$T > 0$: There already exist some excitations which can collide with the wall and can interchange energy and momentum $\rightsquigarrow$ friction caused by the noncondensated particles. But up to T_U there is a macroscopic condensate present.

3.2 Field theory for interacting Bose gas

Start with evolution equation for the field operators $\hat{\Psi}(\mathbf{r},t)$ (Heisenberg equation):

$$\imath\hbar\frac{\partial}{\partial t}\hat{\Psi}(\mathbf{r},t) = \left[\hat{\Psi}(\mathbf{r},t),\hat{H}\right]$$

with $\hat{H} = \hat{H}^{(1)} + \hat{H}^{(2)}$

$$\hat{H}^{(1)} = \int d^3\mathbf{r}\,\hat{\Psi}^\dagger(\mathbf{r})\left\{-\frac{\hbar^2}{2m}\Delta\right\}\hat{\Psi}(\mathbf{r}),$$

$$\hat{H}^{(2)} = \frac{1}{2}\int d^3\mathbf{r_1}d^3\mathbf{r_2}\,U(\mathbf{r_1}-\mathbf{r_2})\hat{\Psi}^\dagger(\mathbf{r_1})\hat{\Psi}^\dagger(\mathbf{r_2})\hat{\Psi}(\mathbf{r_2})\hat{\Psi}(\mathbf{r_1}).$$

The commutators give:

$$\left[\hat{\Psi}(\mathbf{r}),\hat{H}^{(1)}\right] = -\frac{\hbar^2}{2m}\int d^3\mathbf{r}' \underbrace{\left[\hat{\Psi}(\mathbf{r}),\hat{\Psi}^\dagger(\mathbf{r}')\Delta\hat{\Psi}(\mathbf{r}')\right]}_{\substack{=\hat{\Psi}^\dagger(\mathbf{r}')\left[\hat{\Psi}(\mathbf{r}),\Delta\hat{\Psi}(\mathbf{r}')\right] \quad +\left[\hat{\Psi}(\mathbf{r}),\hat{\Psi}^\dagger(\mathbf{r}')\right]\Delta\hat{\Psi}(\mathbf{r}') \\ =0 \qquad\qquad\qquad\qquad +\,\delta(\mathbf{r}-\mathbf{r}')\Delta\hat{\Psi}(\mathbf{r}')}}$$

$$= -\frac{\hbar^2}{2m}\int d^3\mathbf{r}'\,\delta(\mathbf{r}-\mathbf{r}')\Delta\hat{\Psi}(\mathbf{r}') = -\frac{\hbar^2}{2m}\Delta\hat{\Psi}(\mathbf{r}),$$

and

$$\left[\hat{\Psi}(\mathbf{r}),\hat{H}^{(2)}\right] = \frac{1}{2}\int d^3\mathbf{r_1}d^3\mathbf{r_2}\,U(\mathbf{r_1}-\mathbf{r_2}) \underbrace{\left[\hat{\Psi}(\mathbf{r}),\hat{\Psi}^\dagger(\mathbf{r_1})\hat{\Psi}^\dagger(\mathbf{r_2})\hat{\Psi}(\mathbf{r_2})\hat{\Psi}(\mathbf{r_1})\right]}_{=\delta(\mathbf{r}-\mathbf{r_2})\hat{\Psi}^\dagger(\mathbf{r_1})\hat{\Psi}(\mathbf{r_2})\hat{\Psi}(\mathbf{r_1})+\delta(\mathbf{r}-\mathbf{r_1})\hat{\Psi}^\dagger(\mathbf{r_2})\hat{\Psi}(\mathbf{r_2})\hat{\Psi}(\mathbf{r_1})}$$

$$= \int d^3\mathbf{r_1}U(\mathbf{r}-\mathbf{r_1})\hat{\Psi}^\dagger(\mathbf{r_1})\hat{\Psi}(\mathbf{r_1})\hat{\Psi}(\mathbf{r}).$$

Assume (for simplicity: model) contact potential: $U(\mathbf{r}) = U\delta(\mathbf{r})$, we have:

$$\left[\hat{\Psi}(\mathbf{r}),\hat{H}^{(2)}\right] = U\hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}(\mathbf{r})\hat{\Psi}(\mathbf{r}),$$

and the evolution equation (or Heisenberg Equation) becomes

$$\boxed{\imath\hbar\frac{\partial}{\partial t}\hat{\Psi} = -\frac{\hbar^2}{2m}\Delta\hat{\Psi} + U\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi}}. \tag{3.1}$$

Consider a set of NIB ground state $|N\rangle$ with $N \gg 1$. Then

$$\langle N|\,\hat{b}_0^\dagger\hat{b}_0\,|N\rangle = N \qquad \text{and} \qquad \langle N|\,\hat{b}_0\hat{b}_0^\dagger\,|N\rangle = N+1.$$

Since $N \gg 1$ we have:

$$\langle\hat{b}_0^\dagger\hat{b}_0\rangle \simeq \langle\hat{b}_0\hat{b}_0^\dagger\rangle \gg \langle[\hat{b}_0,\hat{b}_0^\dagger]\rangle.$$

We can neglect the commutators of the field operators $\hat{b}_0$ and $\hat{b}_0^\dagger$, i.e. $\hat{b}_0$ and $\hat{b}_0^\dagger$ are simple, complex numbers:

$$\boxed{\hat{\Psi}(\mathbf{r},t) = \underbrace{b_0}_{\text{number}}\psi(\mathbf{r},t) + \sum_{\mathbf{k}\neq 0}\underbrace{\hat{b}_\mathbf{k}}_{\text{operator!}}\psi_\mathbf{k}(\mathbf{r},t).} \tag{3.2}$$

Simplest solution of Eq. (3.1):
The condensate (ground state) is

$$\hat{\Psi}(\mathbf{r},t) = b_0\psi(\mathbf{r},t) \equiv \psi(t). \qquad \text{(classical field)}$$

This corresponds to the state $\psi(\mathbf{r},t)$ with momentum $\mathbf{k} = 0$, and it does not depend on $\mathbf{r}$. Eq. (3.1) then becomes:

$$\imath\hbar\frac{\partial\psi}{\partial t}(t) = U|\psi(t)|^2\psi(t). \tag{3.3}$$

The solution of Eq. (3.3) with time-independent modulus is:

$$\psi(t) = \psi_0 e^{-\frac{\imath}{\hbar}\mu t}, \qquad |\psi(t)|^2 = |\psi_0|^2$$

Remember that $\hat{\Psi}^\dagger\hat{\Psi}$ is the density operator hence the solution describes the Bose condensate with density $\rho(\mathbf{r}) = |\psi_0|^2$. The parameter μ is related to the density via Eq. (3.3):

$$\mu = U\rho.$$

It is the chemical potential of the condensate: adding one more particle to the condensate absorbs the interaction energy U multiplied by the local density of bosons ρ.

3.3 Oscillatory excitations

Linearize equations of motion around the simplest (homogeneous) solution.

$$\text{Ansatz}: \qquad \hat{\Psi}(\mathbf{r},t) = \psi(\mathbf{r},t) + \delta\hat{\Psi}(\mathbf{r},t)e^{-\frac{\imath}{\hbar}\mu t}.$$

Inserting this expression of $\hat{\Psi}$ in Eq. (3.1) (Heisenberg equation) and keeping only the terms to first order in $\delta\hat{\Psi}$, we obtain:

$$\imath\hbar\frac{\partial}{\partial t}\delta\hat{\Psi} + \mu\delta\hat{\Psi} = -\frac{\hbar^2}{2m}\Delta\delta\hat{\Psi} + U\psi_0^2\delta\hat{\Psi}^\dagger + 2U|\psi_0|^2\delta\hat{\Psi}.$$

To simplify, we assume that ψ_0 is real:

$$U\psi_0^2 = U|\psi_0|^2 = U\rho = \mu.$$

Therefore,

$$\imath\hbar\frac{\partial}{\partial t}\delta\hat{\Psi} = -\frac{\hbar^2}{2m}\Delta\delta\hat{\Psi} + \mu\left(\delta\hat{\Psi}^\dagger + \delta\hat{\Psi}\right). \tag{3.4}$$

Obviously plane waves satisfy this equation. Expressing the corrections to the condensate operators as in Eq. (3.2), we can search for a solution of the form

$$\delta\hat{\Psi}(\mathbf{r},t) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}}\hat{b}_{\mathbf{k}}(t)e^{\imath\mathbf{k}\cdot\mathbf{r}}.$$

Inserting in Eq. (3.4) we obtain:

$$\frac{1}{\sqrt{V}}\sum_{\mathbf{k}}e^{\imath\mathbf{k}\cdot\mathbf{r}}\left(\imath\hbar\frac{\partial}{\partial t}\hat{b}_{\mathbf{k}}\right) = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}}e^{\imath\mathbf{k}\cdot\mathbf{r}}\left[E(\mathbf{k})+\mu\right]\hat{b}_{\mathbf{k}} + \frac{1}{\sqrt{V}}\sum_{\mathbf{k}}e^{-\imath\mathbf{k}\cdot\mathbf{r}}\mu\hat{b}^\dagger_{\mathbf{k}}$$

Multiply both sides with $\frac{1}{\sqrt{V}}e^{-\imath\mathbf{q}\cdot\mathbf{r}}$ and then sum over $\mathbf{r}$:

$$\sum_{\mathbf{k}}\underbrace{\frac{1}{V}\sum_{\mathbf{r}}e^{\imath(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}}_{=\delta_{\mathbf{k},\mathbf{q}}}\left(\imath\hbar\frac{\partial}{\partial t}\hat{b}_{\mathbf{k}}\right)=\sum_{\mathbf{k}}\underbrace{\frac{1}{V}\sum_{\mathbf{r}}e^{\imath(\mathbf{k}-\mathbf{q})\cdot\mathbf{r}}}_{=\delta_{\mathbf{k},\mathbf{q}}}\left[E(\mathbf{k})+\mu\right]\hat{b}_{\mathbf{k}}+\sum_{\mathbf{k}}\underbrace{\frac{1}{V}\sum_{\mathbf{r}}e^{-\imath(\mathbf{k}+\mathbf{q})\cdot\mathbf{r}}}_{=\delta_{\mathbf{k},-\mathbf{q}}}\mu\hat{b}^{\dagger}_{\mathbf{k}}$$

which gives:

$$\boxed{\imath\hbar\frac{\partial}{\partial t}\hat{b}_{\mathbf{q}}=\left[E(\mathbf{q})+\mu\right]\hat{b}_{\mathbf{q}}+\mu\hat{b}^{\dagger}_{-\mathbf{q}}.}\tag{3.5}$$

Without the last term $\propto \hat{b}^{\dagger}_{-\mathbf{q}}$, one would recover the usual equation of motion for non-interacting boson - like particles with energies $E(\mathbf{q})+\mu$. The presence of the $\hat{b}^{\dagger}_{-\mathbf{q}}$ term indicate that $\hat{b}_{\mathbf{k}}$'s are not the right operators to work with (i.e. do not diagonalize the Hamiltonian).
Bogoliubov introduced the following new Bose-operators:

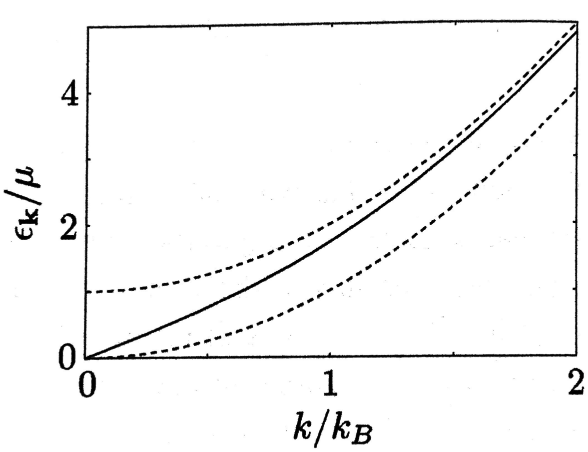
$$\begin{aligned}\hat{b}_{\mathbf{k}}&=u_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}+v_{\mathbf{k}}\hat{\alpha}_{-\mathbf{k}}\\ \hat{b}^{\dagger}_{\mathbf{k}}&=u_{\mathbf{k}}\hat{\alpha}^{\dagger}_{\mathbf{k}}+v_{\mathbf{k}}\hat{\alpha}^{\dagger}_{-\mathbf{k}}\end{aligned}\tag{3.6}$$

such that Eq. (3.5) transforms into:

$$\boxed{\imath\hbar\frac{\partial}{\partial t}\hat{\alpha}_{\mathbf{k}}=\varepsilon_{\mathbf{k}}\hat{\alpha}_{\mathbf{k}}}.\tag{3.7}$$

where $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are real coefficients and $u_{\mathbf{k}}^2-v_{\mathbf{k}}^2=1$ due to Bose operator $\hat{\alpha}_{\mathbf{k}}$.
The "wrong" creation/annihilation-operators $\hat{b}_{\mathbf{k}}$, $\hat{b}^{\dagger}_{\mathbf{k}}$ describe particles and the "right" c/a operators $\hat{\alpha}_{\mathbf{k}}$, $\hat{\alpha}^{\dagger}_{\mathbf{k}}$ describe quasi-particles.
To find the quasiparticle energies $\varepsilon_{\mathbf{k}}$ along with the coefficients $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$, one substitutes Eq. (3.6) into Eq. (3.5) and requires that it can be written as Eq. (3.7) (see exercise). One then obtains a linear algebra problem for an unknown vector with eigenvalues $\varepsilon_{\mathbf{k}}$.
The quasi particles energies, the energies of the elementary excitations of the interacting Bose condensate, are given by:

$$\begin{aligned}\varepsilon_{\mathbf{k}}&=\sqrt{E(\mathbf{k})[E(\mathbf{k})+2\mu]}=\sqrt{\frac{\hbar^2\mathbf{k}^2}{2m}\left(\frac{\hbar^2\mathbf{k}^2}{2m}+2\mu\right)}\\ &=\hbar k\sqrt{\frac{\mu}{m}}\sqrt{1+\frac{\hbar^2\mathbf{k}^2}{4\mu m}}=\hbar k\sqrt{\frac{\mu}{m}}+\mathcal{O}(\mathbf{k}^2).\end{aligned}$$



Hence

$$\frac{\varepsilon_{\mathbf{k}}}{\mu}=\frac{k}{k_{\mathrm{B}}}\sqrt{1+\frac{k^2}{2k_{\mathrm{B}}^2}},\quad k_{\mathrm{B}}=\frac{\sqrt{2\mu m}}{\hbar}$$

Small-$\mathbf{k}$ behavior:

$$\begin{aligned}\varepsilon_{\mathbf{k}}&=\hbar v_p k+\mathcal{O}(k^2),\\ \omega_{\mathbf{k}}&=v_p k+\mathcal{O}(k^2),\\ v_p&=\sqrt{\frac{\mu}{m}}=\frac{1}{\hbar}\lim_{k\to 0}\frac{\partial\varepsilon_{\mathbf{k}}}{\partial k}.\end{aligned}$$

For small k the excitations are density waves (sound waves) and v_p is the sound velocity. The feature $\min\{\omega_{\mathbf{k}}/k\}=v_p>0$ leads to superfluidity: two-fluid model of superfluidity.

3.4 Topological excitations

It turns out that many field theories possess excitations not captured by a Taylor expansion: topological excitations. Configurations of quantum fields in such theories can be separated into classes such that no infinitesimally small change of the field configuration would cause a change from one class to the other.
In superfluidity the relevant configurations of the complex field $\langle\hat{\Psi}(\mathbf{r},t)\rangle$ have constant modulus (related to the particle density) while the phase can change rather freely. There exist topologically non-trivial configurations of the phase which are called vortices: emergent excitations.
Simplification: Resort to a closed equation for $\langle\hat{\Psi}(\mathbf{r},t)\rangle = \psi(\mathbf{r},t)$: "quasiclassical approximations".
From Heisenberg equation (3.1), with mean field approximation:

$$\imath\hbar\frac{\partial}{\partial t}\langle\hat{\Psi}\rangle = -\frac{\hbar^2}{2m}\Delta\langle\hat{\Psi}\rangle + U\underbrace{\langle\hat{\Psi}^\dagger\hat{\Psi}\hat{\Psi}\rangle}_{\simeq\langle\hat{\Psi}^\dagger\rangle\langle\hat{\Psi}\rangle\langle\hat{\Psi}\rangle}.$$

Including factor $e^{\frac{\imath}{\hbar}\mu t}$ into $\psi(\mathbf{r},t)$, one obtains the time-dependent Gross-Pitaevskii (GP) equation:

$$\boxed{\imath\hbar\frac{\partial\psi}{\partial t}(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\Delta - \mu + U|\psi(\mathbf{r},t)|^2\right]\psi(\mathbf{r},t).} \tag{3.8}$$

Quasiclassical approximation requires a large number of bosons: average interatomic distance $\sim\rho^{-1/3}$. Characteristic length scale (healing length) of GP:

$$\xi \equiv \sqrt{\frac{\hbar^2}{2m}\frac{1}{U\rho}} = \frac{\hbar}{\sqrt{2mU\rho}}.$$

If $\xi \gg \rho^{-1/2}$ is consistent, i.e. for $mU \ll \hbar^2\rho^{-1/2}$ (weak interaction). For superfluid Helium: $\xi \sim 0.1\text{nm} \simeq \rho^{-1/2}$.
GP is a classical Hamiltonian equation, can be obtained from Hamiltonian:

$$H_{\text{Cl}} = \int d^3\mathbf{r}\left(\frac{\hbar^2}{2m}|\nabla\psi(\mathbf{r})|^2 - \mu|\psi(\mathbf{r})|^2 + \frac{U}{2}|\psi(\mathbf{r})|^4\right)$$

by variation with respect to $\psi^*(\mathbf{r})$ and $\psi(\mathbf{r})$. It is

$$H_{\text{Cl}} = \langle\hat{H} - \mu\hat{N}\rangle.$$

$\Longrightarrow$ Total energy $E = H_{\text{Cl}}$ is conserved.

How to relate $\psi(\mathbf{r},t)$ to more classical quantities characterizing a liquid?
It is clear that density $\rho(\mathbf{r},t) = \langle\hat{\Psi}^\dagger(\mathbf{r},t)\hat{\Psi}(\mathbf{r},t)\rangle \simeq |\psi(\mathbf{r},t)|^2 \Leftrightarrow$ modulus of ψ!
What about the phase? With Eq. (3.8) one finds:

$$\frac{\partial\rho}{\partial t}(\mathbf{r},t) = \frac{\imath\hbar}{2m}\nabla\cdot\left[\psi^*(\mathbf{r},t)\nabla\psi(\mathbf{r},t) - \psi(\mathbf{r},t)\nabla\psi^*(\mathbf{r},t)\right],$$

since $\psi\Delta\psi^* - \psi^*\Delta\psi = \nabla\cdot[\psi\nabla\psi^* - \psi^*\nabla\psi]$, we define the current density

$$\boxed{\mathbf{j}(\mathbf{r},t) = -\frac{\imath\hbar}{2m}\left[\psi^*(\mathbf{r},t)\nabla\psi(\mathbf{r},t) - \psi(\mathbf{r},t)\nabla\psi^*(\mathbf{r},t)\right]},$$

then the particle density satisfy the continuity equation

$$\boxed{\frac{\partial \rho}{\partial t}(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0}\,.$$

Since $\mathbf{j}$ is on one hand a particle current density, $\mathbf{j} = \rho \mathbf{v_s}$, with $\mathbf{v_s}$ the local velocity field and on the other hand with $\psi = \sqrt{\rho} e^{\imath\phi}$:

$$\mathbf{j}(\mathbf{r}, t) = -\frac{\imath\hbar}{2m}\left[\sqrt{\rho}e^{-\imath\phi}\left(\nabla\sqrt{\rho} + \imath\sqrt{\rho}\nabla\phi\right)e^{\imath\phi} - \sqrt{\rho}e^{\imath\phi}\left(\nabla\sqrt{\rho} - \imath\sqrt{\rho}\nabla\phi\right)e^{-\imath\phi}\right] = \frac{\hbar}{m}\rho\nabla\phi.$$

Hence the velocity is

$$\boxed{\mathbf{v_s}(\mathbf{r}, t) = \frac{\hbar}{m}\nabla\phi(\mathbf{r}, t)}\,,$$

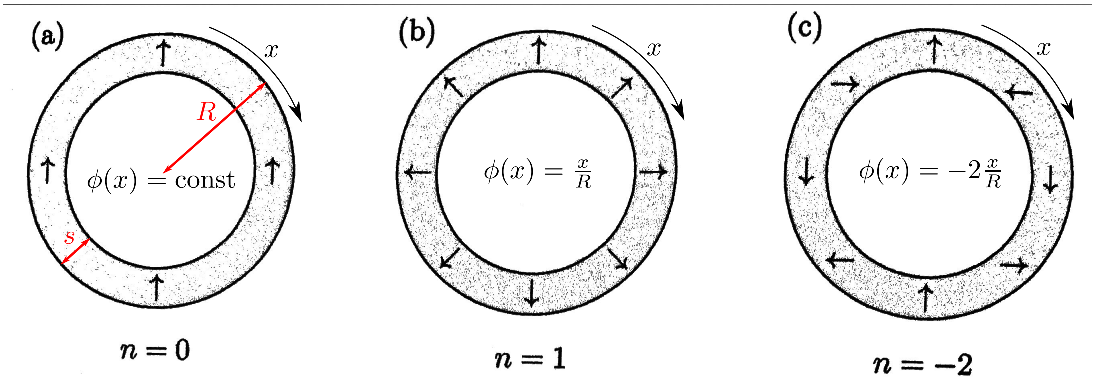
i.e. the gradient of the phase ϕ of ψ is proportional to the local vector of the fluid. Note that if $\psi(\mathbf{r}, t)$ is a plane wave, the phase is $\phi = \mathbf{k} \cdot \mathbf{r}$ and the velocity is trivially

$$\mathbf{v_s} = \frac{\hbar}{m}\mathbf{k} = \frac{\mathbf{p}}{m}.$$

Now we illustrate the existence of topological excitations:
Consider one-dimensional field theory first, and confine the superfluid to a thin ring of cross section s and radius R with $\phi(0) = \phi(2\pi R)$:

$$\oint dx\, \frac{\partial \phi}{\partial x} = 2\pi n, \qquad n \in \mathbb{Z}.$$

The integer n is a topological number, it cannot be changed by a small variation of ψ.



GP in 1d with $\rho = \text{const}$ and stationary $\phi(x)$ (no time dependence):

$$0 = \left[-\frac{\hbar^2}{2m}\phi'' \underbrace{-\mu + U\rho}_{=0}\right]\sqrt{\rho}e^{\imath\phi}$$

$$\implies \phi'' = \frac{m}{\hbar}v_s' = 0$$

$$\implies v_s = \text{const}.$$

The condensate moves with a constant velocity v_s along the ring.

Each field configuration with a non-zero constant density in all points of the ring is characterized by a certain n, and those that differ in n belong to different sectors. For $\psi = \sqrt{\rho} e^{\imath n x/R}$

$$E = s \oint dx \left[\frac{\hbar^2}{2m} \phi'^2 \rho - \mu\rho + \frac{U}{2}\rho^2 \right] = E_0 + n^2 \frac{\pi\hbar\rho s}{mR}.$$

True ground state is $n = 0$.
The relation $\oint dx\, \partial_x \phi = 2\pi n$ implies a quantization of the velocity of the condensate:

$$v_n = \frac{\hbar}{m}\phi' = n\frac{\hbar}{mR}.$$

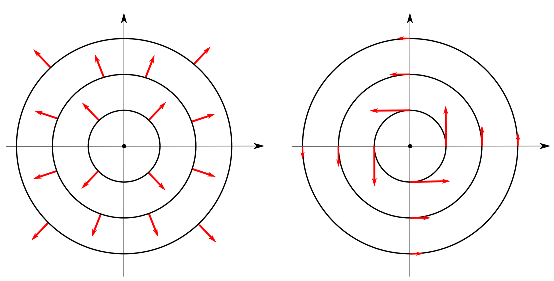
To understand this: compute total angular momentum L_n of the superfluid with respect to the symmetry axis of the ring:
Momentum of an infinitesimal element of the fluid: $dl = v_n m\rho s dx$

$$L_n = R\oint dl = R\int_0^{2\pi R} dx v_n m\rho s = 2\pi R n\hbar\rho s = n\hbar N_p$$

with $N_p = 2\pi R s\rho$, the number of particles in the condensate.
In a topological sector n, each particle of the superfluid acquires a quantized value of the angular momentum $\hbar n$. It is different from the angular momentum quantization of non-interacting bosons: clear manifestation of the collective nature of topological excitations.

3.4.1 Vortices

Consider 2d, use polar coordinates $(x, y) \to (r\cos\theta, r\sin\theta)$.



$\phi(r,\theta)$ $\qquad$ $\mathbf{v_s}(r,\theta)$

$$\phi(r,\theta) = n\theta$$

$$\Rightarrow \qquad \mathbf{v_s}(r,\theta) = \frac{n\hbar}{mr}\mathbf{e}_\theta.$$

Note that the phase accumulation along any close loop around the origin yields the same amount

$$\Delta\phi = \oint d\mathbf{r}\cdot\nabla\phi = 2\pi n.$$

n is also called the winding number of the vortex. Note that $\mathbf{v_s}$ diverges for $r \to 0$ and the phase becomes undefined at $r = 0$: something special goes on close to the center of the vortex (i.e. tornado, whirl-pool sink, ...).
Go back to GP and seek for cylindrically symmetric solutions of the form

$$\psi(\mathbf{r}) = \sqrt{\rho_0} f(r) e^{\imath n\theta}$$

when ρ_0 is the equilibrium density of the superfluid that is reached far away from the vortex center, and $f(r)$ is a dimensionless function. The continuity of ψ gives $f(r) \simeq r^n$ for $r \to 0$, i.e. the density of the condensate must reach zero precisely in the vortex center!
From the stationary form of the Eq. (3.8):

$$0 = \left[-\frac{\hbar^2}{2m}\Delta - \mu + U|\psi|^2 \right]\psi$$

with the Laplace operator in polar coordinates

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}.$$

Hence

$$0 = \left[-\frac{\hbar^2}{2m}\left(f''(r) + \frac{1}{r} f'(r) - \frac{n^2}{r^2} f(r) \right) - \mu f(r) + u\rho_0 f(r)^3 \right] \sqrt{\rho_0} e^{\imath n\theta}.$$

We substitute $u = r/\xi$ with $\xi = \hbar/\sqrt{2mU\rho_0}$, $dr = \xi du$.

$$0 = -\underbrace{\frac{\hbar^2}{2m}\frac{1}{\xi^2}}_{=U\rho_0=\mu} \left(\underbrace{f''(u) + \frac{1}{u} f'(u)}_{\frac{1}{u}\frac{d}{du}\left(u\frac{df}{du}\right)} - \frac{n^2}{u^2} f(u) \right) - \mu f(u) + U\rho_0 f(u)^3$$

$$\Rightarrow \qquad \frac{1}{u}\frac{d}{du}\left(u\frac{df}{du} \right) + \left(1 - \frac{n^2}{u^2} \right) f - f^3 = 0.$$

This equation indeed has a solution satisfying $f \simeq u^n$ for $u \to 0$:

$$\frac{1}{u}\frac{d}{du}\left(u\frac{du^n}{du} \right) = n^2 u^{n-2}, \qquad \left(1 - \frac{n^2}{u^2} \right) f = -n^2 u^{n-2} + \mathcal{O}(u^n)$$

and $f \simeq 1$ for $u \to \infty$:

$$\frac{df}{du} = 0, \qquad \frac{n^2}{u^2} f \to 0, \qquad \text{and} \qquad f - f^3 \to 0.$$

Estimate the (kinetic) energy stored in a single vortex in a 3d slab of height b:

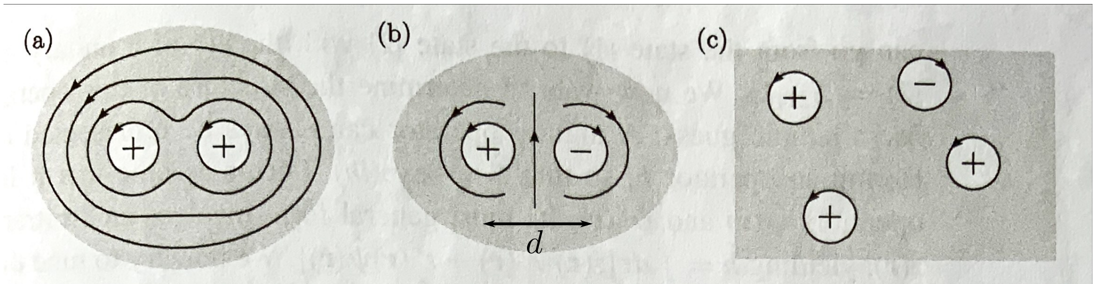
$$E_n = \int d^3\mathbf{r} \frac{mv(\mathbf{r})^2}{2} \rho(\mathbf{r}) = \int_0^b dz \int drr \int_0^{2\pi} d\theta \frac{m}{2}\frac{\hbar^2 n^2}{m^2 r^2}\rho_0 = n^2 b\pi \frac{\hbar^2 \rho_0}{m} \underbrace{\int \frac{dr}{r}}_{I}.$$

I diverges at the upper and lower bounds: cut-off. Lower limit is naturally set by size of the vortex core where the density is suppressed (see above): ξ. Upper limit is nothing but the typical size of the superfluid: L.

$$I = \int_\xi^L \frac{dr}{r} = \ln\frac{L}{\xi} \qquad \Rightarrow \qquad \boxed{E_n = n^2 b \frac{dE}{dl} \ln\frac{L}{\xi}, \qquad \frac{dE}{dl} = \pi\frac{\hbar^2\rho_0}{m}}.$$

where $\frac{dE}{dl}$ denotes energy per unit thickness. Note that E_n scales with n^2: vortices with lowest winding numbers $n = \pm 1$ are preferred.

Multi-vertex configurations:



Total velocity:

$$\mathbf{v}_{\rm tot}(\mathbf{r}) = \mathbf{v_1}(\mathbf{r}) + \mathbf{v_2}(\mathbf{r}) + \cdots .$$

Total kinetic energy of the fluid is prop. to ${\mathbf{v}_{\rm tot}}^2$: pairwise vortex-vortex interactions.

(a) Assume we have $N_{\rm v}$ vortices of winding number $n = +1$ (or $n = -1$). They all carry separately the same energy E_1, since all circulate in the same way. Full energy including interactions:

$$E = b\frac{dE}{dl}\left[N_{\rm v}\ln\frac{L}{\xi} + \frac{1}{2}\sum_{i\neq j}\ln\frac{L}{|\mathbf{r_i} - \mathbf{r_j}|}\right],$$

with $\mathbf{r_i}$ are the vortex coordinates. Interaction energy is lowest when the vortices are far apart. Hence for fixed concentration of vortices, they form a regular lattice.

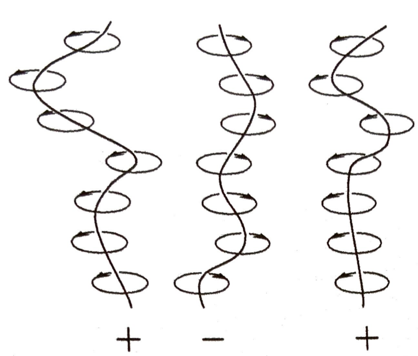
(b) Pair of vortices with opposite winding number. Energy:

$$E \propto b\frac{dE}{dl}\ln\frac{d}{\xi},$$

with d the distance between the two vortex centers. attraction, independent of the system size L: zero topological charge. Then topologically connected to the ground state. Hence it can be seen as a superposition of elementary excitations (sound quanta) of the ground state.

(c) Several vortex arrangement.

3.4.2 Vortex lines (in 3d)



In a realistic 3d liquid, the vortex cores are long lines that must start and end at the boundaries of the superfluid and penetrate the whole volume of the fluid:

$$E_1 = L\frac{dE}{dl}\ln\frac{L}{\xi}.$$

These vortex lines can be simply produced by setting the superfluid into rotation.

Rotating a normal rigid body: $\mathbf{v} = \boldsymbol{\omega}_0 \times \mathbf{r}$.
Given $\mathbf{v}(x, y, z)$, consider surface Ω:

$$\int_\Omega (\nabla \times \mathbf{v}) \cdot d\mathbf{S} = \oint_{\partial\Omega} \mathbf{v} \cdot d\mathbf{r} = \Gamma.$$

Clearly this contour integral is a measure of the circulation Γ of the field $\mathbf{v}$ along the contour $\partial\Omega$. For a normal rotating rigid body, the vorticity is:

$$\begin{aligned}\boldsymbol{\omega} \equiv \nabla \times \mathbf{v} = \nabla \times (\boldsymbol{\omega}_0 \times \mathbf{r}) &= (\nabla \cdot \mathbf{r})\boldsymbol{\omega}_0 - (\boldsymbol{\omega}_0 \cdot \nabla)\mathbf{r} \\ &= 3\boldsymbol{\omega}_0 - \boldsymbol{\omega}_0 = 2\boldsymbol{\omega}_0.\end{aligned}$$

The vorticity is thus simply twice the angular frequency of the rotation.

Superflow:
The vorticity is

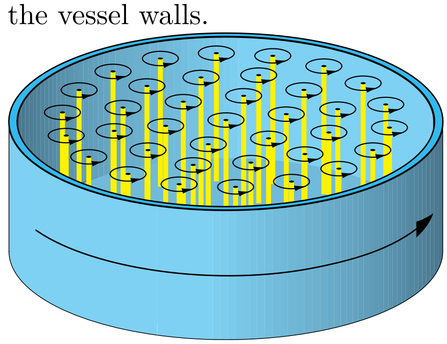
$$\boldsymbol{\omega} = 2\pi N_\mathrm{v} \frac{\hbar}{m},$$

with N_v is the number of vortices penetrating the surface.
Remember: for one vortex:

$$\mathbf{v} = \frac{\hbar}{m}\nabla\phi, \quad \oint \mathbf{v} \cdot d\mathbf{r} = 2\pi\frac{\hbar}{m}.$$

$\Longrightarrow$ Superflow without vortices: zero vorticity, zero angular momentum, non-rotating.
$\Longrightarrow$ Superfluid in a rotating vessel just slips along the vessel walls.

Enforce rotation: rotate in normal state, cool below superfluid-transition temperature.
$\Longrightarrow$ angular momentum cannot disappear
$\Longrightarrow$ lattice of vortices forms. The number of vortex lines is equal to the initial angular momentum.



O. V. Lounasmaa and E. Thuneberg, *Vortices in rotating superfluid ^{3}He*, PNAS **96**, 7760-7767 (1999).

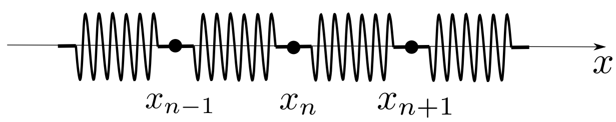
Note: The picture is the same for ^{4}He and ^{3}He.

Chapter 4

Quantization of the classical radiation field

4.1 Classical Fields

Chain of coupled oscillators



For a system of coupled oscillators, the Hamiltonian can be written as:

$$H = \sum_n \left[\frac{p_n^2}{2m} + \frac{1}{2} K (x_{n+1} - x_n)^2 \right],$$

where the Hamilton's equations of motion read:

$$\dot{x}_n = \frac{\partial H}{\partial p_n}, \qquad \dot{p}_n = -\frac{\partial H}{\partial x_n}.$$

which further implies:

$$\frac{d^2 x_n}{dt^2} = \frac{K}{m} \left(x_{n+1} - 2x_n + x_{n-1} \right). \tag{4.1}$$

Solution: Assume the solution of Eq. (4.1) in the form of plane waves:

$$x_n(t) = u_n \exp\{\imath(kn - \omega_k t)\} + u_n^* \exp\{-\imath(kn - \omega_k t)\} \tag{4.2}$$

Inserting Eq. (4.2) in Eq. (4.1), we obtain:

$$-\omega_k^2 = 2\frac{K}{m} \left(\cos k - 1 \right),$$

$$\Longrightarrow \boxed{\omega_k = 2\sqrt{\frac{K}{m}} \left| \sin \frac{k}{2} \right| \simeq |k| \sqrt{\frac{K}{m}}}. \tag{4.3}$$

It is the dispersion relation.
Note: Eq. (4.2) and Eq. (4.3) are periodic in k with period $2\pi \Rightarrow k \in [-\pi, \pi]$.
Boundary condition: allowed k-values are discrete.

Periodic boundary condition (for N oscillators):

$$k = \frac{2\pi l}{N}; \quad l = -\frac{N}{2}, -\frac{N}{2}+1, \cdots, \frac{N}{2}.$$

Hence, the general solution of Eq. (4.1) can be written as:

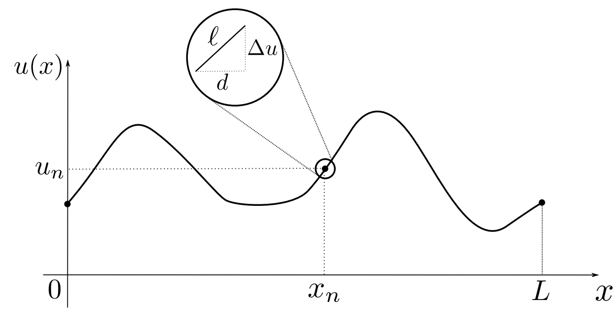
$$\boxed{x_n(t) = \sum_k \left[u_k e^{\imath(kn-\omega t)} + u_k^* e^{-\imath(kn-\omega t)}\right]}. \tag{4.4}$$

Continuous elastic string

Let us consider $u(x,t)$ as the deformation field.

Hamiltonian:
Let us first discretize:

$$\Delta x = x_{n+1} - x_n = d,$$
$$\Delta u = u_{n+1} - u_n,$$



Δm is the mass of the piece of string between x_n and x_{n+1}: $\Delta m = \rho d$ where ρ is the mass density.
Momentum:

$$p_n = \Delta u \frac{du_n}{dt} = \rho d \frac{du_n}{dt}.$$

From the sketch, deformation of the string piece (length):

$$\ell = \sqrt{d^2 + \Delta u^2}.$$

Potential energy:

$$\frac{1}{2}\kappa\ell^2 = \frac{1}{2}\kappa\Delta u^2 + \text{const.}$$

The Hamiltonian then takes the form:

$$H = \sum_n \left[\frac{p_n^2}{2\Delta m} + \frac{1}{2}\kappa\Delta u^2\right] = \sum_n d\left[\frac{1}{2}\frac{p_n^2}{\rho d^2} + \frac{1}{2}\kappa d\left(\frac{u_{n+1}-u_n}{d}\right)^2\right].$$

It gives the equation of motion:

$$\frac{d^2 u_n}{dt^2} = \frac{\kappa d}{\rho}\frac{u_{n+1} - 2u_n + u_{n-1}}{d^2}.$$

Continuum limit: $d \to 0$
$\kappa d = K =$ const. is the string tension.
Definition of momentum density:

$$p(x) = \frac{p_n}{d} \quad \text{for} \quad d \to 0.$$

Hamiltonian for the continuous elastic string:

$$\boxed{H = \int dx \quad \underbrace{\left[\frac{p^2(x)}{2\rho} + \frac{K}{2}\left(\frac{\partial u}{\partial x}\right)^2\right]}_{\text{Hamiltonian (or energy) density}}}. \tag{4.5}$$

Equation of motion:

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\delta H}{\delta p(x)} = \frac{p(x)}{\rho} \\ \frac{\partial p}{\partial t} &= -\frac{\delta H}{\delta u(x)} = K\frac{d^2u(x,t)}{dx^2} \end{aligned}$$

These set of equations implies a wave equation (linear):

$$\boxed{\frac{d^2u(x,t)}{dt^2} = \frac{K}{\rho}\frac{d^2u(x,t)}{dx^2}}. \tag{4.6}$$

Eq. (4.6) is similar to sound waves in solids, spin waves in ferromagnets, etc.

Solution:
Consider

$$u_k(x,t) = u_k e^{\imath(kx-\omega_k t)} + u_k^* e^{-\imath(kx-\omega_k t)}. \tag{4.7}$$

Inserting Eq. (4.7) in Eq. (4.6), we get the dispersion relation

$$\boxed{\omega_k = |k|\sqrt{\frac{K}{\rho}}}.$$

Impose periodic boundary conditions (string length L): $u(x,t) = u(x+L,t) \implies$ discrete k-values:

$$k = \frac{2\pi l}{L}, \quad l = 0, \pm 1, \pm 2, \cdots.$$

General solution:

$$\boxed{u(x,t) = \sum_k \left[u_k e^{\imath(kx-\omega_k t)} + u_k^* e^{-\imath(kx-\omega_k t)}\right]}.$$

Express Hamiltonian in terms of the Fourier-components u_k of $u(x,t)$:
Definition:

$$u_k(t) = u_k e^{-\imath\omega_k t}, \qquad u_k^*(t) = u_k^* e^{\imath\omega_k t}.$$

Then,

$$u(x,t) = \sum_k \left[u_k(t)e^{\imath kx} - u_k^*(t)e^{-\imath kx}\right]$$

$$\begin{aligned} \Rightarrow \frac{\partial u}{\partial x} &= \sum_k \imath k \left[u_k(t)e^{\imath kx} - u_k^*(t)e^{-\imath kx}\right], \\ \Rightarrow \frac{\partial u}{\partial t} &= \sum_k \imath\omega_k \left[u_k(t)e^{\imath kx} - u_k^*(t)e^{-\imath kx}\right]. \end{aligned}$$

And,

$$\left(\frac{\partial u}{\partial x}\right)^2 = \sum_{k,k'}(-kk')\left[u_k(t)e^{\imath kx} - u_k^*(t)e^{-\imath kx}\right]\left[u_{k'}(t)e^{\imath k'x} - u_{k'}^*(t)e^{-\imath k'x}\right],$$
$$\left(\frac{\partial u}{\partial t}\right)^2 = \sum_{k,k'}(-\omega_k\omega_{k'})\left[u_k(t)e^{\imath kx} - u_k^*(t)e^{-\imath kx}\right]\left[u_{k'}(t)e^{\imath k'x} - u_{k'}^*(t)e^{-\imath k'x}\right].$$

Now use:

$$\frac{1}{L}\int_0^L dx\, e^{i(k-k')} = \delta_{k,k'}, \qquad \frac{1}{L}\int_0^L dx\, e^{i(k+k')} = \delta_{-k,k'},$$

and from Eq. (4.5), we obtain

$$\begin{aligned} H = &\int_0^L dx\left[\frac{\rho^2}{2\rho}\left(\frac{\partial u}{\partial t}\right)^2 + \frac{K}{2}\left(\frac{\partial u}{\partial x}\right)^2\right] \\ =&\frac{\rho}{2}L\sum_k \omega_k^2\left[-u_k(t)u_{-k}(t) + u_k(t)u_k^*(t) + u_k^*(t)u_k(t) - u_k^*(t)u_{-k}^*(t)\right] \\ &+\frac{K}{2}L\sum_k k^2\left[u_k(t)u_{-k}(t) + u_k(t)u_k^*(t) + u_k^*(t)u_k(t) + u_k^*(t)u_{-k}^*(t)\right] \\ =&\sum_k 2L\rho\omega_k^2\left(u_k u_k^* + u_k^* u_k\right), \end{aligned}$$

where we use the dispersion relation $Kk^2 = \rho\omega_k^2$.
Definition:

$$d_k = u_k\sqrt{4L\rho\omega_k} \qquad \Rightarrow \qquad u_k = \frac{d_k}{\sqrt{4L\rho\omega_k}}$$

Then, H could be written as:

$$H = \frac{1}{2}\sum_k \omega_k\left(d_k^* d_k + d_k d_k^*\right).$$

As long as d_k and d_k^* are complex numbers:

$$H = \sum_k \omega_k d_k^* d_k.$$

d_k = normal coordinates of the field $u(x,t)$.
Time dependence of the field can be assigned to the d_k

$$d_k(t) = d_k e^{-\imath\omega_k t}, \qquad \ddot{d}_k(t) = -\omega_k^2 d_k(t)$$

One can introduce real variables:

$$Q_k = \frac{1}{\sqrt{2\omega_k}}\left(d_k + d_k^*\right), \qquad \text{and} \qquad P_k = -\imath\sqrt{\frac{\omega_k}{2}}\left(d_k - d_k^*\right).$$

Then, for a set of oscillators

$$\boxed{H = \sum_k \frac{1}{2}\left(P_k^2 + \omega_k^2 Q_k^2\right)} \tag{4.8}$$

P_k, Q_k = generalized coordinates/momenta of the displacement field $u(x,t)$.
Note: All oscillators in nature (electromagnetic wave, sound, pendula, skee ball hanging on a spring) are very similar and can be regarded in a unified way.
Eq. (4.8) is a classical Hamiltonian function, so the equation of motions are:

$$\dot{Q}_k = \frac{\partial H}{\partial P_k}, \qquad \dot{P}_k = -\frac{\partial H}{\partial Q_k},$$

fully equivalent to Eq. (4.6).

Quantization rules:

$$Q_k, P_k \to \hat{Q}_k, \hat{P}_k$$

with the commutation rules:

$$[\hat{Q}_k, \hat{Q}_l] = [\hat{P}_k, \hat{P}_l] = 0, \quad \text{and} \quad [\hat{P}_k, \hat{Q}_l] = \frac{1}{\imath}\delta_{kl} \quad (\hbar = 1).$$

Equivalent to:

$$d_k, d_k^* \to \hat{d}_k, \hat{d}_k^\dagger$$

with bosonic commutation rules:

$$[\hat{d}_k, \hat{d}_l] = [\hat{d}_k^\dagger, \hat{d}_l^\dagger] = 0, \quad \text{and} \quad [\hat{d}_k, \hat{d}_l^\dagger] = \delta_{kl}.$$

4.2 Quantization of the free electromagnetic field

Free electromagnetic fields:
Expressed in the Coulomb gauge ($\nabla \cdot \mathbf{A} = 0$), Maxwell's equations for the vector potential $\mathbf{A}(\mathbf{x}, t)$ and the scalar potential $\phi(\mathbf{x}, t)$ in vacuum (without sources) are reduced to

$$\begin{aligned} \nabla^2\phi = 0, \qquad & \nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}, \\ \Box\mathbf{A} = 0, \qquad & \Box \equiv \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2. \end{aligned} \tag{4.9}$$

The corresponding fields are obtained through

$$\mathbf{B} = \nabla \times \mathbf{A} \qquad \text{and} \qquad \mathbf{E} = -\frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} - \nabla\phi. \tag{4.10}$$

The solution of the free Maxwell's equations (4.9) can be choosen as $\phi = 0$, because the potential is vanishing at infinite distance.

Transversal electromagnetic fields:
The fields $\mathbf{E}$ and $\mathbf{B}$ are *transversal* fields like $\mathbf{A}$, because for a plane wave

$$\mathbf{A} = \mathbf{A_0} e^{\imath(\mathbf{k}\cdot\mathbf{x} - \omega t)}$$

results $\nabla \cdot \mathbf{A} = 0$ in $\mathbf{k} \cdot \mathbf{A} = 0$. Hence the Coulomb gauge is also called *transversal gauge*. It proved favorable to use the Coulomb gauge in the quantization process.

Field energy:
No quantization without Hamilton operator, and for this we need the expression for the total energy

$$E_{\text{cl}} = \frac{1}{8\pi}\int(\mathbf{E}^2 + \mathbf{B}^2)d^3\mathbf{r}$$

of the radiation field. We are now looking for an operator $\hat{\mathbf{A}}_{\text{op}}$ for the vector potential so that

$$i\hbar\frac{d}{dt}\hat{\mathbf{A}}_{\text{op}} = [\hat{\mathbf{A}}_{\text{op}}, \hat{H}] \qquad \Longleftrightarrow \qquad \Box\hat{\mathbf{A}}_{\text{op}} = 0 \tag{4.11}$$

where $\hat{H} = E_{\text{cl}}$ applies.

Periodic boundary conditions:
The quantization is easier to do if there are only countable many degrees of freedom. But the vector field is continuous and have uncountable many degrees of freedom. Therefore we use periodic boundary conditions

$$\mathbf{A}(x + L, y, z, t) = \mathbf{A}(x, y, z, t)$$

for a finite volume $V = L^3$. At the end of the calculations, we will expand it to infinity.

Fourier Series:
Fields which exist on a finite hypercube can be expanded in a Fourier series. The general solution of (4.9) then reads

$$\mathbf{A}(\mathbf{r}, t) = \sum_{\mathbf{k}}\sum_{\lambda}\sqrt{\frac{2\pi\hbar c}{k}}\frac{1}{\sqrt{V}}\Big(A_\lambda(\mathbf{k}, t)e^{\imath\mathbf{k}\cdot\mathbf{r}} + A^*_\lambda(\mathbf{k}, t)e^{-\imath\mathbf{k}\cdot\mathbf{r}}\Big)\mathbf{u}_\lambda(\mathbf{k})$$

The $\mathbf{k}$ sum runs over all valid $\mathbf{k}$ vectors. In the case of periodic boundary conditions they are given by

$$\mathbf{k} = \frac{2\pi}{L}(n_1, n_2, n_3), \quad \text{with} \quad n_i \in \mathbb{Z}.$$

The index λ runs over 1 and 2 and accounts for the polarization. The prefactor under the root will be usefull later but has no further physical meaning. The unit vectors $\mathbf{u_1}$ and $\mathbf{u_2}$ are orthogonal to each other and together with the wave vector $\mathbf{k}$ they form an orthogonal trihedron (transversal gauge):

$$\mathbf{k}\cdot\mathbf{u}_\lambda(\mathbf{k}) = 0, \qquad \text{and} \qquad \mathbf{u}_\lambda(\mathbf{k})\cdot\mathbf{u}_\mu(\mathbf{k}) = \delta_{\mu\lambda}.$$

Additionally we chose without loss of generality $\mathbf{u}_\lambda(\mathbf{k}) = \mathbf{u}_\lambda(-\mathbf{k})$.

Harmonic Oscillator:
It is important to note that due to (4.9) every Fourier coefficient $A_\lambda(\mathbf{k}, t)$ satisfies the equation

$$\Box\mathbf{A} = 0 \qquad \Rightarrow \qquad \frac{\partial^2 A_\lambda}{\partial t^2}(\mathbf{k}, t) = -c^2\mathbf{k}^2 A_\lambda(\mathbf{k}, t) \tag{4.12}$$

which corresponds to the differential equation of a harmonic oscillator. This fact will later on provide the basis for the quantization of the light field.

General solution of the Wave Equation:
To satisfy (4.12), we set

$$A_\lambda(\mathbf{k},t) = A_\lambda(\mathbf{k})e^{-\imath\omega_{\mathbf{k}}t}, \qquad \omega_{\mathbf{k}} = c|\mathbf{k}|$$

The general solution of the wave equation (4.9) is then given by

$$\boxed{\mathbf{A}(\mathbf{r},t) = \sum_{\mathbf{k}}\sum_{\lambda}\sqrt{\frac{2\pi\hbar c}{k}}\frac{1}{\sqrt{V}}\Big(A_\lambda(\mathbf{k})e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} + A^*_\lambda(\mathbf{k})e^{-\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}\Big)\mathbf{u}_\lambda(\mathbf{k})} \tag{4.13}$$

The time-independent field amplitudes $A_\lambda(\mathbf{k})$ will become operators in the Schrödinger picture when the quantization is carried out.

Energy of the light field:
With the help of (4.13) we want to express the total energy of the radiation field through the $A_\lambda(\mathbf{k})$ only. With (4.10) and $\phi = 0$ follows

$$E_{\text{cl}} = \frac{1}{8\pi}\int(\mathbf{E}^2 + \mathbf{B}^2)d\mathbf{r} = \frac{1}{8\pi}\int\left[\frac{1}{c^2}\left(\frac{\partial\mathbf{A}}{\partial t}\right)^2 + (\nabla\times\mathbf{A})^2\right]d^3\mathbf{r} \tag{4.14}$$

We will calculate both parts of the integrals in separate steps.

The ∂_tA-term of the field energy:
It is

$$\begin{aligned}\frac{1}{8\pi c^2}\int\left(\frac{\partial\mathbf{A}}{\partial t}\right)^2 d^3\mathbf{r} = \frac{1}{8\pi c^2}\int\frac{2\pi\hbar c^2}{V}\sum_{\mathbf{k},\mathbf{k}'}\sum_{\lambda,\lambda'}\Bigg[-\frac{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}{\sqrt{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}}\mathbf{u}_\lambda(\mathbf{k})\cdot\mathbf{u}_{\lambda'}(\mathbf{k}')\\ \times(A_\lambda(\mathbf{k},t)e^{\imath\mathbf{k}\cdot\mathbf{r}} - A^*_\lambda(\mathbf{k},t)e^{-\imath\mathbf{k}\cdot\mathbf{r}})(A_{\lambda'}(\mathbf{k}',t)e^{\imath\mathbf{k}'\cdot\mathbf{r}} - A^*_{\lambda'}(\mathbf{k}',t)e^{-\imath\mathbf{k}'\cdot\mathbf{r}})\Bigg]d^3\mathbf{r}\end{aligned} \tag{4.15}$$

One can make use of the relation

$$\frac{1}{V}\int e^{\imath(\mathbf{k}-\mathbf{k}')\mathbf{r}}d^3\mathbf{r} = \delta_{\mathbf{k},\mathbf{k}'} \qquad \text{and} \qquad \frac{1}{V}\int e^{\imath(\mathbf{k}+\mathbf{k}')\mathbf{r}}d^3\mathbf{r} = \delta_{\mathbf{k},-\mathbf{k}'}. \tag{4.16}$$

Furthermore

$$\sum_{\lambda,\lambda'}\mathbf{u}_\lambda(\mathbf{k})\cdot\mathbf{u}_{\lambda'}(\mathbf{k}) = \sum_\lambda$$

because $\mathbf{u}_\lambda(\mathbf{k})\cdot\mathbf{u}_{\lambda'}(\mathbf{k}) = \delta_{\lambda,\lambda'}$. After this (4.15) transforms to

$$\begin{aligned}\frac{1}{8\pi c^2}\int(\partial_t\mathbf{A})^2 d^3\mathbf{r} = \frac{1}{4}\sum_{\mathbf{k},\lambda}\hbar\omega_{\mathbf{k}}[&A_\lambda(\mathbf{k},t)A^*_\lambda(\mathbf{k},t) + A^*_\lambda(\mathbf{k},t)A_\lambda(\mathbf{k},t)\\ &-A_\lambda(\mathbf{k},t)A_\lambda(-\mathbf{k},t) - A^*_\lambda(-\mathbf{k},t)A^*_\lambda(\mathbf{k},t)].\end{aligned}$$

The $\nabla\times$ A-term of the field energy:
The second integral provides the same result (except for the sign) as the first

$$\begin{aligned}\frac{1}{8\pi}\int(\nabla\times\mathbf{A})^2 d^3r = \frac{1}{4}\sum_{\mathbf{k},\lambda}\hbar\omega_{\mathbf{k}}[&A_\lambda(\mathbf{k},t)A^*_\lambda(\mathbf{k},t) + A^*_\lambda(\mathbf{k},t)A_\lambda(\mathbf{k},t)\\ &+A_\lambda(\mathbf{k},t)A_\lambda(-\mathbf{k},t) + A^*_\lambda(-\mathbf{k},t)A^*_\lambda(\mathbf{k},t)].\end{aligned}$$

The last two terms will therefore cancel out and we find

$$\boxed{E_{\text{cl}} = \frac{1}{2}\sum_{\mathbf{k}}\sum_{\lambda} \hbar\omega_{\mathbf{k}}\left[A_\lambda(\mathbf{k})A^*_\lambda(\mathbf{k}) + A^*_\lambda(\mathbf{k})A_\lambda(\mathbf{k})\right]} \qquad \omega_{\mathbf{k}} = c|\mathbf{k}| \tag{4.17}$$

Time dependence was already neglected because it will drop out. In the present case, A_λ and A^*_λ are still numbers, so one could summarize the bracket. But the goal is to perform a quantization. Therefore the order of quantities that will become operators is of importance and needs to be respected.

4.3 Quantization of the light field

The classical expression (4.17) for the electrmagnetic field energy is represented by a sum over harmonic oscillators. We can adopt this quantization template.

Photons are Bosons:
Now follows the decisive step to quantization. We take in the classical total energy (4.17) the substitutions

$$\begin{aligned} A_\lambda(\mathbf{k}) &\to \hat{a}_\lambda(\mathbf{k}), \\ A^*_\lambda(\mathbf{k}) &\to \hat{a}^\dagger_\lambda(\mathbf{k}) \end{aligned} \tag{4.18}$$

where the ladder operators satisfy the bosonic commutation relation

$$[\hat{a}_\lambda(\mathbf{k}), \hat{a}^\dagger_{\lambda'}(\mathbf{k'})] = \delta_{\mathbf{k},\mathbf{k'}}\delta_{\lambda,\lambda'}. \tag{4.19}$$

The vector potential now becomes an *operator*. For simplification, we will merge the index of the polarization λ into the index $\mathbf{k}$, so that (4.19) now shortens to:

$$[\hat{a}_{\mathbf{k}}, \hat{a}^\dagger_{\mathbf{k'}}] = \delta_{\mathbf{k},\mathbf{k'}}.$$

Hamiltonian:
The Hamiltonian operator of the electromagnetic field results from the classical field energy (4.17) by using (4.18):

$$\boxed{\hat{H}_{\text{em}} = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}\left(\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} + \frac{1}{2}\right) = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}}\left(\hat{N}_{\mathbf{k}} + \frac{1}{2}\right).} \tag{4.20}$$

This completes the analogy of the electromagnetic field with a harmonic oscillator: the field can be described as an infinite number of harmonic oscillators, which are distinguished by the wave vector $\mathbf{k}$.

Operator of the vector potential:
With the canonical substitutions (4.18), the vector potential transform into an Hermitian operator, which is given by a linear combination of ladder operators

$$\boxed{\hat{\mathbf{A}}_{\text{op}}(\mathbf{r}, t) = \sum_{\mathbf{k}} \sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{k}}}}\Big(\hat{a}_{\mathbf{k}} e^{\imath(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)} + \hat{a}^\dagger_{\mathbf{k}} e^{-\imath(\mathbf{k}\cdot\mathbf{r} - \omega_{\mathbf{k}} t)}\Big)\mathbf{u}_{\mathbf{k}}, \qquad \omega_{\mathbf{k}} = c|\mathbf{k}|} \tag{4.21}$$

all properties of the quantized light field can be derived directly from this representation.

Equation of motion in the Heisenberg picture:
The Heisenberg equation

$$\imath\hbar\frac{\partial\hat{\mathbf{A}}_{\text{op}}}{\partial t}=[\hat{\mathbf{A}}_{\text{op}},\hat{H}],\tag{4.22}$$

for the above operator is equivalent to the wave equation (4.9), i.e. with

$$\Box\hat{\mathbf{A}}_{\text{op}}(\mathbf{r},t)=0,\qquad\Box e^{\pm\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}=0$$

which is already satisfied for every single wave.
Considering every separate term and using $[\hat{a}^\dagger\hat{a},\hat{a}]=-\hat{a}$:

$$\imath\hbar(-\imath\omega_{\mathbf{k}})\hat{a}_{\mathbf{k}}-\hbar\omega[\hat{a}_{\mathbf{k}},\hat{N}_{\mathbf{k}}]=\hbar\omega_{\mathbf{k}}\hat{a}_{\mathbf{k}}-\hbar\omega_{\mathbf{k}}\hat{a}_{\mathbf{k}}=0.$$

Therefore the equation of motion is satisfied too.

Time dependence:
The ladder operators appearing in (4.21) are completely time independent, i.e. in the Schrödinger picture. The time dependence can be transferred back onto them via

$$\hat{a}_{\mathbf{k}}(t)=e^{\imath\hat{H}t/\hbar}\hat{a}_{\mathbf{k}}e^{-\imath\hat{H}t/\hbar}.$$

Then is

$$\frac{d}{dt}\hat{a}_{\mathbf{k}}(t)=\frac{1}{\imath\hbar}e^{\imath\hat{H}t/\hbar}[\hat{a}_{\mathbf{k}},\hat{H}]e^{-\imath\hat{H}t/\hbar}=\frac{1}{\imath\hbar}e^{\imath\hat{H}t/\hbar}(\hbar\omega_{\mathbf{k}}a_{\mathbf{k}})e^{-\imath\hat{H}t/\hbar}=-\imath\omega_{\mathbf{k}}\hat{a}_{\mathbf{k}},$$

which leads to

$$\boxed{\hat{a}_{\mathbf{k}}(t)=e^{-\imath\omega_{\mathbf{k}}t}\hat{a}_{\mathbf{k}}}\qquad\text{and}\qquad\boxed{\hat{a}^\dagger_{\mathbf{k}}(t)=e^{\imath\omega_{\mathbf{k}}t}\hat{a}^\dagger_{\mathbf{k}}}.$$

This is obviously consistent with (4.21).

Field operators:
The operators for the electric and the magnetic fields are, according to Eq. (4.10), given by $\mathbf{B}=\nabla\times\mathbf{A}$ and $\mathbf{E}=-\frac{1}{c}\partial_t\mathbf{A}$ in Coulomb gauge. This leads to

$$\hat{\mathbf{E}}_{\text{op}}(\mathbf{r},t)=\imath\sum_{\mathbf{k}}\sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}}\Big(\hat{a}_{\mathbf{k}}e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}-\text{h.c.}\Big)\mathbf{u}_{\mathbf{k}},\tag{4.23}$$

$$\hat{\mathbf{B}}_{\text{op}}(\mathbf{r},t)=\imath\sum_{\mathbf{k}}\mathbf{k}\times\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{k}}}}\Big(\hat{a}_{\mathbf{k}}e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}-\text{h.c.}\Big)\mathbf{u}_{\mathbf{k}}.\tag{4.24}$$

The abbreviation "h.c." describes the Hermitic conjugate of the first expression in brackets, in this case $\hat{a}^\dagger_{\mathbf{k}}e^{-\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)}$.

Momentum:
The expression of the momentum of the quantized light field will be mentioned. Classically, the momentum density of the electromagnetic field reads

$$\mathbf{P}=\frac{1}{4\pi c}\int\mathbf{E}\times\mathbf{B}\,d^3\mathbf{r}.$$

From (4.23) and (4.24)

$$\boxed{\hat{\mathbf{P}}_{\text{op}} = \sum_{\mathbf{k}} \hbar\mathbf{k}\hat{a}^\dagger_{\mathbf{k}}\hat{a}_{\mathbf{k}} = \sum_{\mathbf{k}} \hbar\mathbf{k}\hat{N}_{\mathbf{k}}.}$$

The momentum of a single photon is given by $\hbar\mathbf{k}$.

Summary: The following rules for the quantum mechanical description of the light field can be stated:

a) *Vacuum*: There exists a vacuum state $|0\rangle$ with

$$\hat{a}_{\mathbf{k}} |0\rangle = 0 \quad \forall\mathbf{k} \qquad \text{and} \qquad \langle 0|0\rangle = 1. \tag{4.25}$$

b) *Photons*: A photon with a fixed momentum $\hbar\mathbf{k}$ is described by $\hat{a}^\dagger_{\mathbf{k}} |0\rangle$.

c) *General state*: A general state of photons with $n_{\mathbf{k_i}}$ photons per momentum $\hbar\mathbf{k_i}$ (one also says "in the mode $\mathbf{k_i}$") is described by

$$\frac{(\hat{a}^\dagger_{\mathbf{k}_1})^{n_{\mathbf{k_1}}}}{\sqrt{n_{\mathbf{k_1}}!}} \frac{(\hat{a}^\dagger_{\mathbf{k_2}})^{n_{\mathbf{k_2}}}}{\sqrt{n_{\mathbf{k}_2}!}} \cdots |0\rangle = \prod_{i=0}^{\infty} \frac{(\hat{a}^\dagger_{\mathbf{k_i}})^{n_{\mathbf{k_i}}}}{\sqrt{n_{\mathbf{k_i}}!}} |0\rangle . \tag{4.26}$$

Or in short $|n_{\mathbf{k_1}}, n_{\mathbf{k_2}}, \cdots\rangle$ or $|\{n_{\mathbf{k}}\}\rangle$.

d) *Occupation number operator*: The occupation number operator $\hat{N}_{\mathbf{k_i}}$ has the property

$$\hat{N}_{\mathbf{k_i}} |\cdots, n_{\mathbf{k_i}}, \cdots\rangle = n_{\mathbf{k_i}} |\cdots, n_{\mathbf{k_i}}, \cdots\rangle . \tag{4.27}$$

The Hamiltonian (4.20) separates in the contributions of the different modes. Therefore the general state $|\{n_{\mathbf{k}}\}\rangle$ can be written as direct product

$$|n_{\mathbf{k_1}}\rangle \otimes |n_{\mathbf{k_2}}\rangle \otimes \cdots = |n_{\mathbf{k_1}}\rangle |n_{\mathbf{k_2}}\rangle \cdots \tag{4.28}$$

For every mode $\mathbf{k}$ the $\{|n_{\mathbf{k}}\rangle\}$ $\forall n_{\mathbf{k}}$ form a complete set of orthonormal states. If one is interested in a single mode, one writes for the considered state only $|n_{\mathbf{k}}\rangle$.

e) *Photons are Bosons*: Because the occupation numbers $n_{\mathbf{k}}$ can take on arbitrary values of the set $\mathbb{N}_0$, one deals with bosons: An energy level (here a mode) can be arbitrary strong populated. Therefore coherent state and lasers exists, what will be seen in the next section.

Zero Point Energy:
Forming the expectation value of the Hamiltonian (4.20) with the vacuum state, one finds a surprising result:

$$\langle 0|\hat{H}_{\text{em}}|0\rangle = \frac{1}{2}\sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \to \infty. \tag{4.29}$$

The energy of the vacuum seems to be divergent!

- In general we only consider energy differences where an infinite vacuum energy is of no concern.
- The vacuum energy is dependent of the boundary conditions and changes within restricted geometries, e.g. the intermediate space between two conducting plates, which can be experimentally seen in the *Casimir effect*.

4.4 Properties of the radiation field : Coherent states

Vanishing fields:
Following (4.23) the operator of the electric field has the complete representation

$$\hat{\mathbf{E}}_{\text{op}}(\mathbf{r},t) = -\frac{1}{c}\frac{\partial \hat{\mathbf{A}}_{\text{op}}}{\partial t} = \imath \sum_{\mathbf{k}} \sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}} \left(\hat{a}_{\mathbf{k}} e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} - \text{h.c.}\right)\mathbf{u}_{\mathbf{k}}.$$

We are now only interested in a single mode $\mathbf{k}$. For this mode the above equation simply reads

$$\hat{\mathbf{E}}_{\text{op}}(\mathbf{k},t) = \imath \sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}} \left(\hat{a}_{\mathbf{k}} e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} - \text{h.c}\right)\mathbf{u}_{\mathbf{k}}.$$

The expectation value of this operator in a state $|n_{\mathbf{k}}\rangle$ with fixed population $n_{\mathbf{k}}$ of photons is

$$\boxed{\langle n_{\mathbf{k}}|\hat{\mathbf{E}}_{\text{op}}(\mathbf{k},t)|n_{\mathbf{k}}\rangle = 0}$$

since $\hat{\mathbf{E}}_{\text{op}}(\mathbf{k},t)$ is linear in creation and annihilation operators and the $\{|n_{\mathbf{k}}\rangle\}$ forms a complete set of orthonormal states.

Non-classical fields:
The expectation value of the electromagnetic field in states of fixed population vanishes.
States with fixed photon numbers are non-classical.

Finite energy density:
On the other hand, the energy density in the same states holds

$$\langle n_{\mathbf{k}}|\frac{1}{8\pi}(\hat{\mathbf{E}}^2_{\text{op}} + \hat{\mathbf{B}}^2_{\text{op}})|n_{\mathbf{k}}\rangle = \langle n_{\mathbf{k}}|\frac{1}{4\pi}\hat{\mathbf{E}}^2_{op}|n_{\mathbf{k}}\rangle = \frac{1}{V}\hbar\omega_{\mathbf{k}}\left(n_{\mathbf{k}} + \frac{1}{2}\right),$$

as was expected. This hints, there is something special with the photon number.

We will show now, that the occupation operator does not commute with the phase operator. In an eigenstate of $N_{\mathbf{k}}$, the phase of the fields is completely uncertain and therefore the classical expectation values vanish. To describe a correct transition to the classical field theory, one has to consider coherent superpositions of states with different photon populations.

Phase Operator:
For the reminder of this section we will deal with a single mode of the radiation field and will therefore omit the $\mathbf{k}$-dependence of all operators.
In a first step we define the phase operator as

$$\hat{a} = \sqrt{\hat{N}+1}e^{\imath\hat{\phi}}, \qquad \hat{a}^\dagger = e^{-\imath\hat{\phi}^\dagger}\sqrt{\hat{N}+1}, \qquad \hat{N} = \hat{a}^\dagger\hat{a} \tag{4.30}$$

which corresponds to a separation of the creation and annihilation operators in amplitude and phase. $\hat{N} = \hat{a}^\dagger\hat{a}$ is verified even if not obvious. This procedure can be in general performed in a bosonic system. We will further see, that the phase operator is *almost* self-adjoint, $\hat{\phi} \simeq \hat{\phi}^\dagger$, special care has only to be taken when looking at the vacuum state $|0\rangle$.

First we have to show that the representation (4.30) is unitary. We face the task to find such commutation relations, so that

$$[\hat{N}, \hat{\phi}] = ? \qquad \Leftrightarrow \qquad [\hat{a}, \hat{a}^\dagger] = 1. \tag{4.31}$$

Properties of Phase Operator:
Under consideration of the operation order, one can invert Eq. (4.30):

$$\left(\sqrt{\hat{N}+1}\right)^{-1} \hat{a} = e^{\imath\hat{\phi}} \qquad \hat{a}^\dagger \left(\sqrt{\hat{N}+1}\right)^{-1} = e^{-\imath\hat{\phi}^\dagger}. \tag{4.32}$$

Reminder:

$$\hat{a}\,|n\rangle = \sqrt{n}\,|n-1\rangle \qquad \hat{a}^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle$$

This gives:

$$e^{\imath\hat{\phi}}\,|n\rangle = \left(\sqrt{\hat{N}+1}\right)^{-1} \hat{a}\,|n\rangle = (1-\delta_{n,0})\left(\sqrt{(n-1)+1}\right)^{-1}\sqrt{n}\,|n-1\rangle = \begin{cases} |n-1\rangle & ; n>0 \\ 0 & ; n=0 \end{cases},$$

and

$$e^{-\imath\hat{\phi}^\dagger}\,|n\rangle = \hat{a}^\dagger\left(\sqrt{\hat{N}+1}\right)^{-1}|n\rangle = (n+1)^{-1/2}\hat{a}^\dagger\,|n\rangle = |n+1\rangle\,.$$

From these two relations follows the matrix representation of the phase operators

$$\langle n|e^{\imath\hat{\phi}}|m\rangle = \delta_{n,m-1},$$
$$\langle n|e^{-\imath\hat{\phi}^\dagger}|m\rangle = \delta_{n-1,m},$$

and therefore

$$\langle m|e^{\imath\hat{\phi}}e^{-\imath\hat{\phi}^\dagger}|n\rangle = \delta_{m,n} \qquad \langle m|e^{-\imath\hat{\phi}^\dagger}e^{\imath\hat{\phi}}|n\rangle = (1-\delta_{n,0})\delta_{m,n}. \tag{4.33}$$

If $\hat{\phi}$ would be self-adjoint, $e^{\pm\imath\hat{\phi}}$ would permute. Eq. (4.33) shows, that this is almost the case – except for $n=0$ – especially for large particle numbers.

Observable Phases:
The operators are non Hermitian, because from the above relations it follows that $(e^{\imath\hat{\phi}})^\dagger = e^{-\imath\hat{\phi}^\dagger}$. Therefore, they do not represent physical observables in this form. However it is possible to combine the phase operators to Hermitian operators:

$$\sin\hat{\phi} \equiv \frac{e^{\imath\hat{\phi}} - e^{-\imath\hat{\phi}^\dagger}}{2\imath}, \qquad \cos\hat{\phi} \equiv \frac{e^{\imath\hat{\phi}} + e^{-\imath\hat{\phi}^\dagger}}{2}. \tag{4.34}$$

In the case of self-adjoint $\hat{\phi}$, this definition would correspond to the real and imaginary part. For the general operator $\hat{\phi}$, one defines via (4.34) new operators $\sin\hat{\phi}$ and $\cos\hat{\phi}$.

Commutation Relations:
In the following we will make the approximation $\hat{\phi} \simeq \hat{\phi}^\dagger$, which is exact except for the vacuum. The commutation relations for $\hat{\phi}$ and $\hat{N}$ are obtained as follows:

$$1 = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \sqrt{\hat{N}+1}e^{\imath\hat{\phi}}e^{-\imath\hat{\phi}}\sqrt{\hat{N}+1} - e^{-\imath\hat{\phi}}(\hat{N}+1)e^{\imath\hat{\phi}} = \hat{N} - e^{-\imath\hat{\phi}}\hat{N}e^{\imath\hat{\phi}}$$

Multiplying both sides with $e^{\imath\hat{\phi}}$ yields:

$$e^{\imath\hat{\phi}} = e^{\imath\hat{\phi}}\hat{N} - \hat{N}e^{\imath\hat{\phi}} = [e^{\imath\hat{\phi}}, \hat{N}].$$

Therefore:

$$[\hat{N}, e^{\imath\hat{\phi}}] = -e^{\imath\hat{\phi}}, \qquad [\hat{N}, e^{-\imath\hat{\phi}}] = e^{-\imath\hat{\phi}}.$$

With this we obtain

$$[\hat{N}, \cos\hat{\phi}] = \left[\hat{N}, \frac{e^{\imath\hat{\phi}} + e^{-\imath\hat{\phi}}}{2}\right] = \frac{-e^{\imath\hat{\phi}} + e^{-\imath\hat{\phi}}}{2} = -i\frac{e^{\imath\hat{\phi}} - e^{-\imath\hat{\phi}}}{2\imath} = -\imath\sin\hat{\phi},$$

and

$$[\hat{N}, \sin\hat{\phi}] = \left[\hat{N}, \frac{e^{\imath\hat{\phi}} - e^{-i\hat{\phi}}}{2\imath}\right] = \frac{-e^{\imath\hat{\phi}} - e^{-\imath\hat{\phi}}}{2\imath} = \imath\frac{e^{\imath\hat{\phi}} + e^{-\imath\hat{\phi}}}{2} = \imath\cos\hat{\phi}.$$

Obviously $\hat{N}$ acts on $\hat{\phi}$ like a derivative with respect to $\hat{\phi}$, meaning $\hat{N} \equiv \imath\frac{\partial}{\partial\hat{\phi}}$ like the momentum operator $\hat{p}$ and the position operator $\hat{x}$. Therefore

$$\boxed{[\hat{N}, \hat{\phi}] = \imath} \tag{4.35}$$

which express, that is in principle impossible to exactly measure phase and particle number at the same time, both measurements are incompatible.

Uncertainty Relation:
The phase $\hat{\phi}$ and the particle number operator $\hat{N} = \hat{a}^\dagger\hat{a}$ are for bosons canonically conjugated variables.

One brings to mind the Heisenberg uncertainty principle

$$(\Delta\hat{A})(\Delta\hat{B}) \geqslant \frac{1}{2}|\langle[\hat{A}, \hat{B}]\rangle| = \frac{1}{2}, \qquad [\hat{A}, \hat{B}] = \imath,$$

where the last relation is valid for canonical conjugated operators $\hat{A}$ and $\hat{B}$.

Digression: Superconductivity:
This result is essential for superfluidity (see chapter 3, where we discussed the meaning of the phase of the condensate wave function) and for superconductivity. Superconductivity comes into being through singlet pairing of electrons and one can – in a very crude approximation – view this pairs as bosons, because following the spin statistics theorem, this particles possess integer spin – like bosons.
The superconductive condensate is characterized by a fixed phase, one also speaks of a spontaneous breaking of the global gauge invariance.
But when the phase is fixed, then the particle number cannot be according to (4.35). Therefore the BCS wave function is

$$|\psi_{BCS}\rangle = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} \underbrace{\hat{c}^\dagger_{\mathbf{k},\uparrow}\hat{c}^\dagger_{-\mathbf{k},\downarrow}}_{\text{Electron Pair}})\,|0\rangle$$

given by a coherent superposition of states with a different number of singlet pairs.

Variance:
In a pure state $|n\rangle$ with fixed photon number, the natural fluctuation of the occupation number operator vanishes:

$$\Delta N = \sqrt{\langle n|\hat{N}^2|n\rangle - \langle n|\hat{N}|n\rangle^2} = 0$$

In contrast, $\cos\phi$ has a finite fluctuation. It is $\langle \cos\phi\rangle = 0$ and

$$\langle \cos^2\hat{\phi}\rangle = \frac{1}{4}\left\langle e^{\imath\hat{\phi}}e^{-\imath\hat{\phi}^\dagger} + e^{-\imath\hat{\phi}^\dagger}e^{\imath\hat{\phi}}\right\rangle = \frac{2-\delta_{n,0}}{4}$$

in a pure state $|n\rangle$, and therefore $\Delta\cos\phi = \Delta\sin\phi$:

$$\Delta\cos\phi = \sqrt{\langle\cos^2\hat{\phi}\rangle - \langle\cos\hat{\phi}\rangle^2} = \begin{cases} 1/\sqrt{2} & ; n > 0, \\ 1/2 & ; n = 0, \end{cases}.$$

Coherent States:
One can do a linear combination of states with different particle numbers to achieve a transition to macroscopic electrodynamics. One defines a coherent state $|c\rangle$ (also called a Glauber state, Nobel price 2005) through

$$\boxed{|c\rangle \equiv e^{-|c|^2/2}\sum_{n=0}^{\infty}\frac{c^n}{\sqrt{n!}}\,|n\rangle} \qquad \text{with} \qquad c\in\mathbb{C}, \qquad c = |c|e^{\imath\theta}$$

By using the representation (4.26) for the state $|n\rangle$, one can write in a more compact fashion:

$$|c\rangle = e^{-|c|^2/2}\sum_{n=0}^{\infty}\frac{c^n}{\sqrt{n!}}\frac{(\hat{a}^\dagger)^n}{\sqrt{n!}}\,|0\rangle = \exp\Big(-\frac{|c|^2}{2} + c\hat{a}^\dagger\Big)\,|0\rangle$$

A Glauber state $|c\rangle$ only contains the $\{|n\rangle\}$ of a single mode, so $\mathbf{k}$ is still sharply defined.

Properties of a Glauber state:
The coherent states are eigenstates of $\hat{a}$. Proof:

$$\begin{aligned}\hat{a}\,|c\rangle &= e^{-|c|^2/2}\sum_{n=0}^{\infty}\frac{c^n}{\sqrt{n!}}\,\hat{a}\,|n\rangle = e^{-|c|^2/2}\sum_{n=1}^{\infty}\frac{c^n}{\sqrt{(n-1)!}}\,|n-1\rangle \\ &= e^{-|c|^2/2}\sum_{n=0}^{\infty}\frac{c^{n+1}}{\sqrt{n!}}\,|n\rangle = c|c\rangle.\end{aligned}$$

The Glauber state is thus an eigenstate of the annihilation operator. We summarize the relations:

$$\boxed{\hat{a}\,|c\rangle = c\,|c\rangle}, \qquad \langle c|\hat{a}|c\rangle = c, \qquad \langle c|\hat{a}^\dagger|c\rangle = c^*, \qquad \langle c|c\rangle = 1 \tag{4.36}$$

We notice that the coherent states do not build an orthogonal basis, because in general $\langle c|c'\rangle \neq 0$.

Electric field of a coherent state:
The expectation value

$$\begin{aligned}\langle c|\hat{\mathbf{E}}_{\text{op}}|c\rangle &= \imath\sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}}\Big(ce^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t)} - \text{c.c.}\Big)\mathbf{u}_{\mathbf{k}} = \imath\sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}}|c|\Big(e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t+\theta)} - \text{c.c.}\Big)\mathbf{u}_{\mathbf{k}} \\ &= -2\sqrt{\frac{2\pi\hbar\omega_{\mathbf{k}}}{V}}|c|\sin(\mathbf{k}\cdot\mathbf{r}-\omega_{\mathbf{k}}t+\theta)\mathbf{u}_{\mathbf{k}}.\end{aligned} \tag{4.37}$$

of the electrical field in a coherent state is equivalent to the classical value.
Hence there exists a one-to-one relation between the plane waves of classical electrodynamics and the coherent states $|c\rangle$, because through $c = |c|e^{\imath\theta}$ the amplitude as well as the phase of the plane wave can be determined by use of Eq. (4.37).

Fluctuation of the photon number:
From relation (4.36) and $\hat{N}^2 = \hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a} = \hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}$ results

$$\langle c|\,\hat{N}\,|c\rangle = \langle c|\,\hat{a}^\dagger\hat{a}\,|c\rangle = \langle c|\,c^*c\,|c\rangle = |c|^2\,\langle c|c\rangle = |c|^2$$

and

$$\langle c|\,\hat{N}^2\,|c\rangle = \langle c|\,\hat{a}^\dagger\hat{a}\hat{a}^\dagger\hat{a}\,|c\rangle = \langle c|\,\hat{a}^\dagger(1+\hat{a}^\dagger\hat{a})\hat{a}\,|c\rangle = \langle c|\,\hat{a}^\dagger\hat{a}\,|c\rangle + \langle c|\,\hat{a}^\dagger\hat{a}^\dagger\hat{a}\hat{a}\,|c\rangle = |c|^2 + |c|^4,$$

so that

$$\Delta N = \sqrt{\langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2} = |c|. \tag{4.38}$$

The relative fluctuation of the photon number is therefore

$$\frac{\Delta N}{\langle\hat{N}\rangle} = \frac{1}{|c|} = \frac{1}{\sqrt{\langle\hat{N}\rangle}}. \tag{4.39}$$

The bigger the particle number, the smaller the fluctuations. The probability of finding exactly m photons in a measurement is

$$|\,\langle m|c\rangle\,|^2 = \left|\frac{c^m}{\sqrt{m!}}e^{-|c|^2/2}\right|^2 = e^{-|c|^2}\frac{|c|^{2m}}{m!},$$

which matches a Poisson distribution.
One can show that for large N the expectation value of the phase operator in the coherent states is identical to the phase of c, meaning $\langle c|\cos\hat{\phi}\,|c\rangle = \cos\theta$, where $c = |c|e^{i\theta}$.
Proof:

$$e^{\imath\hat{\phi}} = \frac{1}{\sqrt{\hat{N}+1}}\hat{a} \qquad \text{and} \qquad e^{-\imath\hat{\phi}} = \hat{a}^\dagger\frac{1}{\sqrt{\hat{N}+1}},$$

hence

$$\cos\hat{\phi} = \frac{1}{2}\left(\frac{1}{\sqrt{\hat{N}+1}}\hat{a} + \hat{a}^\dagger\frac{1}{\sqrt{\hat{N}+1}}\right).$$

Since

$$\left\langle c\left|\frac{1}{\sqrt{\hat{N}+1}}\hat{a}\right|c\right\rangle = c\left\langle c\left|\frac{1}{\sqrt{\hat{N}+1}}\right|c\right\rangle \qquad \text{and} \qquad \left\langle c\left|\hat{a}^\dagger\frac{1}{\sqrt{\hat{N}+1}}\right|c\right\rangle = c^*\left\langle c\left|\frac{1}{\sqrt{\hat{N}+1}}\right|c\right\rangle$$

one has

$$\langle c|\cos\hat{\phi}\,|c\rangle = \frac{1}{2}(c+c^*)\left\langle c\left|\frac{1}{\sqrt{\hat{N}+1}}\right|c\right\rangle$$

In the limit $N\to\infty$ one has

$$\left\langle\frac{1}{\sqrt{\hat{N}+1}}\right\rangle_c \to \frac{1}{\sqrt{\langle\hat{N}+1\rangle_c}} \approx \frac{1}{\sqrt{\langle\hat{N}\rangle_c}} = \frac{1}{|c|}.$$

Therefore

$$\langle c|\cos\hat{\phi}\,|c\rangle = \frac{c+c^*}{2|c|} = \cos\theta.$$

Fluctuations of the phase:
We assume the uncertainty relation of to general Hermitian operators A and B:

$$\Delta\hat{A}\Delta\hat{B} \geq \frac{1}{2}\Big|\langle[\hat{A},\hat{B}]\rangle\Big|.$$

Through (4.35) for the commutation relation $[\hat{N},\sin\hat{\phi}] = \imath\cos\hat{\phi}$ we find for the fluctuations $\Delta\sin\hat{\phi}$ of $\sin\hat{\phi}$:

$$\Delta\hat{N}\Delta\sin\hat{\phi} \geq \frac{1}{2}\Big|\langle\cos\hat{\phi}\rangle\Big|$$

and through (4.38) for $\Delta N = |c|$ and $\Delta\sin\hat{\phi} = \Delta\cos\hat{\phi}$ one calculates

$$\frac{\Delta\cos\hat{\phi}}{|\langle\cos\hat{\phi}\rangle|} \geq \frac{1}{2|c|}. \tag{4.40}$$

This estimate provides strictly speaking only a lower bound of the relative fluctuations of the phase, but saves the need of costly calculations. In general, the actual fluctuations are determined by two operators of the same magnitude as the corresponding uncertainty relation.
The relative fluctuations of the phase thus vanish in the limit of large photon numbers $\langle\hat{N}\rangle = |c|^2$, just as the relative fluctuations of the photon numbers itself, see Eq. (4.39).

Classical Limit:
The definition of phase and particle number of a light field becomes sharper and sharper, the more photons it contains. In the limiting case of a large number of photons, we arrive at the classical description.

By intuition, this seems comprehensible. For a small amount of photons, their quantum mechanical properties will manifest themselves. But in the limit of large numbers, they will average out.

4.5 Interaction of radiation and matter

Here only emission and absorption of photons by matter (bound electrons) is studied.

Minimal coupling:
The total Hamiltonian of matter and radiation reads

$$\hat{H} = \hat{H}_{\text{em}} + \hat{H}_{\text{mat}} + \hat{H}_{\text{I}}\,, \tag{4.41}$$

where $\hat{H}_{\text{em}}$ describes the radiation field alone, $\hat{H}_{\text{mat}}$ the matter and $\hat{H}_{\text{I}}$ the interaction between both:

$$\hat{H}_{\text{em}} = \sum_{\mathbf{k}} \hbar\omega_{\mathbf{k}} \left(\hat{N}_{\mathbf{k}} + \frac{1}{2}\right), \qquad \hat{H}_{\text{mat}} = \sum_i \frac{\hat{\mathbf{p}}_{\mathbf{i}}^2}{2m_i} + \hat{V}(\mathbf{r_1}, \mathbf{r_2}, \cdots).$$

We will neglect spin effects. The index i runs over all particles. After the introduction of electromagnetic field, the interaction H_{I} results from minimal coupling in Coulomb gauge via:

$$\boxed{\hat{\mathbf{p}}_{\mathbf{i}} \to \hat{\mathbf{p}}_{\mathbf{i}} - \frac{e}{c}\hat{\mathbf{A}}_{\text{op}}(\mathbf{r_i}, t)},$$

where e describes the elementary charge. Take note, that the vector potential is given by the operator (4.21), which describes the vector potential at location $\mathbf{r_i}$ of the i^{th} particle.

Light-Matter Interaction:
By using $\hat{\mathbf{A}}^i_{\text{op}} \equiv \hat{\mathbf{A}}_{\text{op}}(\mathbf{r_i}, t)$, one arrives at

$$\begin{aligned} \hat{H}_{\text{I}} &= \sum_i \left[-\frac{e}{2m_i c}\left(\hat{\mathbf{p}}_{\mathbf{i}} \cdot \hat{\mathbf{A}}^i_{\text{op}} + \hat{\mathbf{A}}^i_{\text{op}} \cdot \hat{\mathbf{p}}_{\mathbf{i}}\right) + \frac{e^2}{2m_i c^2}\left(\hat{\mathbf{A}}^i_{\text{op}}\right)^2 \right] \\ &= -\sum_i \underbrace{\frac{e}{m_i c}\hat{\mathbf{A}}^i_{\text{op}} \cdot \hat{\mathbf{p}}_{\mathbf{i}}}_{\text{paramagnetic}} + \sum_i \underbrace{\frac{e^2}{2m_i c^2}\left(\hat{\mathbf{A}}^i_{\text{op}}\right)^2}_{\text{diamagnetic}} \equiv \hat{H}'_{\text{I}} + \hat{H}''_{\text{I}}. \end{aligned} \tag{4.42}$$

for the interaction between light and matter. Due to $\nabla \cdot \hat{\mathbf{A}} = 0$, it is possible to set

$$\hat{\mathbf{p}} \cdot \hat{\mathbf{A}} = \frac{\hbar}{i}\nabla \cdot \hat{\mathbf{A}} + \hat{\mathbf{A}} \cdot \hat{\mathbf{p}} = \hat{\mathbf{A}} \cdot \hat{\mathbf{p}}.$$

Both terms in (4.42) are called paramagnetic and diamagnetic part, respectively. The diamagnetic term $\sim \hat{\mathbf{A}}^2$ couples with the matter only via the position operator $\hat{\mathbf{r}}_{\mathbf{i}}$ in the argument of the vector potential $\hat{\mathbf{A}}^i_{\text{op}}(\hat{\mathbf{r}}_{\mathbf{i}}, t)$.

State Space:
The whole Hamiltonian (4.41) acts on a state, which contains light field as well as matter:

$$|\text{state of matter}\rangle \otimes |\text{state of light field}\rangle$$

Perturbation operator for a single electron:
In the following we will consider a special case: we ask for the transition rates of a single bound

electron in an atom (e.g. the hydrogen atom) which are introduced through the presence of a radiation field. The Hamiltonian of the interaction reads now:

$$\boxed{\hat{H}_{\mathrm{I}}' = -\frac{e}{mc}\sum_{\mathbf{k}}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{k}}}}\left(\hat{a}_{\mathbf{k}}e^{\imath\mathbf{k}\cdot\hat{\mathbf{r}}} + \mathrm{h.c.}\right)\mathbf{u}_{\mathbf{k}}\cdot\hat{\mathbf{p}}.}$$

Two simplifications were made: first, the $\mathbf{A}^2$-term was neglected. Second, $\hat{H}_{\mathrm{I}}$ is time independent, because every exponential factors would disappear anyway. One can also transform the operator $\hat{\mathbf{A}}_{\mathrm{op}}(\hat{\mathbf{r}}, t)$ in the Schrödinger picture and would arrive at the same result. In this case, the appearing states in the following calculation would be time dependent, what would not be of any consequence.

Fermi's Golden Rule:
We will treat $\hat{H}_{\mathrm{I}}$ as a perturbation. The Golden Rule for a transition rate from an initial state $|i\rangle$ to a final state $|f\rangle$ then reads:

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\delta(E_i - E_f)|\langle f|\,\hat{H}_{\mathrm{I}}'\,|i\rangle\,|^2.$$

Total energies:
The energies E_i and E_f are the total energy of the radiation field and matter before and after a transition, just like $|i\rangle$ and $|f\rangle$ describe the states in *both* Hilbert spaces. We will assume, that initial and final state respectively are eigenstates of $\hat{H}_0 = \hat{H}_{\mathrm{em}} + \hat{H}_{\mathrm{mat}}$:

$$\hat{H}_{\mathrm{mat}}\,|\varepsilon_i\rangle = \varepsilon_i\,|\varepsilon_i\rangle\,, \quad \hat{H}_{\mathrm{mat}}\,|\varepsilon_f\rangle = \varepsilon_f\,|\varepsilon_f\rangle\,,$$
$$\hat{H}_{\mathrm{em}}\,|\{n^i_{\mathbf{k}}\}\rangle = \sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}\left(n^i_{\mathbf{k}} + \frac{1}{2}\right)|\{n^i_{\mathbf{k}}\}\rangle\,, \quad \hat{H}_{\mathrm{em}}\,|\{n^f_{\mathbf{k}}\}\rangle = \sum_{\mathbf{k}}\hbar\omega_{\mathbf{k}}\left(n^f_{\mathbf{k}} + \frac{1}{2}\right)|\{n^f_{\mathbf{k}}\}\rangle\,.$$

The states then read

$$|i\rangle = |\varepsilon_i\rangle \otimes |\{n^i_{\mathbf{k}}\}\rangle\,, \quad |f\rangle = |\varepsilon_f\rangle \otimes |\{n^f_{\mathbf{k}}\}\rangle\,.$$

We will successively consider now the emission and the absorption of a photon.

Emission of a photon $\hbar\mathbf{k}$:
The energies of initial and final state are given by

$$E_i = \varepsilon_i + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\left(n_{\mathbf{k}'} + \frac{1}{2}\right),$$
$$E_f = \varepsilon_f + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\left(n_{\mathbf{k}'} + \frac{1}{2}\right) + \hbar\omega_{\mathbf{k}},$$

because exactly one photon of energy $\hbar\omega_{\mathbf{k}}$ should be emitted. The state vectors read:

$$|i\rangle = |\varepsilon_i\rangle \otimes |\cdots, n_{\mathbf{k}}, \cdots\rangle\,,$$
$$|f\rangle = |\varepsilon_f\rangle \otimes |\cdots, n_{\mathbf{k}} + 1, \cdots\rangle\,.$$

The Golden Rule states, that a corresponding transition must satisfy

$$E_i - E_f = \varepsilon_i - (\varepsilon_f + \hbar\omega_{\mathbf{k}}) = 0.$$

This is exactly the conservation of energy. Further applies

$$\langle f|\,\hat{H}_{\mathrm{I}}'\,|i\rangle = -\frac{e}{mc}\sum_{\mathbf{k}'}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{k}'}}}\,\langle\varepsilon_f|\,e^{-\imath\mathbf{k}'\cdot\hat{\mathbf{r}}}\mathbf{u}_{\mathbf{k}'}\cdot\hat{\mathbf{p}}\,|\varepsilon_i\rangle\,\langle\cdots,n_{\mathbf{k}}+1,\cdots|\,\hat{a}^{\dagger}_{\mathbf{k}'}\,|\cdots,n_{\mathbf{k}},\cdots\rangle\,.$$

The annihilators do not appear anymore, because the corresponding matrix elements will disappear (more photons appear on the left hand side than on the right hand side). Only the summand with $\mathbf{k}=\mathbf{k}'$ survives. Only then is a photon in the right state created and the inner product will not vanish. The second term in the brakets reads therefore

$$\langle\cdots,n_{\mathbf{k}}+1,\cdots|\,\hat{a}^{\dagger}_{\mathbf{k}'}\,|\cdots,n_{\mathbf{k}},\cdots\rangle = \sqrt{n_{\mathbf{k}}+1}\,\delta_{\mathbf{k},\mathbf{k}'}$$

and the transition rate of the emission is given by:

$$\boxed{\Gamma^{e}_{i\to f} = \frac{4\pi^2 e^2}{m^2 V\omega_{\mathbf{k}}}\delta(\varepsilon_i-\varepsilon_f-\hbar\omega_{\mathbf{k}})(n_{\mathbf{k}}+1)|\,\langle\varepsilon_f|\,e^{-\imath\mathbf{k}\cdot\hat{\mathbf{r}}}\mathbf{u}_{\mathbf{k}}\cdot\hat{\mathbf{p}}\,|\varepsilon_i\rangle\,|^2.} \tag{4.43}$$

Absorption of a photon $\hbar\mathbf{k}$:
The energies of initial and final states are

$$E_i = \varepsilon_i + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\left(n_{\mathbf{k}'}+\frac{1}{2}\right),$$
$$E_f = \varepsilon_f + \sum_{\mathbf{k}'}\hbar\omega_{\mathbf{k}'}\left(n_{\mathbf{k}'}+\frac{1}{2}\right) - \hbar\omega_{\mathbf{k}},$$

because now a photon will be “extracted” from the light field. The state vectors are given by

$$|i\rangle = |\varepsilon_i\rangle\otimes|\cdots,n_{\mathbf{k}},\cdots\rangle\,,$$
$$|f\rangle = |\varepsilon_f\rangle\otimes|\cdots,n_{\mathbf{k}}-1,\cdots\rangle\,.$$

In this case, the creation operators do not contribute to the calculation of the matrix elements $\langle f|\,\hat{H}_{\mathrm{I}}'\,|i\rangle$. Furthermore, only the annihilation operator with $\mathbf{k}=\mathbf{k}'$ remains. Analogous to the emission one finds:

$$\boxed{\Gamma^{a}_{i\to f} = \frac{4\pi^2 e^2}{m^2 V\omega_{\mathbf{k}}}\delta(\varepsilon_i-\varepsilon_f+\hbar\omega_{\mathbf{k}})n_{\mathbf{k}}|\,\langle\varepsilon_f|\,e^{\imath\mathbf{k}\cdot\hat{\mathbf{r}}}\mathbf{u}_{\mathbf{k}}\cdot\hat{\mathbf{p}}\,|\varepsilon_i\rangle\,|^2.} \tag{4.44}$$

Discussion: Absorption vs Emission
Both expressions for emission and absorption processes are identical, except for the factors of the occupation numbers.

- *Spontaneous emission*: One speaks of a spontaneous emission if a photon is emitted in absence of other photons. Spontaneous emission is possible, because the factor $n_{\mathbf{k}}+1$ in Eq. (4.43) will not disappear if a external photon field is missing ($n_{\mathbf{k}}=0$).
- *Stimulated emission*: The factor $n_{\mathbf{k}}+1$ in Eq. (4.43) implies, that in presence of a external field with the same quantum numbers, the emission probability is increased, proportional to the intensity of the external light field. One speaks of stimulated emission – which is essential for the laser – because a mode $\hbar\mathbf{k}$ can only stimulate an emission of a photon of the same wave length $\lambda=2\pi/|\mathbf{k}|$. One obtains coherent radiation.

- *Absorption*: The interpretation of the occupation factor $n_{\mathbf{k}}$ in Eq. (4.44) of the absorption process is relatively trivial. Photons can only be absorbed, if any are present.

Electric dipole transition:
We consider the *electric dipole transition*, which occurs if the exponential function $e^{\imath \mathbf{k}\cdot\hat{\mathbf{r}}}$ in the matrix elements can be presumed equal to 1. This is possible if

$$\mathbf{k}\cdot\hat{\mathbf{r}} \simeq \frac{2\pi a_0}{\lambda} \ll 1,$$

which is the case if the wavelength λ of the participating radiation is big compare to the characteristic scales of the system (here the Bohr radius a_0). It is called *electric dipole approximation*, if the matrix element is further rearranged. We use

$$\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}, x\right] = \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}x - x\frac{\partial^2}{\partial x^2}\right) = \frac{\hbar^2}{m}\frac{\partial}{\partial x} = \frac{i\hbar}{m}p_x$$

and find

$$\begin{aligned}\langle\varepsilon_f|\,\hat{\mathbf{p}}\,|\varepsilon_i\rangle &= \langle\varepsilon_f|\,\frac{im}{\hbar}[\hat{H}_{\mathrm{mat}},\hat{\mathbf{r}}]\,|\varepsilon_i\rangle = \frac{im}{\hbar}\,\langle\varepsilon_f|\,\hat{H}_{\mathrm{mat}}\hat{\mathbf{r}} - \hat{\mathbf{r}}\hat{H}_{\mathrm{mat}}\,|\varepsilon_i\rangle \\ &= \frac{im}{\hbar}\,\langle\varepsilon_f|\,\hat{\mathbf{r}}\,|\varepsilon_i\rangle\,(\varepsilon_f - \varepsilon_i). \end{aligned} \tag{4.45}$$

This is exactly the dipole matrix element, which also results if one directly uses the electric dipole moment in a field

$$\hat{E}_{\mathrm{dip}} = -e\hat{\mathbf{r}}\cdot\hat{\mathbf{E}}_{\mathrm{op}}$$

as interaction term.

Selection rules:
The matrix elements appearing in Eqs. (4.43) and (4.44) determine if a transition ever takes place and if it does, the probability of it. They govern the section rules.
In the case of the electric dipole transition, the matrix element (4.45) states, that initial and final state in any case need different parity, if the considered transition should be permitted, because $\hat{\mathbf{r}}$ is odd under parity transformations.
In an atom, this means that electric dipole transition are permitted from the s-level to the p-level or f-level, but not to the d-level.

Transition of higher orders:
Transition which are forbidden in zeroth order can nonetheless occur if higher orders are considered, i.e. the exponential function is further expanded:

$$e^{\pm\imath\mathbf{k}\cdot\hat{\mathbf{r}}} \simeq 1 \pm \imath\mathbf{k}\cdot\hat{\mathbf{r}} + \ldots.$$

The next order (linear in $\mathbf{k}\cdot\hat{\mathbf{r}}$) describes magnetic dipole and electric quadrupole transitions.

4.6 Lifetime of an excited state

It seems surprising, that the periodic volume V still occurs in Eqs. (4.43) and (4.44). Rather the transition rates should not depend on this auxiliary variable. In the following calculations, we will build the limit $V \to +\infty$. To guarantee meaningful results, one has to consider transition to a group of final states and sum up all final states as well as all $\mathbf{k}$ vectors of the photon. The δ-distribution ensures the energy conservation. As an first example we will look at the spontaneous emission from an arbitrary initial state to a set of final states.

Lifetime of an excited state:
We define the lifetime τ of an excited state about the spontaneous emission in a target level $|\varepsilon_f\rangle$:

$$\frac{1}{\tau} \equiv \sum_{f,\mathbf{k}} \Gamma_{i\to f} = \sum_{f,\mathbf{k},\lambda} \frac{4\pi^2 e^2}{\hbar^2 V \omega_{\mathbf{k}}} \delta(\varepsilon_f - \varepsilon_i + \hbar\omega_{\mathbf{k}})(\varepsilon_i - \varepsilon_f)^2 |\langle\varepsilon_f|\, \mathbf{u}_\lambda(\mathbf{k}) \cdot \hat{\mathbf{r}}\, |\varepsilon_i\rangle|^2. \tag{4.46}$$

where the expression (4.45) for the dipole moment is used.

- The expression (4.46) consists of the portion of spontaneous emission in Eq. (4.43), summed up over all target levels f of the atoms and all wave vectors $\mathbf{k}$ of the photons.
- The δ-distribution ensures, that only summands remain, for which the released energy merges into the radiation field.
- The polarization λ explicitly shows up again, where $\mathbf{u}_\lambda(\mathbf{k})$ describes the unity polarization vector of the light field.

Thermodynamic limit:
V will now approach infinity. This is done by the substitution

$$\frac{1}{V}\sum_{\mathbf{k}} \to \frac{1}{(2\pi)^3}\int d^3\mathbf{k}$$

because the volume of a mode in the reciprocal $\mathbf{k}$-space is given by $(2\pi)^3/V$ under periodic boundary conditions. For continuous $\mathbf{k}$ it is given by $d^3\mathbf{k}$ instead.

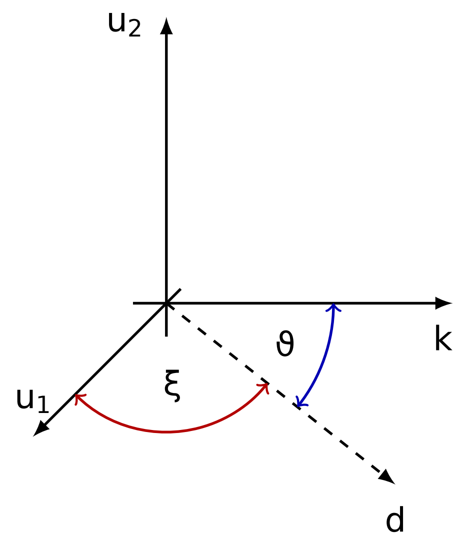
Summation over different polarizations:
First we will perform the λ-summation. We have to calculate:

$$\sum_{\lambda=1}^{2} \left| \mathbf{u}_\lambda(\mathbf{k}) \cdot \underbrace{\langle\varepsilon_f|\, \hat{\mathbf{r}}\, |\varepsilon_i\rangle}_{\equiv \mathbf{d}} \right|^2$$

Other than building an orthogonal trihedron with $\mathbf{k}$, $\mathbf{u}_\lambda$ can be chosen freely. E.g. one can choose $\mathbf{u}_2$ to be perpendicular to the dipole matrix element $\mathbf{d}$, which will result in a dependence of the sum on $\mathbf{u}_1$ alone. Let the angle between $\mathbf{d}$ and $\mathbf{u}_1$ be ξ, the angle between $\mathbf{d}$ and $\mathbf{k}$ reads $\theta = \pi/2 - \xi$. The above sum then yields

$$|\langle\varepsilon_f|\, \hat{\mathbf{r}}\, |\varepsilon_i\rangle|^2 \sin^2\theta.$$

The orthogonal trihedron consisting of the two polarization vectors $\mathbf{u}_1$, $\mathbf{u}_2$ *and the wave vector of the photon* $\mathbf{k}$ *can be arranged in such a way, so that the dipole matrix element* $\mathbf{d}$ *lies within the plane spanned by* $\mathbf{u}_1$ *and* $\mathbf{k}$*.*



Photon momentum integration:
Favorably one places the coordinate system in such a way, that $\mathbf{d}$ point in the k_z-direction. Under this condition, the appearing $\sin^2\theta$ of an integration in spherical coordinates comes in handy:

$$\begin{aligned}\frac{1}{\tau} &= \sum_f \frac{4\pi^2 e^2}{\hbar^2}(\varepsilon_f-\varepsilon_i)^2 |\langle\varepsilon_f|\,\hat{\mathbf{r}}\,|\varepsilon_i\rangle|^2 \frac{1}{(2\pi)^3}\int k^2\sin\theta\sin^2\theta\frac{\delta(\varepsilon_f-\varepsilon_i+\hbar\omega_{\mathbf{k}})}{\omega_{\mathbf{k}}}dkd\theta d\varphi \\ &= \sum_f \frac{e^2}{2\pi\hbar^4c^3}(\varepsilon_f-\varepsilon_i)^2 |\langle\varepsilon_f|\,\hat{\mathbf{r}}\,|\varepsilon_i\rangle|^2 \underbrace{\int\sin^3\theta d\theta d\varphi}_{=8\pi/3}\underbrace{\int\varepsilon\delta(\varepsilon_f-\varepsilon_i+\varepsilon)d\varepsilon}_{=\varepsilon_i-\varepsilon_f}\end{aligned}$$

In the last step the $\mathbf{k}$-integration was shifted to the variable $\varepsilon=\hbar\omega_{\mathbf{k}}$. The angle integration results in $8\pi/3$, which leads to the final result

$$\boxed{\frac{1}{\tau}=\frac{4e^2}{3\hbar c^3}\sum_f\left(\frac{\varepsilon_i-\varepsilon_f}{\hbar}\right)^3 |\langle\varepsilon_f|\,\hat{\mathbf{r}}\,|\varepsilon_i\rangle|^2.}$$

As one can see, spontaneous emission and absorption rules are “antagonists”:

- If a system is in a state from which only forbidden transition lead to a lower level, then this excited state will be durable.

- If one manages to populate such a level in a “top-down fashion”, one can achieve a population inversion.

This principle is applied in every laser.
The matrix element $\mathbf{r}_{if}=|\langle\varepsilon_f|\,\hat{\mathbf{r}}\,|\varepsilon_i\rangle|^2$ contains selection rules for electric dipole transitions → cf. Stark effect.
Hydrogen atom: $\tau(2p\to1s)=1.6\cdot10^{-9}$ s, lifetime of magnetic dipole or electric quadrupole transitions is four times longer. Interestingly $2s\to1s$: forbidden in every multipole expansion ⇒ long lifetime of $1/7$ s, multi-photon process.

Light scattering on atoms:
In such a process the photon number is conserved

$$|i\rangle = |\underbrace{(\mathbf{k}, \varepsilon, \omega)}_{1\text{ photon}}, \underbrace{A}_{\text{atomic state}} \rangle ,$$
$$|f\rangle = |(\mathbf{k}', \varepsilon', \omega'), B\rangle .$$

Term $\mathbf{A}^2$ in H_I causes such processes in first order perturbation theory.
Term $\mathbf{A} \cdot \mathbf{p}$ in H_I causes such processes in second order perturbation theory.
Both processes are in general important.
Kramer-Heisenberg (KH) formula ($\xi \gg a_0$):

$$\frac{d\sigma}{d\Omega} = r_0^2 \frac{\omega'}{\omega} \left| (\varepsilon^* \cdot \varepsilon')\delta_\mathrm{AB} - \frac{1}{m} \sum_I \left\{ \frac{(\varepsilon'^* \cdot \mathbf{p}_\mathrm{BI})(\varepsilon \cdot \mathbf{p}_\mathrm{IA})}{E_\mathrm{I} - E_\mathrm{A} - \hbar\omega} + \frac{(\varepsilon \cdot \mathbf{p}_\mathrm{BI})(\varepsilon'^* \cdot \mathbf{p}_\mathrm{IA})}{E_\mathrm{I} - E_\mathrm{A} + \hbar\omega} \right\} \right|^2$$

where $r_0 = 2.8 \cdot 10^{-13}$ cm is the classical electron radius, $\mathbf{p}_\mathrm{BI} = \langle B | \, \mathbf{p} \, | I \rangle$, and $\sum_I$ is the sum over intermediate states of the atom I.

Elastic scattering: $\omega' = \omega$, B = A.
Limiting case $\omega \ll \omega_\mathrm{IA} \equiv (E_\mathrm{I} - E_\mathrm{A})/\hbar$: **Rayleigh scattering**. Expansion in powers of ω/ω_{IA}:

$$\left(\frac{d\sigma}{d\Omega}\right)_\mathrm{Rayl} = \left(\frac{r_0 m}{\hbar}\right)^2 \omega^4 \left| \sum_I \frac{1}{\omega_\mathrm{IA}} \left[(\varepsilon'^* \cdot \mathbf{r}_\mathrm{AI})(\varepsilon \cdot \mathbf{r}_\mathrm{IA}) + (\varepsilon \cdot \mathbf{r}_\mathrm{AI})(\varepsilon'^* \cdot \mathbf{r}_\mathrm{IA}) \right] \right|^2$$

Limiting case $\omega \gg \omega_{IA}$: **Thomson scattering**

$$\left(\frac{d\sigma}{d\Omega}\right)_\mathrm{Thom} = r_0^2 \left| \varepsilon \cdot \varepsilon'^* \right|$$

also applies when $\omega_\mathrm{IA} = 0$, i.e. for free electrons, the **Compton scattering**.

Inelastic scattering:
Raman scattering: $E_A + \hbar\omega = E_B + \hbar\omega'$, only the process of second order contributes. In general:

$$\left(\frac{d\sigma}{d\Omega}\right)_\mathrm{Raman} \approx r_0^2.$$

Special situation: $E_I = E_A + \hbar\omega \to$ resonant Raman squattering, KH-formula fails. Energy uncertainty has to be considered.

4.7 Interaction between light and matter in Second Quantization

Our goal is now, in association with the first part of the lesson, to examine the interaction of light and matter. The representation of matter states in the second quantization formalism will allow us to introduce the concept of *Feynman diagrams*, which play an important role in the theory of many particles as well as the theory of fundamental particles.
Because everything will be expressed as an operator now, we will neglect emphasis of operators via bold letters.

Light-matter Hamiltonian in second quantization:
We describe the interaction of photons and electrons completely in second quantization. The Hamiltonian reads

$$\hat{H} = \hat{H}_{\text{mat}} + \hat{H}_{\text{I}} + \hat{H}_{\text{em}} \,,$$

where $\hat{H}_{\text{mat}}$ describes the electrons alone, $\hat{H}_{\text{I}}$ the interaction with the radiation field (4.41) and $\hat{H}_{\text{em}}$ the electromanetic field alone.

$$\begin{aligned}
\hat{H}_{\text{mat}} &= \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}) \left(-\frac{\hbar^2}{2m}\Delta + V(\mathbf{r}) \right) \hat{\psi}(\mathbf{r}) \\
\hat{H}_{\text{I}} &= \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}) \left[\frac{e}{mc}\hat{\mathbf{A}}_{\text{op}} \cdot \mathbf{p} + \frac{e^2}{2mc^2} \left(\hat{\mathbf{A}}_{\text{op}} \right)^2 \right] \hat{\psi}(\mathbf{r}) \\
\hat{H}_{\text{em}} &= \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} \left(\hat{a}^\dagger_{\mathbf{q}} \hat{a}_{\mathbf{q}} + \frac{1}{2} \right) \,,
\end{aligned}$$

where

$$\hat{\mathbf{A}}_{\text{op}} = \sum_{\mathbf{q}} \sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{q}}}} \left(\hat{a}_{\mathbf{q}} e^{\imath \mathbf{q}\cdot\mathbf{r}} + \hat{a}^\dagger_{\mathbf{q}} e^{-\imath \mathbf{q}\cdot\mathbf{r}} \right) \mathbf{u}_{\mathbf{q}} \,.$$

- The operators $\hat{\psi}^\dagger(\mathbf{r})$ and $\hat{\psi}(\mathbf{r})$ are the creation and annihilation operators of electrons at position $\mathbf{r}$.
- The summation over the polarisation index is incorporated in the sum over $\mathbf{q}$.
- the ladder operators $\hat{a}^\dagger_{\mathbf{q}}$ and $\hat{a}_{\mathbf{q}}$ of the radiations field are given in the Heisenberg picture, i.e. time independent.
- The total Hamiltonian acts on a product states consisting of both Fock spaces of electrons and photons: $\mathcal{H}_{\text{matter}} \otimes \mathcal{H}_{\text{photons}}$.

Field operators:
First we want to investigate the case of *free electrons*, thus it is $V(\mathbf{r}) = 0$. Plane waves pose a good candidate for a complete orthonormal system to express the field operators:

$$\hat{\psi}_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{\imath \mathbf{k}\cdot\mathbf{r}} \hat{c}_{\mathbf{k}} \qquad\qquad \hat{\psi}^\dagger_{\mathbf{k}}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{-\imath \mathbf{k}\cdot\mathbf{r}} \hat{c}^\dagger_{\mathbf{k}}$$

where the following (anti-)commutation rules apply:

$$\left\{\hat{\psi}^\dagger(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right\} = 0\,, \quad \left\{\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r}')\right\} = 0\,, \quad \left\{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r}')\right\} = \delta(\mathbf{r}-\mathbf{r}')$$

$$\left\{\hat{c}^\dagger_{\mathbf{k}}, \hat{c}^\dagger_{\mathbf{k}'}\right\} = 0\,, \qquad \left\{\hat{c}_{\mathbf{k}}, \hat{c}_{\mathbf{k}'}\right\} = 0\,, \qquad \left\{\hat{c}_{\mathbf{k}}, \hat{c}^\dagger_{\mathbf{k}'}\right\} = \delta_{\mathbf{k},\mathbf{k}'}\,.$$

Dispersion relation:
Thus we are able to express $\hat{H}_{\text{mat}}$ completely in terms of ladder operators:

$$\hat{H}_{\text{mat}} = \sum_{\mathbf{k},\mathbf{k}'} \underbrace{\frac{1}{V}\int d\mathbf{r} e^{-\imath\mathbf{k}\cdot\mathbf{r}}\left(-\frac{\hbar^2}{2m}\Delta\right) e^{\imath\mathbf{k}'\cdot\mathbf{r}}}_{=\delta_{\mathbf{k},\mathbf{k}'}\frac{\hbar^2\mathbf{k}^2}{2m}} \hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{k}'}$$

where $\varepsilon_{\mathbf{k}} = \hbar^2\mathbf{k}^2/2m$ is called dispersion relation.

$$\boxed{\hat{H}_{\text{mat}} = \sum_{\mathbf{k}} \frac{\hbar^2\mathbf{k}^2}{2m}\hat{c}^\dagger_{\mathbf{k}}\hat{c}_{\mathbf{k}} = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}}\hat{n}_{\mathbf{k}}} \tag{4.47}$$

when using the occupation number operator $\hat{n}_{\mathbf{k}}$. The interpretation of (4.47) is intuitive: The energy of a many particle state (without interaction) is simply given by the sum over the different single particle levels. But one has to note that this simple form breaks down as soon as the Coulomb interaction between electrons is considered.

$$\begin{aligned} H_{\text{I}}' &= \frac{1}{V}\int d\mathbf{r}\sum_{\mathbf{k}_1} e^{-\imath\mathbf{k}_1\cdot\mathbf{r}}\hat{c}^\dagger_{\mathbf{k}_1}\left(-\frac{e\hbar}{\imath mc}\sum_{\mathbf{q}}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{q}}}}\left(\hat{a}_{\mathbf{q}}e^{\imath\mathbf{q}\cdot\mathbf{r}} + \hat{a}^\dagger_{\mathbf{q}}e^{-\imath\mathbf{q}\cdot\mathbf{r}}\right)\mathbf{u}_{\mathbf{q}}\cdot\nabla\right)\sum_{\mathbf{k}_2} e^{\imath\mathbf{k}_2\cdot\mathbf{r}}\hat{c}_{\mathbf{k}_2} \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}}\left(M_1(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}_{\mathbf{q}} + M_1(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{q})\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}^\dagger_{\mathbf{q}}\right) \end{aligned} \tag{4.48}$$

where again the polarization index is contained in $\mathbf{q}$. One calculates

$$\begin{aligned} M_1(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}) &= \frac{1}{V}\int d\mathbf{r}\, e^{-\imath\mathbf{k}_1\cdot\mathbf{r}}\left(-\frac{e\hbar}{\imath mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{q}}}}e^{\imath\mathbf{q}\cdot\mathbf{r}}\mathbf{u}_{\mathbf{q}}\cdot(\imath\mathbf{k}_2)\,e^{\imath\mathbf{k}_2\cdot\mathbf{r}}\right) \\ &= -\frac{e\hbar}{Vmc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{q}}}}\left(\mathbf{u}_{\mathbf{q}}\cdot\mathbf{k}_2\right)\int d\mathbf{r}\, e^{\imath(\mathbf{q}+\mathbf{k}_2-\mathbf{k}_1)\cdot\mathbf{r}} \\ &= -\frac{e\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{q}}}}\left(\mathbf{u}_{\mathbf{q}}\cdot\mathbf{k}_2\right)\,\delta_{\mathbf{k}_1,\mathbf{q}+\mathbf{k}_2}\,. \end{aligned} \tag{4.49}$$

The last expression in (4.49) represents the conservation of momentum. The partial Hamiltonian $\hat{H}_{\text{I}}'$ describes two kinds of processes via its two terms in (4.48):

- The first term destroys a photon $\mathbf{q}$ and an electron k_2 and creates on the other hand an electron $\mathbf{k}_1$. The total momentum is thereby conserved: $\mathbf{k}_1 = \mathbf{q} + \mathbf{k}_2$.
- The second term creates a photon $\mathbf{q}$ and an electron $\mathbf{k}_1$ but destroys on the other hand an electron $\mathbf{k}_2$. Again the total momentum is conserved via $\mathbf{k}_2 = \mathbf{q} + \mathbf{k}_1$.

Simplification:
It is easy to show that the second term in (4.48) is the Hermitian conjugate of the first term. This is because the first term reads

$$\mathbf{u_q} \cdot \mathbf{k}_2 = \mathbf{u_q} \cdot (\mathbf{k}_1 - \mathbf{q}) = \mathbf{u_q} \cdot \mathbf{k}_1 \,,$$

so one can instead of $\mathbf{q} \to -\mathbf{q}$ do the substitution $\mathbf{k}_1 \leftrightarrow \mathbf{k}_2$ when doing the transition to the second term. The Hermitian conjugate of the second term satisfies then

$$\begin{aligned}\left(\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} M_1(\mathbf{k}_2,\mathbf{k}_1,\mathbf{q})\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}^\dagger_{\mathbf{q}}\right)^\dagger &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} M_1(\mathbf{k}_2,\mathbf{k}_1,\mathbf{q})\hat{c}^\dagger_{\mathbf{k}_2}\hat{c}_{\mathbf{k}_1}\hat{a}_{\mathbf{q}} \\ &= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} M_1(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}_{\mathbf{q}}\end{aligned}$$

and this corresponds to the first term. The paramagnetic part of $\hat{H}'_\mathrm{I}$ of the light-matter interaction can therefore be written as

$$\boxed{\hat{H}'_\mathrm{I} = \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} \left(M_1(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q})\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}_{\mathbf{q}} + \text{h.c.}\right).} \tag{4.50}$$

Feynman diagrams:
Both processes described by $\hat{H}'_\mathrm{I}$ can be visualized by simple diagrams. Fig. 4.1 shows on the left the first process: the annihilation of a photon $\mathbf{q}$ while scattering an electron from the state $\mathbf{k}_2$ to $\mathbf{k}_1$. The diagram on the right hand side represents the hermetic conjugated process, namely the creation of a photon under scattering of an electron.

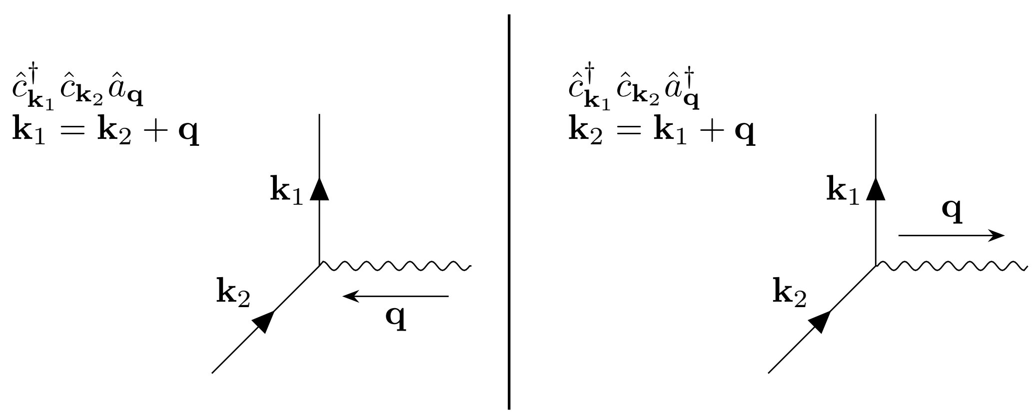


Figure 4.1: Processes resulting from first order perturbation theory in $\hat{H}'_\mathrm{I}$. The right process corresponds to the Hermitian conjugate of the left one.

Feynman diagrams:
Feynman diagrams are a graphical representation of perturbation theoretical processes. Lines represent participating incoming or outgoing particles and the vertices correspond to the matrix elements of the interaction.

Feynman diagrams do not only serve the purpose of visualisation. In many body theory and the theory of fundamental particles every Feynman diagram represents a precise mathematical expression of perturbation theory.

Conservation of momentum at the vertices:
A point were different particle lines meet is called a vertex. The Kronecker delta in M_1 demands at a vertex that the total momentum of annihilated particles is equal to the total momentum of created particles.

Diamagnetic perturbation term:
$\hat{H}_{\mathrm{I}}''$ as part of the whole Hamiltonian contains four terms which arise from the product $\hat{\mathbf{A}}^2$:

$$\begin{aligned}\hat{H}_{\mathrm{I}}'' = \sum_{\mathbf{k_1},\mathbf{k_2}}\sum_{\mathbf{q}_1,\mathbf{q}_2}\Big(&M_2(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}_1,\mathbf{q}_2)\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}_{\mathbf{q}_1}\hat{a}_{\mathbf{q}_2} + M_2(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{q}_1,\mathbf{q}_2)\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}^\dagger_{\mathbf{q}_1}\hat{a}_{\mathbf{q}_2}\\ &+M_2(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}_1,-\mathbf{q}_2)\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}_{\mathbf{q}_1}\hat{a}^\dagger_{\mathbf{q}_2} + M_2(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{q}_1,-\mathbf{q}_2)\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}^\dagger_{\mathbf{q}_1}\hat{a}^\dagger_{\mathbf{q}_2}\Big)\\ = \sum_{\mathbf{k_1},\mathbf{k_2}}\sum_{\mathbf{q}_1,\mathbf{q}_2}\Big(&M_2(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}_1,\mathbf{q}_2)\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}_{\mathbf{q}_1}\hat{a}_{\mathbf{q}_2} + M_2(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{q}_1,\mathbf{q}_2)\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}^\dagger_{\mathbf{q}_1}\hat{a}_{\mathbf{q}_2} + \text{h.c.}\Big)\end{aligned} \tag{4.51}$$

Where

$$\begin{aligned}M_2(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}_1,\mathbf{q}_2) &= \frac{2\pi\hbar c^2}{V}\frac{1}{\sqrt{\omega_{\mathbf{q}_1}\omega_{\mathbf{q}_2}}}\frac{1}{V}\frac{e^2}{2mc^2}\int d\mathbf{r}\, e^{\imath\mathbf{k}_1\cdot\mathbf{r}}e^{\imath(\mathbf{q}_1+\mathbf{q}_2)\cdot\mathbf{r}}e^{\imath\mathbf{k}_2\cdot\mathbf{r}}\,(\mathbf{u}_{\mathbf{q}_1}\cdot\mathbf{u}_{\mathbf{q}_2})\\ &= \frac{2\pi\hbar c^2}{V}\frac{1}{\sqrt{\omega_{\mathbf{q}_1}\omega_{\mathbf{q}_2}}}\frac{e^2}{2mc^2}\,(\mathbf{u}_{\mathbf{q}_1}\cdot\mathbf{u}_{\mathbf{q}_2})\,\delta_{\mathbf{k}_1,\mathbf{k}_2+\mathbf{q}_1+\mathbf{q}_2}\end{aligned} \tag{4.52}$$

The four terms in (4.51) describe vertices, at which two electrons and two photons are involved each. Fig. 4.2 shows the corresponding Feynman graphs. The quantities M_1 and M_2 determine the probability of the occurrence of these processes.

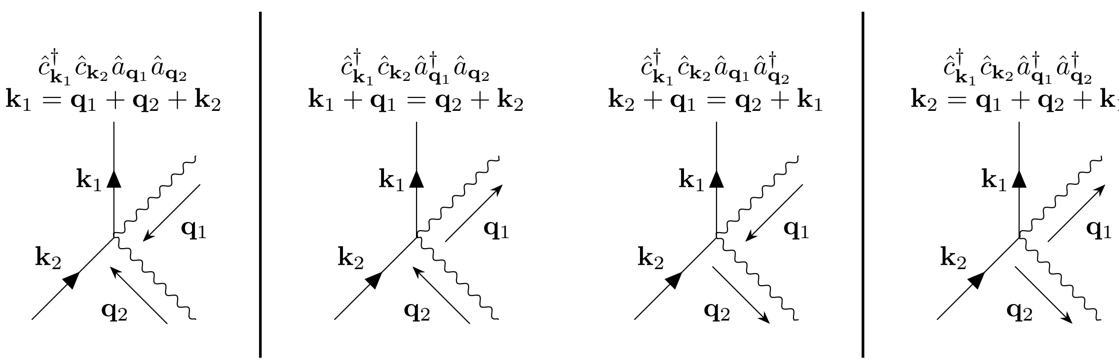


Figure 4.2: Processes associated with first order perturbation theory in $\hat{H}_{\mathrm{I}}''$. Both graphs in the middle describe contributions to Compton scattering. The two diagrams to the right are the Hermitian conjugate of the left ones.

Compton Scattering:
Both graphs in the middle of the Fig. 4.2 show the scattering of a photon on a (free) electron,

what is called *Compton scattering* (note that basically we are not looking at one "single photon", a photon gets annihilated while another is created - at least this is a good visualisation). The other diagrams describe emission and absorption processes involving two photons: Always two photon lines are involved at a vertex created via H_I''.

4.8 Non-relativistic Bremsstrahlung

In the following we will examine the scattering of an electron at a potential, e.g. at a static (because much heavier compared to the electron) nucleus. The charged particle will be hereby accelerated and will radiate energy in the form of photons. This effect is known as *Bremsstrahlung* and is for example used in a dentist's office to produce the appropriate radiation for a X-ray scan. We will assume that $v/c \ll 1$, namely we are looking at the non-relativistic limiting case.

Perturbation terms:
We are interested in the emission of a single photon, therefore the interaction term is given by H_I'. Furthermore we will consider the potential $V_\mathrm{Nuc}(\mathrm{r})$ of a nucleus from the target as a perturbation. The complete operator of the perturbation then reads

$$\hat{V}_0 = \hat{H}_\mathrm{I}' + V_\mathrm{Nuc}(\mathbf{r}).$$

We note that $\hat{H}_\mathrm{I}''$ is not appearing, because the diamagnetic term of lowest order describes the Rutherford scattering process. We find in second quantization:

$$H_\mathrm{I}' = \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}} \Big(M_1(\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}) \hat{c}^\dagger_{\mathbf{k}_1} \hat{c}_{\mathbf{k}_2} \hat{a}_\mathbf{q} + \mathrm{h.c.} \Big) \tag{4.53}$$

and

$$V_\mathrm{Nuc} = \int d\mathbf{r}\, \hat{\psi}^\dagger(\mathbf{r}) V_\mathrm{Nuc}(\mathbf{r}) \hat{\psi}(\mathbf{r}), \qquad \text{with} \quad \hat{\psi}(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_\mathbf{k} e^{\imath \mathbf{k}\cdot\mathbf{r}} \hat{c}_\mathbf{k}.$$

No conservation of momentum:
The explicit for of the perturbation potential reads

$$V_\mathrm{Nuc} = \frac{1}{V} \sum_{\mathbf{k}_1,\mathbf{k}_2} \int d\mathbf{r}\, e^{\imath(\mathbf{k}_1-\mathbf{k}_2)\cdot\mathbf{r}} V_\mathrm{Nuc}(\mathbf{r}) \hat{c}^\dagger_{\mathbf{k}_1} \hat{c}_{\mathbf{k}_2} = \frac{1}{V} \sum_{\mathbf{k}_1,\mathbf{k}_2} \tilde{V}_\mathrm{Nuc}(\mathbf{k}_1 - \mathbf{k}_2) \hat{c}^\dagger_{\mathbf{k}_1} \hat{c}_{\mathbf{k}_2}$$

$$\text{with} \quad \tilde{V}_\mathrm{Nuc}(\mathbf{k}) = \int d\mathbf{r}\, V_\mathrm{Nuc}(\mathbf{r}) e^{-\imath \mathbf{k}\cdot\mathbf{r}}.$$

The potential V_Nuc is real, therefore the Fourier transform $\tilde{V}_\mathrm{Nuc}$ is Hermitian symmetric, i.e. $\tilde{V}_\mathrm{Nuc}(-\mathbf{k}) = \tilde{V}_\mathrm{Nuc}(\mathbf{k})$. We notice, that the total momentum is not conserved, because the Hamiltonian has no translation invariance. Momentum can be transferred to the lattice when scattering at V_Nuc.

Golden rule:
Using the perturbation operator V_0, we want to induce transitions. Fermi's golden rule for transitions reads:

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar} \delta(E_i - E_f) |M_{if}| \tag{4.54}$$

with

$$M_{if} = M_{if}^{(1)} + M_{if}^{(2)} .$$

The energies E_i and E_f stand for the total energies of electrons and radiation field before and after the transition. Initial and final states are:

$$|i\rangle = \hat{c}_{\mathbf{k}}^\dagger |0\rangle \quad : \quad \text{no photon, one electron } \hbar\mathbf{k}\,, \qquad E_i = \frac{\hbar^2\mathbf{k}^2}{2m} \tag{4.55}$$

$$|f\rangle = \hat{c}_{\mathbf{k}'}^\dagger \hat{a}_{\mathbf{q}}^\dagger |0\rangle : \quad \text{one photon } \hbar\mathbf{q}\text{, one electron } \hbar\mathbf{k}'\,, \quad E_F = \frac{\hbar^2\mathbf{k}'^2}{2m} + \hbar c|\mathbf{q}| \tag{4.56}$$

Differential cross-section

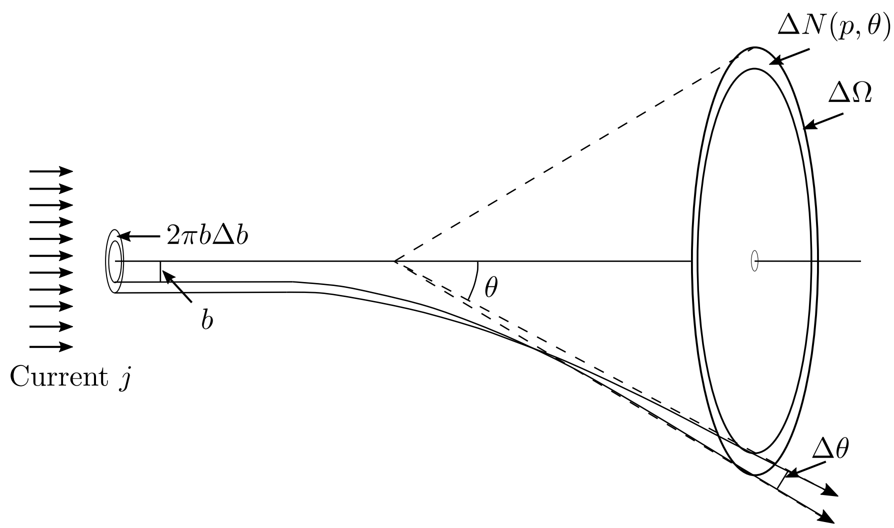


Figure 4.3: Geometry of the elastic scattering. The area $\Delta\sigma$ of the incoming ray reads $\Delta\sigma = 2\pi b\Delta b$. Also shown the solid angle $\Delta\Omega$.

Suppose a particle stream of density j_i (describes particle number per area and time, "i" means "initial") is hitting a scattering potential. In this event, a detector counting the scattered particles at the solid angle $d\Omega$ and in the momentum range between k' and $k' + dk'$ will measure a certain counting rate (events per second). This rate is given by

$$\frac{V}{(2\pi)^3} k'^2 dk'\, d\Omega\, \Gamma_{i\to f} = j_i d\sigma\,, \tag{4.57}$$

where $d\sigma$ is a differential area element perpendicular to the incoming particle stream j_i. $\Gamma_{i\to f}$ describes the transition rate to the final state $\mathbf{k}'$, see Fig. 4.3.

General scattering cross-section:
In the following we have to specify more precisely what a detector will be measuring. In the case of a *wavelength-dispersive* detector, the interesting quantity is

$$\frac{d^2\sigma}{dk' d\Omega}(k', \Omega) = \frac{1}{j_i} \frac{V}{(2\pi)^3} k'^2 \Gamma_{i\to f} .$$

The scattering cross-section is a measure for the magnitude of scattering coming from a centre of diffraction inside a solid angle $d\Omega$ and into the momentum range between k' and $k' + dk'$.

Differential cross-section:
Assuming the detector is not sensitive in a certain momentum range dk' around k' alone but is just counting all scattered particles in $d\Omega$, without regard for their energy. Then we have to integrate over the left hand side of (4.57) with respect to dk' and we are calling

$$\frac{d\sigma}{d\Omega}(\Omega) := \frac{1}{j_i}\frac{V}{(2\pi)^3}\int dk'\, k'^2\, \Gamma_{i\to f}$$

differential cross-section with regard to a scattering into the solid angle Ω.

Final states regarding Bremsstrahlung:
In the case of Bremsstrahlung one is confronted with one obstacle: After the scattering one has to deal with two particles, the electron $\hbar\mathbf{k}'$ and the photon $\hbar\mathbf{q}$. The energy of the photon is not fixed but follows a certain distribution. A detector for photons should work wavelength-dispersive, a detector for the scattered electrons however should not. In the case of Bremsstrahlung we are mainly concerned with the wavelength of the generated photons (important for application like X-ray scans), but we are not interested in the energy of the scattered electrons.

Therefore we are asking for the differential cross-section of the scattering of an electron into the solid angle $d\Omega_{\mathbf{k}'}$ under emission of a photon carrying a momentum between $\hbar q$ and $\hbar(q + \Delta q)$ into the solid angle $d\Omega\mathbf{q}$. This quantity is written as

$$\frac{d^3\sigma}{d\Omega_{\mathbf{k}'}d\Omega_{\mathbf{q}}dq}(\Omega_{\mathbf{k}'}, q, \Omega_{\mathbf{q}}).$$

$$\text{Velocities:} \quad \boldsymbol{\nu} := \frac{\hbar\mathbf{k}}{m} \quad \text{and} \quad \boldsymbol{\nu}' = \frac{\hbar\mathbf{k}'}{m} \quad \Rightarrow \quad \text{particle stream:} \quad j_i = \frac{\nu}{V}$$

$$\Rightarrow \text{cross-section:} \quad \boxed{\frac{d^3\sigma}{d\Omega_{\mathbf{k}'}d\Omega_{\mathbf{q}}dq}(\Omega_{\mathbf{k}'}, q, \Omega_{\mathbf{q}}) = \frac{V}{\nu}\left(\frac{V}{(2\pi)^3}\right)^2 q^2 \int dk'\, k'^2\, \Gamma_{i\to f}.} \tag{4.58}$$

Perturbation theory of first order:
The part V_{Nuc} is not containing any creators of photons which is why it cannot cause transitions between (4.55) and (4.56) in first order. The only contribution will come from the Hermitian conjugate inside of H_{I}'. The terms concerned are proportional to $\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}^\dagger_{\mathbf{q}}$ and the corresponding Feynman diagram is shown on the right of Fig 4.1. However conservation of momentum and energy apply and both requirements can't be satisfied simultaneously. This can be seen via the following:

Let be p^μ and $(p')^\mu$ the four-momentum of the arriving respectively emitting electron. Furthermore let q^μ be the four-momentum of the photon (we will set $\hbar = 1$). Then we find

$$m^2c^2 = p^\mu p_\mu = ((p')^\mu + q^\mu)((p')_\mu + q_\mu)\,.$$

The right hand side gives, considering $q^\mu q_\mu = 0$ (photons own no mass):

$$m^2c^2 + 0 + (p')^\mu q_\mu + q^\mu (p')_\mu = m^2c^2 + 2(p')^\mu q_\mu\,.$$

This leads to $(p')^\mu q_\mu = 0$. In the resting frame of the escaping electron is

$$(p')^\mu = (mc, 0) \qquad \text{and} \qquad q^\mu = (\hbar\omega_{\mathbf{q}}/c, \mathbf{q}),$$

which gives

$$(p')^\mu q_\mu = mc\,\hbar\omega_{\mathbf{q}} = 0.$$

The energy of the photon vanishes, the considered process does not exist. Bremsstrahlung is an effect of second order perturbation theory in V_0.

Second order perturbation theory:
The matrix element $M_{if}^{(2)}$ reads

$$M_{if}^{(2)} = \sum_m \frac{\langle f|V_0|m\rangle \langle m|V_0|i\rangle}{E_i - E_m + \imath\eta\hbar}, \quad \text{where} \quad V_0 = \hat{H}_\mathrm{I}' + V_\mathrm{Nuc}, \tag{4.59}$$

which we already know from Quantum Mechanics I (with $\eta \ll 1$). It needs a little bit of bookkeeping to not lose track of the calculations. For an intermediate state $|m\rangle$ exist two possibilities, so that the numerator of the sum is not vanishing.

a) Intermediate state without photon:
The intermediate state has no photon in it, but only an "intermediate" electron carrying momentum $\hbar\mathbf{k}_z$,

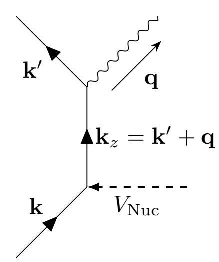
$$|m_a\rangle = \hat{c}^\dagger_{\mathbf{k}_z}|0\rangle, \quad E_m^a = \frac{\hbar^2\mathbf{k}_z^2}{2m}.$$

The numerator of (4.59) then reads

$$\langle f|H_\mathrm{I}' + V_\mathrm{Nuc}|m_a\rangle \langle m_a|H_\mathrm{I}' + V_\mathrm{Nuc}|i\rangle = \langle f|H_\mathrm{I}'|m_a\rangle \langle m_a|V_\mathrm{Nuc}|i\rangle \tag{4.60}$$

because H_I' generates exactly the required photon of the final state (via its h.c. part), V_Nuc on the other hand generates none. The corresponding Feynman graph is shown on the right.

a)



b) Intermediate state with photon:
The intermediate state contains a photon carrying momentum $\hbar\mathbf{q}$ and an electron carrying momentum $\hbar\mathbf{k}_z$:

$$|m_b\rangle = \hat{c}^\dagger_{\mathbf{k}_z}\hat{a}^\dagger_{\mathbf{q}}|0\rangle, \qquad E_m^b = \frac{\hbar^2\mathbf{k}_z^2}{2m} + \hbar cq.$$

The numerator of (4.59) reads

$$\langle f|V_\mathrm{Nuc}|m_b\rangle \langle m_b|H_\mathrm{I}'|i\rangle, \tag{4.61}$$

and the Feynman graph is shown in figure 4.4 on the right hand side. Only the Hermitian conjugate part of H_I' plays a role again in the calculations of the matrix elements, the other part is not contributing. The sum appearing in $M_{if}^{(2)}$ is running over all $\mathbf{k}_z$ of intermediate electrons and over the cases *a*) and *b*).

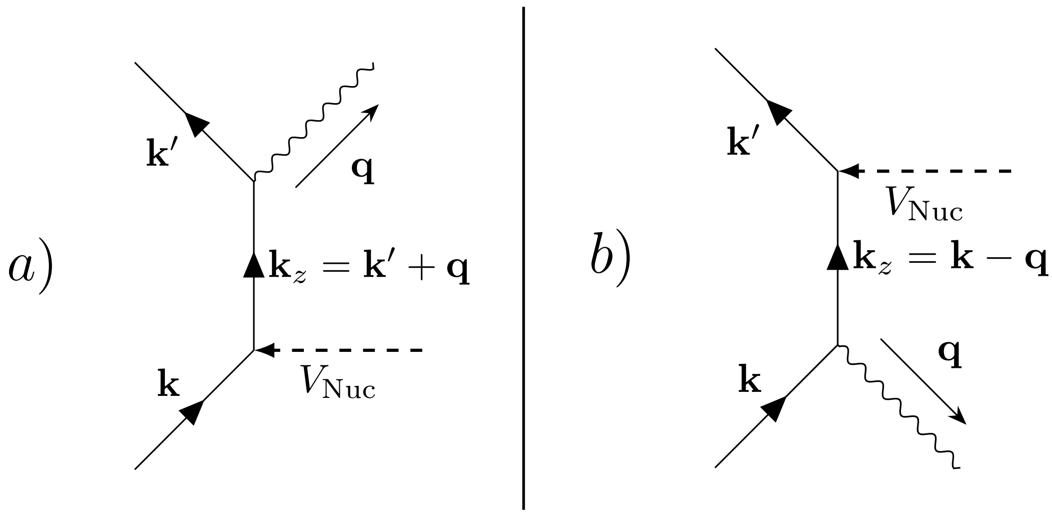


Figure 4.4: Feynman diagrams for the breaking radiation process.

The emission of Bremsstrahlung is carried out in two phases: the scattering at a nucleus and the emission of a photon (or vice versa). The calculation of the matrix elements is following:

a) Matrix elements - Intermediate state without photon:
One has to calculate (4.60). It is

$$
\begin{aligned}
\langle m_a|V_\mathrm{Nuc}|i\rangle &= \langle 0|\hat{c}_{\mathbf{k}_z} \sum_{\mathbf{k}_1,\mathbf{k}_2} \hat{c}^\dagger_{\mathbf{k}_1} \tilde{V}_\mathrm{Nuc}(\mathbf{k}_1-\mathbf{k}_2)\hat{c}_{\mathbf{k}_2}\hat{c}^\dagger_{\mathbf{k}}|0\rangle \\
&= \sum_{\mathbf{k}_1,\mathbf{k}_2} \langle 0|\Big(\hat{c}_{\mathbf{k}_z}\hat{c}^\dagger_{\mathbf{k}_1}\Big)\tilde{V}_\mathrm{Nuc}(\mathbf{k}_1-\mathbf{k}_2)\Big(\hat{c}_{\mathbf{k}_2}\hat{c}^\dagger_{\mathbf{k}}\Big)|0\rangle \\
&= \sum_{\mathbf{k}_1,\mathbf{k}_2} \delta_{\mathbf{k}_z,\mathbf{k}_1}\tilde{V}_\mathrm{Nuc}(\mathbf{k}_1-\mathbf{k}_2)\delta_{\mathbf{k}_2,\mathbf{k}} \\
&= \tilde{V}_\mathrm{Nuc}(\mathbf{k}_z-\mathbf{k})
\end{aligned}
$$

and

$$
\begin{aligned}
\langle f|H_\mathrm{I}'|m_a\rangle &= \langle 0|\hat{c}_{\mathbf{k}'}\hat{a}_{\mathbf{q}} \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}_1} M_1(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{q}_1)\hat{c}^\dagger_{\mathbf{k}_1}\hat{c}_{\mathbf{k}_2}\hat{a}^\dagger_{\mathbf{q}_1}\hat{c}^\dagger_{\mathbf{k}_z}|0\rangle \\
&= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}_1} \langle 0|\Big(\hat{c}_{\mathbf{k}'}\hat{c}^\dagger_{\mathbf{k}_1}\Big)\Big(\hat{a}_{\mathbf{q}}\hat{a}^\dagger_{\mathbf{q}_1}\Big)\Big(\hat{c}_{\mathbf{k}_2}\hat{c}^\dagger_{\mathbf{k}_z}\Big)|0\rangle\ M_1(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{q}_1) \\
&= \sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}_1} \delta_{\mathbf{k}',\mathbf{k}_1}\delta_{\mathbf{q},\mathbf{q}_1}\delta_{\mathbf{k}_2,\mathbf{k}_z}\ M_1(\mathbf{k}_1,\mathbf{k}_2,-\mathbf{q}_1) \\
&= -\frac{e\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{q}}}}\delta_{\mathbf{k}_z,\mathbf{q}+\mathbf{k}'}\Big(\mathbf{u}_{\mathbf{q}}\cdot\mathbf{k}_z\Big)\,.
\end{aligned}
$$

The first contribution to $M_{if}^{(2)}$ is therefore, taking into account that $\mathbf{u_q} \cdot \mathbf{q} = 0$, given by:

$$M_{if}^{(2,a)} = \sum_{\mathbf{k}_z} \frac{\langle f|H_\mathrm{I}'|m_a\rangle \langle m_a|V_\mathrm{Nuc}|i\rangle}{E_i - E_m^a + \imath\eta\hbar} \overset{\eta\to 0}{=} -\frac{e\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_\mathbf{q}}}\, \frac{\tilde{V}_\mathrm{Nuc}(\mathbf{q}+\mathbf{k}'-\mathbf{k})(\mathbf{u_q}\cdot\mathbf{k}')}{\frac{\hbar^2}{2m}\Big(\mathbf{k}^2 - (\mathbf{q}+\mathbf{k}')^2\Big)}.$$

Because of energy conservation,

$$E_f = \frac{\hbar^2 \mathbf{k}'^2}{2m} + \hbar c|\mathbf{q}| = E_i = \frac{\hbar \mathbf{k}^2}{2m}\,,$$

the denominator also writes

$$N_a = \hbar c|\mathbf{q}| - \frac{\hbar \mathbf{q}^2}{2m} - \frac{\hbar^2}{m}\,\mathbf{q}\cdot\mathbf{k}' = \hbar c|\mathbf{q}|\left(1 - \frac{\hbar\mathbf{q}\cdot\mathbf{k}'}{mc|\mathbf{q}|} - \frac{\hbar\mathbf{q}^2}{2mc|\mathbf{q}|}\right). \tag{4.62}$$

But the second term in brackets gives

$$\frac{\hbar\mathbf{k}'}{m}\cdot\frac{\mathbf{q}}{c|\mathbf{q}|} \le \frac{p'}{m}\frac{1}{c}\frac{|\mathbf{q}|}{|\mathbf{q}|} \approx \frac{\nu'}{c}\,,$$

where ν' is the velocity of the electron after the collision. The third term of (4.62) is again one magnitude smaller in ν/c, because $|\mathbf{q}|$ is assumed far smaller then the electron momentum. Therefore the non-relativistic case is approximated by $N_a \approx \hbar c|\mathbf{q}| = \hbar\omega_\mathbf{q}$. Hence

$$\boxed{M_{if}^{(2,a)} = -\frac{e\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_\mathbf{q}}}\, \frac{\tilde{V}_\mathrm{Nuc}(\mathbf{q}+\mathbf{k}'-\mathbf{k})(\mathbf{u_q}\cdot\mathbf{k}')}{\hbar\omega_\mathbf{q}}}.$$

b) Matrix elements - Intermediate state containing a photon:
The calculation is carried out analogous to case a) and the result for the second contribution of $M_{if}^{(2)}$ reads

$$M_{if}^{(2,b)} = \sum_{\mathbf{k}_z} \frac{\langle f|V_\mathrm{Nuc}|m_a\rangle \langle m_a|H_\mathrm{I}'|i\rangle}{E_i - E_m^b + \imath\eta\hbar} \overset{\eta\to 0}{=} -\frac{e\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_\mathbf{q}}}\, \frac{\tilde{V}_\mathrm{Nuc}(\mathbf{q}+\mathbf{k}'-\mathbf{k})(\mathbf{u_q}\cdot\mathbf{k})}{\frac{\hbar^2}{2m}\Big(\mathbf{k}^2 - (\mathbf{q}-\mathbf{k})^2\Big) - \hbar c|\mathbf{q}|}.$$

The denominator one finds then:

$$N_b = \frac{\hbar\mathbf{k}^2}{2m} - \left(\frac{\hbar\mathbf{q}^2}{2m} + \frac{\hbar\mathbf{k}^2}{2m} - \frac{\hbar\mathbf{q}\cdot\mathbf{k}}{m}\right) - \hbar c|\mathbf{q}| = -\hbar c|\mathbf{q}|\left(1 + \frac{\hbar\mathbf{q}^2}{2mc|\mathbf{q}|} - \frac{\hbar\mathbf{q}\cdot\mathbf{k}}{mc|\mathbf{q}|}\right) \approx -\hbar\omega_\mathbf{q}\,.$$

Hence

$$\boxed{M_{if}^{(2,b)} = -\frac{e\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_\mathbf{q}}}\, \frac{\tilde{V}_\mathrm{Nuc}(\mathbf{q}+\mathbf{k}'-\mathbf{k})(\mathbf{u_q}\cdot\mathbf{k})}{-\hbar\omega_\mathbf{q}}}.$$

Sum of the matrix elements - Nucleus potential:

Both intermediate states (with and without photon) together result in:

$$\boxed{M_{if}^{(2)} = M_{if}^{(2,a)} + M_{if}^{(2,b)} = -\frac{e\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_\mathbf{q}}}\frac{(\mathbf{k}'-\mathbf{k})\cdot\mathbf{u_q}}{\hbar\omega_\mathbf{q}}\,\tilde{V}_\mathrm{Nuc}(\mathbf{q}+\mathbf{k}'-\mathbf{k})}. \tag{4.63}$$

Until now we didn't specify the nucleus potential. From now on we choose

$$V_{\text{Nuc}}(\mathbf{r}) = -\frac{Z\,e^2}{r}\,.$$

The Fourier transform $\tilde{V}_{\text{Nuc}}(\mathbf{k})$ gives

$$\tilde{V}_{\text{Nuc}}(\mathbf{k}) = -\frac{Z\,e^2}{V}\int_V d\mathbf{r}\,\frac{e^{\imath\mathbf{k}\cdot\mathbf{r}}}{r} = -\frac{Z\,e^2}{V}\int_V d\mathbf{r}\,\left(-\frac{1}{k^2}\right)\frac{\Delta\,e^{\imath\mathbf{k}\cdot\mathbf{r}}}{r}\,.$$

Two times partial integration and the substitution

$$\Delta\,\frac{1}{r} = -4\pi\delta(\mathbf{r})$$

results in

$$\tilde{V}_{\text{Nuc}}(\mathbf{k}) = -\frac{Z\,e^2}{Vk^2}\int_V d\mathbf{r}\,\left(\Delta\,\frac{1}{r}\right)e^{\imath\mathbf{k}\cdot\mathbf{r}} = -\frac{4\pi Z\,e^2}{Vk^2}\,. \tag{4.64}$$

Finally we arrive at

$$M_{if}^{(2)} = \frac{4\pi Z\,e^3\hbar}{mc}\sqrt{\frac{2\pi\hbar c^2}{V\omega_{\mathbf{q}}}}\,\frac{(\mathbf{k}'-\mathbf{k})\cdot\mathbf{u}_{\mathbf{q}}}{V\,\hbar\omega_{\mathbf{q}}(\mathbf{q}+\mathbf{k}'-\mathbf{k})^{\mathbf{2}}}\,.$$

Low energy scattering:
We will now assume that the energy of the photon $\omega := \omega_{\mathbf{q}}$ is much smaller compared to the electron's and we set

$$(\mathbf{q}+\mathbf{k}'-\mathbf{k})^2 \approx (\mathbf{k}'-\mathbf{k})^2 \quad := \quad (\Delta\mathbf{k})^2 = \frac{m^2}{\hbar^2}(\Delta\boldsymbol{\nu})^2\,.$$

Simultaneously we find that $|\boldsymbol{\nu}| = |\boldsymbol{\nu}'|$ because when the photon is neglected we are confronted with elastic scattering of the electrons. For the transition rate we find

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar}\,\delta(E_f - E_i)\,\left|M_{if}^{(2)}\right|^2 = \frac{64\pi^2 Z^2\,e^6\hbar^2(\mathbf{u}\cdot\Delta\boldsymbol{\nu})^2}{V^3\,\omega^3 m^4(\Delta\boldsymbol{\nu})^4}\,\delta(E_i - E_f)\,.$$

If θ is the angle between the velocities $\boldsymbol{\nu}$ and $\boldsymbol{\nu}'$ before respectively after the collision, we also find

$$|\Delta\boldsymbol{\nu}| = 2|\boldsymbol{\nu}|\sin\frac{\theta}{2}\,.$$

Differential cross-section of Bremsstrahlung:
The differential cross-section (4.58) can now be calculated:

$$\begin{aligned}\frac{d^3\sigma}{d\Omega_{\mathbf{k}'}d\Omega_{\mathbf{q}}dq}(\Omega_{\mathbf{k}'},q,\Omega_{\mathbf{q}}) &= \frac{V}{\nu}\left(\frac{V}{(2\pi)^3}\right)^2 q^2\int dk'\,k'^2\,\Gamma_{i\to f}\\ &= \frac{64\pi^4 Z^2\hbar^2\,e^6\,q^2}{(2\pi)^6\,\omega^3\,m^4}\int dk'\,\frac{(\mathbf{u}\cdot\Delta\boldsymbol{\nu})^2\,k'^2}{16\nu^5\,\sin^4(\theta/2)}\,\delta(E_i - E_f).\end{aligned}$$

We see a Rutherford cross-section is already looming in this result. The integrand is only dependent on k'^2, and the δ-distribution only of k'. Further it is

$$\delta(E_i - E_f) = \delta\left(\frac{\hbar^2\mathbf{k}'^2}{2m} - \frac{\hbar^2\mathbf{k}^2}{2m}\right) = \frac{2m}{\hbar^2}\,\delta(\mathbf{k}'^2 - \mathbf{k}^2)\,.$$

Now it is easy to calculate the integral:

$$\int dk'\,k'^2\,\delta(\mathbf{k}'^2 - \mathbf{k}^2) = \int d\xi\,\frac{\xi}{2\sqrt{\xi}}\,\delta(\xi - \mathbf{k}^2) = \frac{k}{2} = \frac{m\nu}{2\hbar}\,.$$

Along with $q = \omega/c$ we arrive at

$$\frac{d^3\sigma}{d\Omega_{\mathbf{k}'}d\Omega_{\mathbf{q}}d\omega} = \frac{Z^2\,e^4}{m^2\nu^4\sin^4(\theta/2)}\,\frac{(\mathbf{u}\cdot\Delta\boldsymbol{\nu})^2\,e^2}{16\pi^2\,c^2\,\hbar\omega}\,. \tag{4.65}$$

In the first factor, one recognizes the Rutherford cross-section. The second factor represents the probability density of observing an additional photon carrying energy $\hbar\omega_{\mathbf{q}}$ at the solid angle $d\Omega_{\mathbf{q}}$.

Chapter 5

Relativistic quantum mechanics

5.1 Invariances of the Schrödinger equation

Consider a free particle:

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2 = -\frac{\hbar^2}{2m}\Delta$$

Coordinate transformations:

a) *Translation:* $x' = x - a$, $y' = y$, $z' = z$, $t' = t$.

b) *Rotation:* $x'_j = \sum_l a_{jl} x_l$.
Rotations do not change the length:

$$\sum_j x'^2_j = \sum_j \sum_{k,l} a_{jk} a_{jl} x_k x_l \stackrel{!}{=} \sum_j x_j^2 \,.$$

Thus

$$\sum_j a_{jk} a_{jl} = \delta_{kl} \quad \text{and} \quad \sum_k a_{ik} a_{jk} = \delta_{ij}$$

or more compact

$$\mathbf{A} \cdot \mathbf{A}^T = \mathbf{A}^T \cdot \mathbf{A} = \mathbf{1} \quad \text{with} \quad \mathbf{A} = (a_{jl}) \,.$$

c) *Galilean transformation:* The primed coordinate system moves with a constant speed v relative to the unprimed system: $x' = x - vt$, $y' = y$, $z' = z$, $t' = t$.

Schrödinger equation

$$\imath\hbar \frac{\partial}{\partial t}\psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}, t)$$

is *covariant* under the transformations mentioned above, i.e. it is form-invariant during a change of coordinates:

$$\imath\hbar \frac{\partial}{\partial t'}\psi'(\mathbf{r}', t') = -\frac{\hbar^2}{2m}\Delta'\psi'(\mathbf{r}', t') \,.$$

Proof:

a) *Translation:* Use the chain rule:

$$\frac{\partial}{\partial x'} = \frac{\partial x}{\partial x'}\frac{\partial}{\partial x} = \frac{\partial}{\partial x} \,.$$

and analogous for y, z and t. With $\psi'(x') = \psi'(x - a) = \psi(x)$ the covariance under translation becomes obvious.

b) *Rotation:* Use the chain rule:

$$\frac{\partial}{\partial x_k} = \sum_j \frac{\partial x'_j}{\partial x_k}\frac{\partial}{\partial x'_j} = \sum_j a_{jk}\frac{\partial}{\partial x'_j}\,.$$

Thus the Laplacian transforms as

$$\Delta = \sum_k \frac{\partial^2}{\partial x_k^2} = \sum_k\sum_{j,l} a_{jk}a_{lk}\frac{\partial}{\partial x'_j}\frac{\partial}{\partial x'_l} = \sum_{j,l}\delta_{jl}\frac{\partial}{\partial x'_j}\frac{\partial}{\partial x'_l} = \sum_j \frac{\partial^2}{\partial x'^2_j} = \Delta'\,.$$

With $\psi'(\mathbf{r}',t') = \psi(\mathbf{r},t)$ the covariance under rotation is clear.

c) *Galilean transformation:* The momenta in both systems satisfy

$$p'_x = p_x - mv, \quad p'_y = p_y, \quad p'_z = p_z\,.$$

The momentum operators in both systems reads as

$$\hat{p}_x = \frac{\hbar}{\imath}\frac{\partial}{\partial x}, \quad \hat{p}'_x = \frac{\hbar}{\imath}\frac{\partial}{\partial x'}\,.$$

Below, we will show that the Schrödinger equation is covariant under Galilean transformation if the following transformation of the wave function is used

$$\psi(\mathbf{r},t) = e^{-\frac{\imath}{\hbar}mvx'}\psi'(\mathbf{r}',t')\,. \tag{5.1}$$

It is

$$\begin{aligned}\hat{p}_x\psi(\mathbf{r},t) &= (p'_x + mv)\,\psi(\mathbf{r},t) = \left[\frac{\hbar}{\imath}\frac{\partial}{\partial x'} + mv\right]e^{-\frac{\imath}{\hbar}mvx'}\psi'(\mathbf{r}',t') \\ &= e^{-\frac{\imath}{\hbar}mvx'}\frac{\hbar}{\imath}\frac{\partial}{\partial x'}\psi'(\mathbf{r}',t') = e^{-\frac{\imath}{\hbar}mvx'}\hat{p}'_x\psi'(\mathbf{r}',t')\end{aligned}$$

and thus

$$\hat{p}_x^2\psi(\mathbf{r},t) = e^{-\frac{\imath}{\hbar}mvx'}\hat{p}'^2_x\psi'(\mathbf{r}',t')\,.$$

Inserting this into the the Schrödinger equation leads to

$$\begin{aligned}0 &= \left[\imath\hbar\frac{\partial}{\partial t} - \frac{1}{2m}\left(\hat{p}_x^2 + \hat{p}_y^2 + \hat{p}_z^2\right)\right]\psi(\mathbf{r},t) \\ &= e^{-\frac{\imath}{\hbar}mvx'}\left[\imath\hbar\frac{\partial}{\partial t'} - \frac{1}{2m}\left(\hat{p}'^2_x + \hat{p}'^2_y + \hat{p}'^2_z\right)\right]\psi'(\mathbf{r}',t')\,.\end{aligned}$$

This equation is fulfilled if

$$\imath\hbar\frac{\partial}{\partial t'}\psi'(\mathbf{r}',t') = \frac{1}{2m}\left[\hat{p}'^2_x + \hat{p}'^2_y + \hat{p}'^2_z\right]\psi'(\mathbf{r}',t')\,.$$

Importantly, it follows from Eq. (5.1) that

$$|\psi(\mathbf{r},t)|^2 = |\psi'(\mathbf{r}',t')|^2\,,$$

i.e. the probability densities of the original and transformed wave functions are the same and thus also the physics they describe.

We have shown that the Schrödinger equation is form-invariant under the transformations mentioned above. In particular, it fulfills the *classical principle of relativity*: two persons, that move with a speed v relative to each other, observe physical processes in the same way.

However, we know from classical mechanics that Galilean transformations are only valid for $v \ll c$. A correct formulation of the principle of relativity must account for the equality of the speed of light c in all reference frames.

5.2 Recap of special relativity

Before combining special relativity and quantum mechanics we recap the required formalism of relativity. This enables us to generalize Galilean invariance to *Lorentz invariance*.

Please note, that we have to use *Lorentz transformations*

$$x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}} = \gamma(x - \beta ct), \quad y' = y, \quad z' = z, \quad ct' = \frac{ct - \frac{v}{c}x}{\sqrt{1 - \frac{v^2}{c^2}}} = \gamma(ct - \beta x) \tag{5.2}$$

instead of Galilean transformations.

$$\gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{1}{\sqrt{1 - \beta^2}}$$

is the so-called Lorentz factor.

It turns out that the Schrödinger equation is not invariant under Lorentz transformations and thus a relativistic generalization of this equation is needed.

Lets repeat the formalism of relativity. We define a *(contravariant) four-vector* as

$$\boxed{x^\mu = (x^0, x^1, x^2, x^3) = (x^0, x^k) = (x^0, \mathbf{r})},$$

where

$$x^0 = ct, \quad x^1 = x, \quad x^2 = y, \quad x^3 = z\,.$$

Later we will introduce a *(covariant) four-vector* x_μ which is distinct from x^μ.

We define a metric in this four-dimensional *Minkowski space* via a squared distance

$$\boxed{s^2 = c^2t^2 - x^2 - y^2 - z^2 = c^2t^2 - \mathbf{r} = g_{\mu\nu}x^\mu x^\nu} \tag{5.3}$$

with the *Minkowski metric tensor*

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

More precisely, it is a pseudo-Euclidean metric, because it is not positive-definite. Distances with $s^2 < 0$ are called *spacelike*. Events with a spacelike distance are causally independent. On the other hand, events with a *timelike* distance, $s^2 > 0$, can influence each other. For events with a *lightlike* distance, $s^2 = 0$, a communication is only possible via signals that propagate at the speed of light.

Note that, in Eq. (5.3) we have used the so-called *Einstein summation convention*: we sum (from 0 to 3) over indices occurring twice, one of which is a upper and the other a lower index.

In analogy to rotations, we want to describe Lorentz transformations via a real matrix $\Lambda^\mu{}_\nu$ as

$$\boxed{x'^\mu = \Lambda^\mu{}_\nu x^\nu}. \tag{5.4}$$

The Lorentz transformation should leave the distance s^2 unchanged. Just like for rotations, the condition for the matrix $\Lambda^\mu{}_\nu$ reads as

$$s'^2 = g_{\mu\nu} x'^\mu x'^\nu = g_{\mu\nu} \Lambda^\mu{}_\rho x^\rho \Lambda^\nu{}_\lambda x^\lambda \stackrel{!}{=} g_{\rho\lambda} x^\rho x^\lambda = s^2 \, .$$

Thus

$$\boxed{g_{\mu\nu} \Lambda^\mu{}_\rho \Lambda^\nu{}_\lambda = g_{\rho\lambda}} \tag{5.5}$$

or in matrix representation

$$\boxed{\Lambda^T g \Lambda = g} \, .$$

All Lorentz transformations form a group, the so-called *Lorentz group*.

In particular, the matrix representation of the basic Lorentz transformation (5.2) reads as

$$\Lambda^\mu{}_\nu = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} \cosh\xi & -\sinh\xi & 0 & 0 \\ -\sinh\xi & \cosh\xi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with *rapidity* ξ defined via $\tanh\xi = \beta$.

In addition to a contravariant vector x^μ we introduce a *covariant vector* x_μ as

$$\boxed{x_\mu = g_{\mu\nu} x^\nu = (ct, -\mathbf{r})} \tag{5.6}$$

with the inverse operation

$$x^\mu = g^{\mu\nu} x_\nu \, . \tag{5.7}$$

Thus a multiplication with $g^{\mu\nu}$ or $g_{\mu\nu}$ allows raising or lowering of indices. One of the advantages of this is an integration of the metric into a vector and thus a more compact notation. For the Euclidean metric it is $g_{\mu\nu} = \delta_{\mu\nu}$, where $\delta_{\mu\nu}$ is the Kronecker delta, and thus there is no difference between contravariant and covariant vectors.
The consistency of Eq. (5.6) and (5.7) is guaranteed via

$$g_{\mu\rho} g^{\rho\nu} = \delta_\mu{}^\nu \, .$$

For the Lorentz transformation Λ we define in the same way:

$$\Lambda_\mu{}^\nu = g_{\mu\lambda} \Lambda^\lambda{}_\rho g^{\rho\nu} = \Lambda_{\mu\rho} g^{\rho\nu} = g_{\mu\lambda} \Lambda^{\lambda\nu} \, , \tag{5.8}$$

which is generally true for order-2 tensors.

The term "contravariant" and "covariant" reflects the different transformation behavior of the corresponding vectors under Lorentz transformation. Contravariant vectors transform according to Eq. (5.4). On the contrary, covariant vectors transform as

$$\Lambda_\mu{}^\nu x_\nu = g_{\mu\lambda} \Lambda^\lambda{}_\rho g^{\rho\nu} x_\nu = g_{\mu\lambda} \Lambda^\lambda{}_\rho x^\rho = g_{\mu\lambda} x'^\lambda = x'_\mu \, ,$$

where we have used Eqs. (5.8), (5.6) and (5.4).

We became familiar with the behaviour of position vectors under Lorentz transformations. All other four-vectors behave in the same way. Thus we define:
A *contravariant four-vector* a^μ transforms as

$$\boxed{a'^\mu = \Lambda^\mu{}_\nu a^\nu} \tag{5.9}$$

and a *covariant four-vector* a_μ transforms as

$$\boxed{a'_\mu = \Lambda_\mu{}^\nu a_\nu}\,. \tag{5.10}$$

How do four-gradients transform? We define four-gradients as

$$\frac{\partial}{\partial x^\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) = \left(\frac{\partial}{\partial ct}, \nabla\right) = \partial_\mu$$

and

$$\frac{\partial}{\partial x_\mu} = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\frac{\partial}{\partial x}, -\frac{\partial}{\partial y}, -\frac{\partial}{\partial z}\right) = \left(\frac{\partial}{\partial ct}, -\nabla\right) = \partial^\mu\,.$$

As indicated by the notation, the vectors ∂_μ and ∂^μ transform covariantly and contravariantly, respectively, just oppositely to the position vectors used in the derivative.

Proof: We multiply Eq. (5.4) with $g_{\mu\lambda}\Lambda^\lambda{}_\rho$:

$$g_{\mu\lambda}\Lambda^\lambda{}_\rho x'^\mu = g_{\mu\lambda}\Lambda^\lambda{}_\rho \Lambda^\mu{}_\nu x^\nu$$

and obtain

$$x_\rho = \Lambda^\lambda{}_\rho x'_\lambda \tag{5.11}$$

using Eq. (5.5). Using the chain rule we get

$$\frac{\partial}{\partial x'_\mu} = \frac{\partial x_\nu}{\partial x'_\mu}\frac{\partial}{\partial x_\nu} = \Lambda^\mu{}_\nu \frac{\partial}{\partial x_\nu}$$

and thus the contravariance of ∂^μ is evident. The covariance of ∂_μ can be shown in an analogous way.

Multiplying Eq. (5.11) with $\Lambda_\mu{}^\rho$ we get

$$x'_\mu = \Lambda_\mu{}^\rho x_\rho = \Lambda_\mu{}^\rho \Lambda^\lambda{}_\rho x'_\lambda$$

and thus

$$\Lambda_\mu{}^\rho \Lambda^\lambda{}_\rho = \delta^\lambda_\mu\,.$$

This means that the transformation matrices of covariant and contravariant vectors are essentially inverse to one another. In matrix representation:

$$\begin{aligned} \text{Contravariant}: \quad x' &= \Lambda x \\ \text{Covariant}: \quad x' &= \left(\Lambda^{-1}\right)^T x\,. \end{aligned}$$

It useful to know that the scalar product

$$a_\mu b^\mu = g_{\mu\nu} a^\nu b^\mu = a^\mu b_\mu$$

of two four-vectors a_μ and b^μ is invariant under Lorentz transformations and thus the d'Alembertian

$$\Box = \partial^\mu \partial_\mu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$$

is also an invariant scalar.

We consider an electromagnetic field with a scalar potential $\varphi(\mathbf{r}, t)$ and a vector potential $\mathbf{A}(\mathbf{r}, t)$ and combine them into a single four-vector

$$A^\mu = (\varphi, \mathbf{A}) \ .$$

The electric and magnetic fields associated with these four-potentials are

$$\mathbf{E} = -\nabla\varphi - \frac{1}{c}\frac{\partial \mathbf{A}}{\partial t} \quad \text{and} \quad \mathbf{B} = \nabla \times \mathbf{A} \, .$$

Next, we consider a particle with a rest mass m_0 and an electric charge e.
The contravariant four-momentum of a particle with a relativistic energy E and a three-momentum $\mathbf{P} = \gamma m_0 \mathbf{v}$, where $\mathbf{v}$ is the particle's three-velocity and γ the Lorentz factor, is

$$P^\mu = \left(\frac{E}{c}, \mathbf{P}\right) = (\gamma m_0 c, \gamma m_0 \mathbf{v}) \ .$$

The squared length of P^μ is a Lorentz invariant quantity:

$$P_\mu P^\mu = \frac{E^2}{c^2} - \mathbf{P}^2 = \gamma^2 m_0^2 c^2 - \gamma^2 m_0^2 \mathbf{v}^2 = m_0^2 c^2$$

If the particle is exposed to an electromagnetic field with a four-potential A^μ the canonical four-momentum p^μ reads as

$$p^\mu = P^\mu + \frac{e}{c} A^\mu = \left(\frac{E}{c}, \mathbf{p}\right)$$

with

$$E = \gamma m_0 c^2 + e\varphi \quad \text{and} \quad \mathbf{p} = \mathbf{P} + \frac{e}{c}\mathbf{A} \, .$$

In lowest order ($v \ll c$) the energy yields the non-relativistic expression:

$$E = m_0 c^2 + \frac{m_0}{2} v^2 + e\varphi + \mathcal{O}\left(\frac{v^2}{c^2}\right) \ .$$

The dynamics of the classical relativistic mechanics follows from the Hamiltonian

$$\mathcal{H}(\mathbf{r}, \mathbf{p}) = e\varphi + \sqrt{m_0^2 c^4 + c^2 \left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2} \, . \tag{5.12}$$

From Hamilton's equations

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \frac{\partial \mathcal{H}}{\partial \mathbf{p}} \, , \quad \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = -\frac{\partial \mathcal{H}}{\partial \mathbf{r}}$$

one can derive the Lorentz force

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{v} \, , \quad \frac{\mathrm{d}\mathbf{P}}{\mathrm{d}t} = e\left(\mathbf{E} + \frac{\mathbf{v}}{c} \times \mathbf{B}\right) \ .$$

5.3 Klein-Gordon equation

We try to derive a relativistic analogue to the Schrödinger equation.
Correspondence principle reads as

$$E \to \imath\hbar\frac{\partial}{\partial t}\,, \quad \mathbf{p} \to -\imath\hbar\nabla$$

or as a four-vector

$$p^\mu = \left(\frac{E}{c}, \mathbf{p}\right) \to \imath\hbar\left(\frac{\partial}{\partial ct}, -\nabla\right) = \imath\hbar\partial^\mu\,.$$

This leads in case of a non-relativistic free particle with an energy $E = \mathcal{H} = \frac{\mathbf{p}^2}{2m}$ to the Schrödinger equation.

As a first try we apply the correspondence principle to the Hamiltonian (5.12) of a relativistic charged particle in an electromagnetic field and obtain

$$\imath\hbar\frac{\partial}{\partial t}\psi(\mathbf{r},t) = \left[e\varphi + \sqrt{m_0^2c^4 + c^2\left(\frac{\hbar}{\imath}\nabla - \frac{e}{c}\mathbf{A}\right)^2}\,\right]\psi(\mathbf{r},t)\,. \tag{5.13}$$

An expansion in $\frac{1}{c^2}$ leads to

$$\sqrt{m_0^2c^4 + c^2\left(\frac{\hbar}{\imath}\nabla - \frac{e}{c}\mathbf{A}\right)^2} \approx m_0c^2 + \frac{1}{2m_0}\left(\frac{\hbar}{\imath}\nabla - \frac{e}{c}\mathbf{A}\right)^2 + \mathcal{O}\left(\frac{1}{c^4}\right)$$

and the contribution due to the rest energy m_0c^2 vanish using the transformation

$$\psi(\mathbf{r},t) = e^{-\frac{\imath}{\hbar}m_0c^2t}\phi(\mathbf{r},t)\,. \tag{5.14}$$

Thus we end up with a classical Schrödinger equation for ϕ

$$\imath\hbar\frac{\partial}{\partial t}\phi(\mathbf{r},t) = \left[e\varphi + \frac{1}{2m_0}\left(\frac{\hbar}{\imath}\nabla - \frac{e}{c}\mathbf{A}\right)^2\right]\phi(\mathbf{r},t)\,.$$

Problems with the relativistic equation (5.13):

a) The asymmetry of space and time derivatives masks the relativistic invariance.

b) The square root of a differential operator can be defined via a series expansion. This may lead to problems with the convergence. Moreover, in an expansion, arbitrary powers of the differential operator occur. This corresponds to a nonlocal theory since the whole shape of the wave function gets important.

A possible way out is to start with the square of the energy:

$$(E - e\varphi)^2 = m_0^2c^4 + c^2\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2\,. \tag{5.15}$$

As a consequence, two solutions

$$E = e\varphi \pm \sqrt{m_0^2c^4 + c^2\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2}$$

are possible. In particular, a solution with a negative energy exists.

Quantization of Eq. (5.15) gives the Klein-Gordon equation:

$$\boxed{\left[\left(\imath\hbar\frac{\partial}{\partial t}-e\varphi\right)^2-c^2\left(\frac{\hbar}{\imath}\nabla-\frac{e}{c}\mathbf{A}\right)^2\right]\psi(\mathbf{r},t)=m_0^2c^4\psi(\mathbf{r},t)}$$

or using four-vectors

$$\boxed{\left[\left(\partial_\mu+\frac{ie}{\hbar c}A_\mu\right)\left(\partial^\mu+\frac{ie}{\hbar c}A^\mu\right)+\frac{m_0^2c^2}{\hbar^2}\right]\psi(\mathbf{r},t)=\left(D_\mu D^\mu+\frac{m_0^2c^2}{\hbar^2}\right)\psi(\mathbf{r},t)=0} \tag{5.16}$$

The Klein-Gordon equation is relativistically invariant, because the scalar product $D_\mu D^\mu$ is invariant under Lorentz transformations.

The Klein-Gordon equation for a free particle

$$\left(\partial_\mu\partial^\mu+\frac{m_0^2c^2}{\hbar^2}\right)\psi(\mathbf{r},t)=0 \tag{5.17}$$

corresponds to a classical wave equation with an additional mass term.
Their solutions are plane waves

$$\psi(\mathbf{r},t)=\psi_0\exp\left[-\frac{\imath}{\hbar}p_\mu x^\mu\right]=\psi_0\exp\left[-\frac{\imath}{\hbar}\left(Et-\mathbf{p}\cdot\mathbf{r}\right)\right],$$

with a dispersion relation

$$\frac{E^2}{c^2}-\mathbf{p}^2=m_0^2c^2\,.$$

As expected, there are solutions with positive and negative energy

$$E=\pm c\sqrt{m_0^2c^2+\mathbf{p}^2}$$

separated by an energy gap, i.e. states with energies between m_0c^2 and $-m_0c^2$ do not exist. Furthermore, the energy spectrum is not bounded from below, which leads to stability problems. A way out is to interpret states of negative energy as antiparticles.

5.3.1 Continuity equation and interpretation of the wave function

How to interpret the wave functions that evolve according to the Klein-Gordon equation?
The Schrödinger equation obeys a continuity equation

$$\frac{\partial\rho}{\partial t}+\nabla\cdot\mathbf{j}=0\,,$$

where

$$\rho(\mathbf{r},t)=|\psi(\mathbf{r},t)|^2\geq 0 \tag{5.18}$$

can be interpreted as a probability density. The corresponding probability current is given by

$$\mathbf{j}=\frac{\hbar}{2mi}\left(\psi^*\nabla\psi-\psi\nabla\psi^*\right)\,. \tag{5.19}$$

For a relativistic theory we expect a similar continuity equation to hold. Written in a covariant form

$$\partial_\mu j^\mu = 0 \tag{5.20}$$

with a four-current

$$j^\mu = (c\rho, \mathbf{j}) \ .$$

We multiply Eq. (5.17) with ψ^* and subtract the complex conjugate:

$$\begin{aligned} 0 &= \psi^* \left(\partial_\mu \partial^\mu + \frac{m_0^2 c^2}{\hbar^2} \right) \psi - \psi \left(\partial_\mu \partial^\mu + \frac{m_0^2 c^2}{\hbar^2} \right) \psi^* \\ &= \partial_\mu \left(\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^* \right) \ . \end{aligned}$$

Thus the continuity equation (5.20) with the four-current

$$j^\mu = \frac{\imath\hbar}{2m_0} \left(\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^* \right)$$

is fulfilled.
The current-component $\mathbf{j}$ of $j^\mu = (c\rho, \mathbf{j})$,

$$\mathbf{j} = \frac{\hbar}{2m_0 i} \left(\psi^* \nabla \psi - \psi \nabla \psi^* \right) \ ,$$

equals the expression (5.19) of the non-relativistic quantum mechanics.
In contrast to (5.18), the density-component

$$\rho = \frac{\imath\hbar}{2m_0 c^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right)$$

is not positive definite and therefore cannot be interpreted as a probability density. That's because Klein-Gordon equation is second-order in time.

Let's consider the non-relativistic limit. Using the transformation (5.14) one obtains

$$\frac{\partial \psi}{\partial t} \approx -\imath \frac{m_0 c^2}{\hbar} \psi$$

and thus a probability density

$$\rho \approx |\psi|^2 \ .$$

5.3.2 Problems of the Klein-Gordon equation

Problems of the Klein-Gordon (KG) equation:

a) Solutions with negative energy exists and the energy spectrum of free particles is not bounded from below.

b) The wave function ψ cannot be interpreted as a probability amplitude.

c) ψ depends only on $\mathbf{r}$ and t, and it is not possible to incorporate internal degrees of freedom, e.g. a spin.

Problem c) makes a further search for a relativistic equation, that could describe electrons (spin-$\frac{1}{2}$), necessary. At the date of the discovery (1926) the physical relevance of the KG equation was unclear, because at that time only particles with spin-$\frac{1}{2}$ (electrons, protons and neutrons) were known. Later it turned our that KG equation can describe spinless scalar particles, like pions (or pi mesons) discovered in 1947. The fact that KG equation is a field equation for spin-0 particles can be seen from its non-relativistic limit, which is the spinless Schrödinger equation, and from the behavior of the wave function under Lorentz transformations.

With regard to problem b), the question arises: Can we interpret ρ and $\mathbf{j}$ in a different way? Yes, for that we switch to the *charge density*

$$j'^{\mu} = ej^{\mu} = (c\rho', \mathbf{j}') = \frac{ie\hbar}{2m_0}\left(\psi^* \partial^{\mu}\psi - \psi\partial^{\mu}\psi^*\right) , \tag{5.21}$$

where e is an electric charge. ρ' is now a charge density and can have either positive or negative values. $\mathbf{j}'$ is the corresponding current density. Below we will see that this interpretation of j^{μ} is compatible with the interpretation of states with $E < 0$ as antiparticles.

We illustrate this with the free particle. Inserting an ansatz

$$\psi = A \exp\left[\frac{\imath}{\hbar}\left(\mathbf{p}\cdot\mathbf{r} - Et\right)\right]$$

into KG equation leads to the condition

$$E^2 = c^2\left(\mathbf{p}^2 + m_0^2 c^2\right)$$

and thus to two solutions

$$\psi_{\pm} = A_{\pm} \exp\left[\frac{\imath}{\hbar}\left(\mathbf{p}\cdot\mathbf{r} \mp E_p t\right)\right] ,$$

with energies

$$E_p = c\sqrt{\mathbf{p}^2 + m_0^2 c^2} .$$

The corresponding charge density (5.21) reads as

$$\rho'_{\pm} = \pm\frac{eE_p}{m_0 c^2}\left|\psi_{\pm}\right|^2 .$$

This suggests the following interpretation of ψ: ψ_+ describes a particle with charge $+e$ and ψ_- a particle with the same mass m_0, however, with an opposite charge $-e$.

In order to obtain a normalized wave function we consider a particle in a box with an edge length L. From periodic boundary conditions we get

$$\psi_{\pm}^{(n)} = A_{\pm}^{(n)} \exp\left[\frac{\imath}{\hbar}\left(\mathbf{p}_n\cdot\mathbf{r} \mp E_n t\right)\right]$$

with the momentum

$$\mathbf{p}_n = \frac{2\pi}{L}\mathbf{n} \quad \text{with} \quad \mathbf{n} = (n_x, n_y, n_z) \in \mathbb{N}^3$$

and the corresponding energy $E_n = E_{p_n}$.

The normalization condition

$$\pm e = \int_{L^3} \mathrm{d}r^3 \, \rho'_\pm(\mathbf{r}) = \pm \frac{eE_n}{m_0 c^2} \left| A_\pm^{(n)} \right|^2 L^3$$

yields the normalized wave function

$$\psi_\pm^{(n)} = \sqrt{\frac{m_0 c^2}{E_n L^3}} \exp\left[\frac{\imath}{\hbar} \left(\mathbf{p}_n \cdot \mathbf{r} \mp E_n t \right) \right].$$

Both solutions have the same normalization constant and they differ only in the time factor $\exp\left(\mp \frac{\imath}{\hbar} E_n t\right)$. Thus the general solution for positive and negative spin-0 particles, respectively, reads as

$$\begin{aligned} \psi_+ &= \sum_n A_n \psi_+^{(n)} = \sum_n A_n \sqrt{\frac{m_0 c^2}{E_n L^3}} \exp\left[\frac{\imath}{\hbar} \left(\mathbf{p}_n \cdot \mathbf{r} - E_n t \right) \right] \\ \psi_- &= \sum_n B_n \psi_-^{(n)} = \sum_n B_n \sqrt{\frac{m_0 c^2}{E_n L^3}} \exp\left[\frac{\imath}{\hbar} \left(\mathbf{p}_n \cdot \mathbf{r} + E_n t \right) \right]. \end{aligned}$$

Is it possible to describe a neutral particle? From

$$\rho' = \frac{ie\hbar}{2m_0 c^2} \left(\psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) = -\frac{e\hbar}{m_0 c^2} \operatorname{Im} \left(\psi^* \frac{\partial \psi}{\partial t} \right) \tag{5.22}$$

it follows that ψ must be real in this case. Thus we obtain the general wave function of a neutral particle as

$$\begin{aligned} \psi_0^{(n)} &= \frac{1}{\sqrt{2}} \left[\psi_+^{(n)} \left(\mathbf{p}_n \right) + \psi_-^{(n)} \left(-\mathbf{p}_n \right) \right] \\ &= \sqrt{\frac{m_0 c^2}{E_n L^3}} \, 2 \cos \left(\frac{\mathbf{p}_n \cdot \mathbf{r} - E_n t}{\hbar} \right). \end{aligned}$$

Note that $\psi_-^{(n)}$ contributes with an opposite momentum $-\mathbf{p}_n$, therefore $\left(\psi_0^{(n)} \right)^* = \psi_0^{(n)}$ and the charge density (5.22) vanishes, i.e. $\rho' = 0$. However, the current density also disappears, $\mathbf{j}' = 0$, and the continuity equation becomes a trivial identity.

In summary, for the relativistic motion of a free spinless particle there are three solutions of the Klein Gordon equation corresponding to the electric charges $(+, -, 0)$ at each momentum $\mathbf{p}$. Moreover, wave functions ψ and ψ^* describe opposite charges.

Chapter 6

The Dirac equation

6.1 The Dirac equation

The Dirac equation, in contrast to the Klein-Gordon equation, is of first order and only valid in the case of spin-$\frac{1}{2}$ particles. Due to the fact that the Klein-Gordon equation (KGE) expresses nothing more than the relativistic relation between energy, momentum and mass, it must be valid for particles of arbitrary spin.

The Dirac equation has a completely different origin and can be derived from the transformation properties of a spinor under the Lorentz group. We will address this later on – first we want to understand Dirac's original line of thinking.

The KGE suffers from two flaws: The probability density is not positive definite and states with an negative energy appear. For these reasons, the KGE was (historically) initially discarded and Dirac was looking for a replacement of it, namely a relativistic invariant equation of a field function $\psi(x)$, which should describe free electrons.

In the case of *non*-relativistic electrons, Pauli (1927) found the correct description: Within the framework of the Schrödinger picture, an non-relativistic electron is described by a wave function with two components:

$$\psi(\mathbf{x},t) = \begin{pmatrix} \psi_1(\mathbf{x},t) \\ \psi_2(\mathbf{x},t) \end{pmatrix} .$$

Here $|\psi_i(\mathbf{x},t)|^2\, d\mathbf{x}$, $(i = 1,2)$ are the probability densities of finding the electron with a spin in positive $(i = 1)$ or negative $(i = 2)$ 2-direction within the volume element $d\mathbf{x}$ around the position $\mathbf{x}$.

Total angular momentum operator:

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \frac{\hbar}{2}\boldsymbol{\sigma} ,$$

where

$$\hat{\mathbf{L}} = \mathbf{x} \times \frac{\hbar}{\imath}\nabla$$

and

$$\underbrace{\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -\imath \\ \imath & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}_{\text{Pauli spin-matrices}}$$

$\psi(\mathbf{x}, t)$ (respectively every component of it) should satisfy the Schrödinger equation

$$\imath\hbar\frac{\partial}{\partial t}\psi(\mathbf{x}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\mathbf{x}, t)$$

This equation is certainly **not** relativistic invariant, because only one temporal but two spatial derivations appear.

For reasons which would not seem mandatory today, Dirac was looking for a field equation that would be linear in temporal and spatial derivations. We will view this as a heuristic principle and make the general linear ansatz

$$\boxed{(\imath\hbar\gamma^\mu\partial_\mu - a)\,\psi(x) = 0\,,} \tag{6.1}$$

where the number of components of ψ, the nature of the coefficients γ^μ and the constant a are still completely undefined.

Applying the operator $(\imath\hbar\gamma^\mu\partial_\mu)$ again to (6.1) gives

$$\begin{aligned} &\Big[-\hbar^2(\gamma^\mu\partial_\mu)(\gamma^\nu\partial_\nu) - \imath\hbar(\gamma^\mu\partial_\mu)a\Big]\psi = 0 \\ \text{resp.}\qquad &\Big(-\hbar^2\gamma^\mu\gamma^\nu\partial_\mu\partial_\nu + a^2\Big)\psi = 0 \end{aligned}$$

Because of $\partial_\mu\partial_\nu = \partial_\nu\partial_\mu$ one can replace $\gamma^\mu\gamma^\nu$ with the symmetric combination

$$\frac{1}{2}\Big(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu\Big) =: \frac{1}{2}\Big\{\gamma^\mu, \gamma^\nu\Big\}$$

and arrives at

$$\boxed{\left(\frac{1}{2}\Big\{\gamma^\mu, \gamma^\nu\Big\}\partial_\mu\partial_\nu + \frac{a^2}{\hbar^2}\right)\psi = 0} \tag{6.2}$$

On the other hand the principle of relativity demands that the energy-momentum-mass relation is satisfied, i.e. that every component of ψ satisfies the KGE

$$\left(\Box + \frac{m^2c^2}{\hbar^2}\right)\psi(x) = 0$$

From this we derive that $a = mc$ and that the coefficient of $\partial_\mu\partial_\nu$ in (6.2) has to be $g^{\mu\nu}$

$$\boxed{a = mc \quad \text{and} \quad \Big\{\gamma^\mu, \gamma^\nu\Big\} = 2g^{\mu\nu}} \tag{6.3}$$

This relation must be satisfied for the coefficients.
With $\mu = \nu = 0$, $\mu = \nu = i$ and $\mu \neq \nu$ follows successively

$$\Big(\gamma^0\Big)^2 = 1\,, \qquad \Big(\gamma^i\Big)^2 = -1\,, \qquad \gamma^\mu\gamma^\nu = -\gamma^\nu\gamma^\mu \quad (\mu \neq \nu)\,.$$

These conditions can neither be satisfies by complex numbers nor 2×2-matrices as a choice for γ^μ. However it is possible with 4×4-matrices, e.g.:

$$\gamma^0 = \left(\begin{array}{c|c} +\mathbb{1} & 0 \\ \hline 0 & -\mathbb{1} \end{array}\right); \quad \gamma^j = \left(\begin{array}{c|c} 0 & +\sigma^j \\ \hline -\sigma^j & 0 \end{array}\right), \quad j = 1, 2, 3\,.$$

Obviously this is not the only possible choice: $\gamma'^\mu = \mathbf{S}\gamma^\mu\mathbf{S}^{-1}$ with an arbitrary unitary 4×4-matrix $\mathbf{S}$ will also satisfy (6.2). The Dirac equation is then satisfied with $\psi' = \mathbf{S}\psi$.

The 1928 postulated equation of Dirac was

$$\boxed{\Big(\imath\hbar\gamma^\mu\partial_\mu - mc\Big)\psi(x) = 0\,,} \tag{6.4}$$

with

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \\ \psi_4(x) \end{pmatrix},$$

where $\psi(x)$ is a 4-component field function, a so called *Dirac spinor*.

Our goal now is to construct a (probability-)current $\jmath^\mu$ (like in the KGE case) and check if the density is positive. Proceeding from the Dirac equation

$$\Big(\imath\hbar\gamma^0\partial_0 + \imath\hbar\gamma^j\partial_j - mc\Big)\psi = 0\,, \tag{6.4}$$

we will consider now the adjoint (or Hermitian transpose) of the Dirac equation (6.4), given by a complex conjugation and subsequent transposition. This gives:

$$-\imath\hbar\partial_\mu\psi^\dagger\gamma^{\mu\dagger} - mc\psi^\dagger = 0\,, \tag{6.5}$$

where

$$\gamma^{\mu\dagger} = \begin{cases} \gamma^0, & \mu = 0 \\ -\gamma^\mu, & \mu = 1, 2, 3 \end{cases}$$

Definition: $\bar\psi = \psi^\dagger\gamma^0$ represents the **adjoint spinor** of ψ and with this, the current density and other quantities can be written in a more compact form.
Now, from (6.5), we have

$$-\imath\hbar\partial_0\psi^\dagger\gamma^0 + \imath\hbar\partial_j\psi^\dagger\gamma^j - mc\psi^\dagger = 0\,,$$

Multiplying from the right with γ_0 (and using $\gamma^j\gamma^0 = -\gamma^0\gamma^j$) leads to

$$\begin{aligned} -\imath\hbar(\partial_0\psi^\dagger\gamma^0)\gamma^0 - \imath\hbar\partial_j\psi^\dagger\gamma^0\gamma^j - mc\psi^\dagger\gamma^0 = 0 \\ \Longrightarrow \boxed{+\imath\hbar(\partial_\mu\bar\psi)\gamma^\mu + mc\bar\psi = 0} \end{aligned} \tag{6.6}$$

With (6.6) and the Dirac equation (6.4) one can show now that the **4-current density**

$$\boxed{\jmath^\mu := c\bar{\psi}\gamma^\mu\psi}$$

is conserved:

$$\begin{aligned}\frac{1}{c}\partial_\mu \jmath^\mu &= \left(\partial_\mu\bar{\psi}\right)\gamma^\mu\psi + \bar{\psi}\gamma^\mu\left(\partial_\mu\psi\right)\\ &= -\frac{mc}{\imath\hbar}\bar{\psi}\,\psi + \bar{\psi}\,\frac{mc}{\imath\hbar}\psi \\ &= 0\end{aligned} \tag{6.7}$$

$$\Rightarrow \quad \partial_0 \jmath^0 = \nabla\cdot\boldsymbol{\jmath}\,, \quad \text{continuity equation.} \tag{6.8}$$

Now, writing out the left hand term of the above equation explicitly, we have

$$\frac{1}{c}\frac{\partial}{\partial t}\left(c\psi^\dagger\gamma^0\gamma^0\psi\right) = \frac{\partial}{\partial t}\left(\psi^\dagger\psi\right)\,,$$

and because

$$\boxed{\rho := \frac{1}{c}\jmath^0 = \psi^\dagger\psi = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2} \tag{6.9}$$

is *positive*, ρ can serve as probability density for the particles described by the Dirac equation. This brings the continuity equation (6.8) to the form

$$\boxed{\frac{\partial}{\partial t}\rho = \nabla\cdot\boldsymbol{\jmath}\,,} \tag{6.10}$$

with the current density

$$\boxed{\boldsymbol{\jmath} = c\bar{\psi}\boldsymbol{\gamma}\psi} = c\psi^\dagger\underbrace{\gamma^0\boldsymbol{\gamma}}_{=:\boldsymbol{\alpha}}\psi = c\psi^\dagger\boldsymbol{\alpha}\psi\,,$$

where $\boldsymbol{\alpha} := \gamma^0\boldsymbol{\gamma}$.

Each component of ψ satisfies the Klein–Gordon Equation. Multiplying the Dirac Equation (6.4) by $\imath\hbar\gamma^\nu\partial_\nu$ from the left:

$$\begin{aligned}-\hbar^2\gamma^\nu\partial_\nu\gamma^\mu\partial_\mu\psi - \underbrace{\imath\hbar mc\gamma^\nu\partial_\nu\psi}_{=m^2c^2\psi \text{ Dirac eq.}} &= 0\\ \Rightarrow -\hbar^2\underbrace{\frac{1}{2}\left(\gamma^\nu\gamma^\mu + \gamma^\mu\gamma^\nu\right)}_{g^{\mu\nu}}\partial_\nu\partial_\mu\psi &= m^2c^2\psi\end{aligned}$$

$$\Rightarrow \boxed{\underbrace{\partial_\mu\partial^\mu}_{\frac{1}{c^2}\partial_0^2-\nabla^2}\psi + \frac{m^2c^2}{\hbar^2}\psi = 0} \tag{6.11}$$

We will solve this with the **Ansatz:**

$$\psi = Ae^{-\imath(\omega t - \mathbf{k}\cdot\mathbf{x})}\,.$$

After applying Eq. (6.11), we get

$$\begin{aligned} -\frac{\omega^2}{c^2} + k^2 + \frac{m^2c^2}{\hbar^2} &= 0 \\ \Rightarrow \quad (\hbar\omega)^2 &= c^2(\hbar k)^2 + m^2c^4 \\ \text{or,} \qquad E^2 &= c^2p^2 + m^2c^4 \end{aligned}$$

Special case:
Particle at rest, $\mathbf{p} = 0$ and $\psi = Ae^{-\frac{\imath}{\hbar}Et}$. Then,

$$\begin{aligned} \imath\hbar\gamma^0\frac{1}{c}\partial_0\psi = \gamma^0\frac{E}{c}\psi &\overset{!}{=} mc\psi \\ \text{or,} \qquad E\gamma^0 A &= mc^2 A \\ \text{or,} \qquad E &= \pm mc^2 \end{aligned}$$

The eigenvalues of γ^0 are $+1$ (doubly degenerated) and -1 (doubly degenerated), therefore there exist two solutions with positive energy $+mc^2$ and two solutions with negative energy $-mc^2$. Actually it is easy to see (by writing out the four components of the Dirac equation in full), that the eigenvalues are given by

$$E = +\left(m^2c^2 + p^2\right)^{1/2} \qquad \text{(2 times)}$$
$$E = -\left(m^2c^2 + p^2\right)^{1/2} \qquad \text{(2 times)}$$

For every p exist two solutions with $E > 0$, corresponding to the two states of a spin-$\frac{1}{2}$ particle, and two solutions with $E < 0$.
An electron in a state with $E > 0$ can therefore (by interacting with other particles or fields) jump in a state with $E < 0$ and then cascade downwards to $E = -\infty$ while emitting an infinite amount of radiation.

Dirac's solution of this problem: The electrons possess spin-$\frac{1}{2}$, therefore they satisfy the Pauli exclusion principle. Dirac assumed, that states with negative energy are already completely occupied, the Pauli principle prohibits that further electrons fall in the *sea* with $E < 0$.

Remark:
This "Dirac sea" is the **vacuum**. The vacuum is therefore by no means "empty". Important postulate of this theory: **antiparticles**.

Assuming there exists a vacancy ("blank position") within the electron sea – a "hole" with energy $-|E|$.
Then an electron with energy E is able to fill this hole by emitting the energy $2E$ and only leaving a vacuum :

$$\mathrm{e}^- + \text{hole} \rightarrow \text{energy}$$

Thus the "hole" possesses an effective charge $+e$ and a positive energy. Dirac's theory postulated the existence of **antiparticles** for all particles with spin-$\frac{1}{2}$, and over time e^+, $\bar{p}$, $\bar{n}$, $\bar{\gamma}$ and others were all found. It became apparent that bosons also possess antiparticles (see quantized complex Klein-Gordon field).

Remark:
Despite the successful resolution of the negative energy problem, the Dirac equation does *no longer represent a single particle equation*! It describes particles and antiparticles. The only consistent philosophy is to treat the spinor ψ as a **field** and $|\psi|^2$ as a measure of the amount of particles present at a certain point. This field is naturally a quantum field.

6.2 Solution of the Dirac equation

We choose plane waves as an ansatz for a solution:

$$\psi(x) = e^{-\frac{\imath}{\hbar}px}\, u(p) = e^{-\frac{\imath}{\hbar}(p_0 t - \mathbf{p}\cdot\mathbf{x})}\, u(p)\,.$$

Furthermore $\psi(x)$ must satisfy the KGE, which demands $p_0 = E/c = \sqrt{\mathbf{p}^2 + m^2c^2}$ and $\mathbf{p} = (p_x,\, p_y,\, p_z)^{\mathrm{T}}$. Therefore, from Dirac Equation (6.4), we get,

$$\Big(\imath\hbar\gamma^\mu\Big(-\frac{\imath}{\hbar}\Big)p_\mu - mc\Big)\, u(p) = 0$$

$$\Rightarrow \boxed{(\gamma^\mu p_\mu - mc)\, u(p) = 0\,,} \tag{6.12}$$

where $u(p)$ is a spinor to be determined.

First we want to consider the case $\mathbf{p} = 0$, i.e. a particle at rest where $p = (\underbrace{E/c}_{p_0}, 0, 0, 0)^{\mathrm{T}} =: p_{\mathrm{R}}$, with $p_0 = E/c = mc$ or $E = mc^2$ respectively. Calculating the zeroth component from Eq. (6.12), we obtain

$$(\gamma^0 p_0 - mc)u = 0$$

or written out in matrix form

$$\begin{pmatrix} p_0 - mc & & & \\ & p_0 - mc & & \\ & & -p_0 - mc & \\ & & & -p_0 - mc \end{pmatrix} u = \begin{pmatrix} 0 & & & \\ & 0 & & \\ & & -2mc & \\ & & & -2mc \end{pmatrix} u = 0\,.$$

Therefore $(\gamma^0 p_0 - mc)u_s(p_{\mathrm{R}}) = 0$ has two linear independent solutions

$$u_s(p_{\mathrm{R}}) = \begin{pmatrix} \chi_s \\ 0 \end{pmatrix}\,,$$

where $s = \pm\frac{1}{2}$ and

$$\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

are two-spinors.

Now we want to consider $\mathbf{p} \neq 0$. We combine the two upper as well as the two lower components of the Dirac spinor to a two-spinor respectively. For an arbitrary four-vector we make the ansatz

$$u(p) = \begin{pmatrix} \xi \\ \eta \end{pmatrix} ,$$

where ξ and η represent the aforementioned two-spinors. Let us also take, $\psi(x) = u(p)e^{-\frac{i}{\hbar}p^\mu x_\mu} = u(p)e^{-\frac{i}{\hbar}(Et-\mathbf{p}\cdot\mathbf{r})}$.
From the Dirac equation (6.12) follows

$$\left(\begin{array}{c|c} p_0 - mc & -\mathbf{p}\cdot\boldsymbol{\sigma} \\ \hline +\mathbf{p}\cdot\boldsymbol{\sigma} & -p_0 - mc \end{array}\right) \begin{pmatrix} \xi \\ \eta \end{pmatrix} = 0 \,,$$

where we used the definition of the Dirac matrices

$$\gamma_0 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} , \qquad \gamma_i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}$$

and defined

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma^1 \\ \sigma^2 \\ \sigma^3 \end{pmatrix}$$

as a vector with 2×2-matrices as entries. From the above equation, we get:

$$\begin{aligned} (p_0 - mc)\,\xi - (\mathbf{p}\cdot\boldsymbol{\sigma})\,\eta &= 0 \qquad\qquad \text{(a)} \\ (\mathbf{p}\cdot\boldsymbol{\sigma})\,\xi - (p_0 + mc)\,\eta &= 0 \qquad\qquad \text{(b)} \end{aligned}$$

Rearranging of (b) gives us:

$$\eta = \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{p_0 + mc}\xi \,.$$

Substituting the above expression of η in (a):

$$\left(p_0 - mc - \frac{(\mathbf{p}\cdot\boldsymbol{\sigma})^2}{p^0 + mc} \right) \xi = 0 \,. \tag{6.13}$$

The appearing numerator results in

$$\begin{aligned} (\mathbf{p}\cdot\boldsymbol{\sigma})^2 &= (p^1\,\sigma^1)^2 + (p^2\,\sigma^2)^2 + (p^3\,\sigma^3)^2 \\ &\quad + p^1p^2\,\underbrace{(\sigma^1\sigma^2 + \sigma^2\sigma^1)}_{=0} + p^1p^3\,\underbrace{(\sigma^1\sigma^3 + \sigma^3\sigma^1)}_{=0} + p^2p^3\,\underbrace{(\sigma^2\sigma^3 + \sigma^3\sigma^2)}_{=0} \\ &= \mathbf{p}^2 \end{aligned}$$

where we used $\{\sigma^i, \sigma^j\} = 2\delta_{i,j}$ and $(\sigma^i)^2 = 1$. Therefore, from (6.13), we get

$$\frac{(p_0)^2 - m^2c^2 - \mathbf{p}^2}{(p_0 + mc)}\xi = 0 \,.$$

Since $(p_0)^2 = (p^0)^2 = \frac{E^2}{c^2} = \mathbf{p}^2 + m^2c^2$, ξ is arbitrary and we choose $\xi = \chi_s$ and find for u_s:

$$u_s(p) = \mathcal{N} \begin{pmatrix} \chi_s \\ \dfrac{\mathbf{p}\cdot\boldsymbol{\sigma}}{p_0 + mc}\,\chi_s \end{pmatrix} ,$$

where $\mathcal{N}$ handles the normalization. To determine it, we need the conjugated spinor $\bar{u}_s(p)$ given by

$$\bar{u}_s(p) = u^\dagger(p)\gamma^0 = \mathcal{N}\left(\chi_s^\dagger\,, \quad \frac{-\mathbf{p}\cdot\boldsymbol{\sigma}}{p_0 + mc}\,\chi_s^\dagger\right) .$$

Then,

$$\bar{u}_r(p)u_r(p) = \mathcal{N}^2\left(1 - \frac{(\mathbf{p}\cdot\boldsymbol{\sigma})^2}{(p_0 + mc)^2}\right) , \tag{6.14}$$

where we write the numerator as

$$\begin{aligned}(\mathbf{p}\cdot\boldsymbol{\sigma})^2 = \mathbf{p}^2 &= \frac{E^2}{c^2} - m^2c^2 \\ &= p_0^2 - m^2c^2 \\ &= (p_0 + mc)(p_0 - mc)\,.\end{aligned}$$

Now, from (6.14), we calculate further

$$\begin{aligned}\bar{u}_r(p)u_r(p) &= \mathcal{N}^2\left(1 - \frac{(p_0 + mc)(p_0 - mc)}{(p_0 + mc)^2}\right) \\ &= \mathcal{N}^2\frac{p_0 + mc - p_0 + mc}{p_0 + mc} \\ &= \mathcal{N}^2\frac{2mc}{p_0 + mc} \\ &\overset{!}{=} 1\,,\end{aligned}$$

what results in a normalization constant

$$\mathcal{N} = \sqrt{\frac{p_0 + mc}{2mc}} = \sqrt{\frac{E + mc^2}{2mc^2}}\,. \tag{6.15}$$

For different indices we find using (6.15)

$$\begin{aligned}\bar{u}_r(p)u_s(p) &= \mathcal{N}^2\left(\underbrace{\chi_r^\mathrm{T}\chi_s}_{\delta_{rs}} - \frac{\mathbf{p}^2}{(p_0 + mc)^2}\underbrace{\chi_r^\mathrm{T}\chi_s}_{\delta_{rs}}\right) \\ &= \mathcal{N}^2\left(1 - \frac{(p_0 + mc)(p_0 - mc)}{(p_0 + mc)^2}\right)\delta_{rs} \\ &= \delta_{rs}\,. \end{aligned} \tag{6.16}$$

Analogously, for the solutions with negative energies, we choose the ansatz $\psi(x) = e^{+\frac{i}{\hbar}px}\,v(p)$, where $v(p)$ is again a spinor to be determined.

Substitution in the Dirac equation (6.4) gives:

$$\left(\imath\hbar\gamma^\mu\left(+\frac{\imath}{\hbar}\right)p_\mu - mc\right)\,v(p) = 0$$

$$\Rightarrow \boxed{(\gamma^\mu p_\mu + mc)\,v(p) = 0\,.} \tag{6.17}$$

For a particle at rest, $\mathbf{p} = 0$, we have

$$\left(\gamma^0 p_0 + mc\right)\,v(p_R) = 0$$

and with $p_0 = mc$

$$\gamma^0 p_0 + mc = \begin{pmatrix} p_0+mc & & & \\ & p_0+mc & & \\ & & -p_0+mc & \\ & & & -p_0+mc \end{pmatrix} = \begin{pmatrix} 2mc & & & \\ & 2mc & & \\ & & 0 & \\ & & & 0 \end{pmatrix}.$$

We therefore choose

$$v_s(p_R) = \begin{pmatrix} 0 \\ \chi_s \end{pmatrix}.$$

For arbitrary and finite $\mathbf{p} \neq 0$, we take $\psi(x) = e^{+\frac{\imath}{\hbar}p^\mu x_\mu}\,v(p)$, with $v(p) = \begin{pmatrix} \xi \\ \eta \end{pmatrix}$.
From the Dirac equation (6.4), we get

$$\left(\begin{array}{c|c} p_0+mc & -\mathbf{p}\cdot\boldsymbol{\sigma} \\ \hline +\mathbf{p}\cdot\boldsymbol{\sigma} & -p_0+mc \end{array}\right)\begin{pmatrix} \xi \\ \eta \end{pmatrix} = 0\,,$$

and arrive at the two equations:

$$\begin{aligned} (p_0+mc)\,\xi - (\mathbf{p}\cdot\boldsymbol{\sigma})\,\eta &= 0 && \text{(c)} \\ (\mathbf{p}\cdot\boldsymbol{\sigma})\,\xi - (p_0-mc)\,\eta &= 0 && \text{(d)} \end{aligned}$$

From (c) follows $\xi = \frac{\mathbf{p}\cdot\boldsymbol{\sigma}}{p^0+mc}\,\eta$, what substituted in (d) gives:

$$\underbrace{\left(\frac{(\mathbf{p}\cdot\boldsymbol{\sigma})^2}{p^0+mc} - (p^0-mc)\right)}_{=0,\text{ as before}}\eta = 0\,.$$

Therefore, η is arbitrary. We again choose two linear independent solutions $\forall\,p$ and in summary find the two spinors:

$$\boxed{u_s(p) = \sqrt{\frac{p_0+mc}{2mc}}\begin{pmatrix} \chi_s \\ \dfrac{\mathbf{p}\cdot\boldsymbol{\sigma}}{p_0+mc}\chi_s \end{pmatrix}, \qquad v_s(p) = \sqrt{\frac{p_0+mc}{2mc}}\begin{pmatrix} \dfrac{\mathbf{p}\cdot\boldsymbol{\sigma}}{p_0+mc}\chi_s \\ \chi_s \end{pmatrix}}$$

We have following orthogonality relations for the above determined solutions:

$$\begin{aligned}\bar{u}_r(p)u_s(p) &= \delta_{rs}\\ \bar{v}_r(p)v_s(p) &= -\delta_{rs}\\ \bar{u}_r(p)v_s(p) &= 0\\ \bar{v}_r(p)u_s(p) &= 0\,.\end{aligned}$$

Remarks:

a) This normalization is invariant under orthochronous Lorentz transformations. *Proof:* see next section in “Transformations of bilinear forms”.

b) The density $\rho = j^0 = c\bar{\psi}\gamma^0\psi$ is **not** Lorentz invariant since it is the zeroth component of a 4-vector:
E.g. for $\psi_{r,s} = e^{\imath kx}\, u_{r,s}$ one has

$$\begin{aligned}\bar{\psi}_r\gamma^0\psi_s &= \bar{u}_r(k)\gamma^0 u_s(k)\\ &= u_r^\dagger(k)\gamma^0\gamma^0 u_s(k)\\ &= u_r^\dagger u_s(k)\\ &= \frac{p_0+mc}{2mc}\left(\frac{\mathbf{p}^2}{(p_0+mc)^2}+1\right)\delta_{r,s}\\ &= \frac{p_0}{m}\delta_{r,s}\end{aligned}$$

(Note that $\mathbf{p}^2 = p_0^2 - m^2c^2 = (p_0+mc)(p_0-mc)$.) This is plausible since the spinors are normalized such that the density is one in the rest system of the particles. For a Lorentz transformation the product of density times volume must stay constant. Since the volume is reduced by a factor $\gamma = \sqrt{1-(v/c)^2}$ (note that only lengths parallel to the velocity vector are contracted) the density must be increased by a factor $1/\gamma = E/mc^2$ (note that $E = \gamma mc^2$, where m the rest mass of the particle).
Analogously for states with negative energy, $\psi_{r,s} = e^{+\imath kx}\, v_{r,s}$.

Due to the linearity of the Dirac equation, the **general solution** is given by a superposition in the form of a Fourier integral:

$$\boxed{\psi(x) = \int \frac{d\mathbf{p}}{(2\pi)^3} \sum_{s=\pm\frac{1}{2}} \left\{ e^{\frac{\imath}{\hbar}px} v_s(p)\beta_s^*(\mathbf{p}) + e^{-\frac{\imath}{\hbar}px} u_s(p)\alpha_s(\mathbf{p}) \right\}}$$

Here $\alpha_s(\mathbf{p})$ and $\beta_s^*(\mathbf{p})$ represent two arbitrary complex valued functions.

6.3 Non-relativistic limiting case and the magnetic moment of the electron

Particles with a spin possess an “inner” magnetic moment. A charge e, which is moving on an closed circular orbit, interacts with a magnetic field and possesses an effective magnetic moment,

$$\boldsymbol{\mu} = \frac{e}{2m}\mathbf{L}\,.$$

Would nature be "simple", the proportionality between electron spin $\mathbf{S} = \frac{1}{2}\hbar\boldsymbol{\sigma}$ and it's magnetic moment $e/2m$ would be such, that the inner magnetic moment would assume the value $(e/2m) \cdot |\mathbf{S}| = e\hbar/4m$.

The resulting shift in frequencies of the spectral lines would correspond to the "normal" Zeeman effect. However experiments show an "anomalous" Zeeman effect – the proportionality constant is *2 times* the one of the circular orbit motion, i.e. the magnetic moment of the electron is $-\boldsymbol{\mu}$ where

$$\boldsymbol{\mu} = 2\frac{e}{2m}\mathbf{S} = \frac{e}{m}\mathbf{S} = \frac{e\hbar}{2m}\boldsymbol{\sigma}$$

The factor 2 is often called *Landé factor*, $g_s = 2$. This is an immediate result of the Dirac equation. To derive this we have to consider the equation in the case of an electron in presence of an electromagnetic field.

6.3.1 Dirac equation with electromagnetic field

We use the scheme of "**minimal coupling**" (The reason will later on become clear when looking at gauge theories, but is in this case analogous to classical mechanics and electrodynamics):

$$\begin{aligned} \mathbf{p} \to \mathbf{p} - \frac{e}{c}\mathbf{A} \quad &\text{or} \quad -\imath\hbar\frac{\partial}{\partial x^i} \to -\imath\hbar\frac{\partial}{\partial x^i} - \frac{e}{c}A^i \\ E \to E + e\phi \quad &\text{or} \quad \imath\hbar\frac{\partial}{\partial t} \to \imath\hbar\frac{\partial}{\partial t} + e\phi\,. \end{aligned}$$

Using the co- and contravariant definitions of the momentum operator,

$$p_\mu = \imath\hbar\partial_\mu \qquad\qquad p^\mu = \imath\hbar\partial^\mu\,,$$

where $\partial_\mu = \frac{\partial}{\partial x^\mu}$ or $\partial^\mu = \frac{\partial}{\partial x_\mu}$, we have as temporal and spatial components:

$$p^0 = p_0 = \imath\hbar\frac{\partial}{\partial\, ct} \qquad p^i = -p_i = \imath\hbar\frac{\partial}{\partial x_i} = -\imath\hbar\frac{\partial}{\partial x^i}$$

In this formulation, the minimal coupling scheme becomes

$$p_\mu \to p_\mu - \frac{e}{c}A_\mu\,,$$

where $A_\mu = (\phi, -\mathbf{A})$ the (covariant) four-vectorpotential – with ϕ the electric potential and $\mathbf{A}$ the usual vector potential. Expressed as derivations we find:

$$\imath\hbar\partial_\mu = \left(\imath\hbar\frac{\partial}{\partial(ct)}, \imath\hbar\nabla\right) \longrightarrow \left(\underbrace{\imath\hbar\frac{\partial}{\partial(ct)} - \frac{e}{c}\phi}_{\frac{1}{c}\left(\imath\hbar\frac{\partial}{\partial t} - e\phi\right)}, \imath\hbar\boldsymbol{\nabla} - \frac{e}{c}\mathbf{A}\right)$$

Therefore, the Dirac equation under minimal coupling becomes

$$\imath\hbar\gamma^\mu\partial_\mu\psi - mc\psi = 0 \longrightarrow \boxed{\gamma^\mu\left(\imath\hbar\partial_\mu - \frac{e}{c}A_\mu\right)\psi - mc\psi = 0} \tag{6.18}$$

We then get:

$$\left\{\gamma^0\left(\imath\hbar\frac{\partial}{\partial(ct)}-\frac{e}{c}\phi\right)\psi+\gamma^i(p_i-\frac{e}{c}A_i)-mc\right\}\psi=0$$

$$\Rightarrow\ \imath\hbar\frac{\partial\psi}{\partial t}=\left\{c\underbrace{\gamma^0\gamma^i}_{=:\alpha^i}\left(\underbrace{(-p_i)}_{=p^i}-\frac{e}{c}\underbrace{(-A_i)}_{=A^i}\right)+\underbrace{\gamma^0}_{=:\beta}mc^2+e\phi\right\}\psi$$

$$\Rightarrow\ \boxed{\imath\hbar\frac{\partial\psi}{\partial t}=\underbrace{\left\{c\boldsymbol{\alpha}\cdot\left(\mathbf{p}-\frac{e}{c}\mathbf{A}\right)+\beta mc^2+e\phi\right\}}_{=:H_{\text{Dirac}}\text{ (Dirac Hamiltonian)}}\psi=0\,,} \tag{6.19}$$

where the introduced matrices are defined as

$$\beta=\begin{pmatrix}\mathbb{1}&0\\0&-\mathbb{1}\end{pmatrix},\qquad\alpha^i=\begin{pmatrix}0&\sigma^i\\\sigma^i&0\end{pmatrix}\quad\text{and}\quad\boldsymbol{\alpha}=\begin{pmatrix}\alpha^1\\\alpha^2\\\alpha^3\end{pmatrix}.$$

6.3.2 Non-relativistic limit

In a first step, we partition the 4-spinor ψ into two 2-spinors $\tilde{\varphi}$ and $\tilde{\chi}$:

$$\psi=\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix}$$

Using this in (6.19) we get

$$\imath\hbar\frac{\partial}{\partial t}\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix}=c\begin{pmatrix}0&\boldsymbol{\sigma}\\\boldsymbol{\sigma}&0\end{pmatrix}\cdot\underbrace{(\mathbf{p}-\frac{e}{c}\mathbf{A})}_{\boldsymbol{\pi}}\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix}+mc^2\begin{pmatrix}\mathbb{1}&0\\0&-\mathbb{1}\end{pmatrix}\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix}+e\phi\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix}$$

$$\Longrightarrow\ \imath\hbar\frac{\partial}{\partial t}\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix}=c\begin{pmatrix}\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\tilde{\chi}\\\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\tilde{\varphi}\end{pmatrix}+mc^2\begin{pmatrix}\tilde{\varphi}\\-\tilde{\chi}\end{pmatrix}+e\phi\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix} \tag{6.20}$$

In the non-relativistic limit the rest energy mc^2 is the largest energy and we define:

$$\begin{pmatrix}\tilde{\varphi}\\\tilde{\chi}\end{pmatrix}=e^{-\frac{\imath mc^2t}{\hbar}}\begin{pmatrix}\varphi\\\chi\end{pmatrix}$$

Then from Eq. (6.20), we obtain

$$\boxed{\imath\hbar\begin{pmatrix}\dot{\varphi}\\\dot{\chi}\end{pmatrix}=c\begin{pmatrix}\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\chi\\\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\varphi\end{pmatrix}+e\phi\begin{pmatrix}\varphi\\\chi\end{pmatrix}-2mc^2\begin{pmatrix}0\\\chi\end{pmatrix}} \tag{6.21}$$

In the second equation, $\imath\hbar\dot{\chi}=c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\varphi+e\phi\chi-2mc^2\chi$, the last term is much larger than $\dot{\chi}$ and $e\phi\chi$. So, neglecting those two terms we get,

$$0=c(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})\varphi-2mc^2\chi$$
$$\Rightarrow\ \chi=\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\pi}}{2mc}\varphi$$

Note that $\boldsymbol{\pi}/m \sim \mathbf{v}$, i.e. of the same order as the velocity, and therefore $\chi \propto \frac{v}{c}\varphi \ll \varphi$ (in the non-relativistic limit). Therefore one denotes φ as the "large" component and χ as the "small" component.

Inserting the expression of χ in the first line of (6.21), $\imath\hbar\dot{\varphi} = c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\chi + e\phi\varphi$, leads to

$$\boxed{\imath\hbar\frac{\partial\varphi}{\partial t} = \left\{\frac{1}{2m}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) + e\phi\right\}\varphi\,.} \tag{6.22}$$

To evaluate $(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})$, we use that for general $\mathbf{a}$, $\mathbf{b}$

$$\begin{aligned}(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \sigma^i a^i \sigma^j b^j &= \underbrace{\sigma^i\sigma^j}_{=\delta_{ij}+\imath\epsilon^{ijk}\sigma^k} a^i b^j \\ &= a^i b^i + \imath\underbrace{(\epsilon^{ijk}a^i b^j)}_{(\mathbf{a}\times\mathbf{b})^k}\sigma^k\end{aligned}$$

Therefore,

$$(\boldsymbol{\sigma}\cdot\mathbf{a})(\boldsymbol{\sigma}\cdot\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} + \imath\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b})$$

and

$$\begin{aligned}(\boldsymbol{\sigma}\cdot\boldsymbol{\pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\pi}) &= \boldsymbol{\pi}\cdot\boldsymbol{\pi} + \imath\boldsymbol{\sigma}\cdot(\boldsymbol{\pi}\times\boldsymbol{\pi}) \\ &= (\mathbf{p}-\frac{e}{c}\mathbf{A})^2 + \imath\boldsymbol{\sigma}\cdot\underbrace{(\mathbf{p}-\frac{e}{c}\mathbf{A})\times(\mathbf{p}-\frac{e}{c}\mathbf{A})}_{=-\frac{e}{c}(\mathbf{A}\times\mathbf{p}+\mathbf{p}\times\mathbf{A})}\,.\end{aligned}$$

It is

$$\begin{aligned}(\mathbf{A}\times\mathbf{p}+\mathbf{p}\times\mathbf{A})_x &= (A_y p_z - A_z p_y) + (p_y A_z - p_z A_y) \\ &= (p_y A_z - A_z p_y) - (p_z A_y - A_y p_z) \\ &= [p_y, A_z] - [p_z, A_y] \\ &= \frac{\hbar}{\imath}\left(\frac{\partial}{\partial y}A_z - \frac{\partial}{\partial z}A_y\right) = \frac{\hbar}{\imath}(\boldsymbol{\nabla}\times\mathbf{A})_x\end{aligned}$$

and the other components are obtained by cyclic permutation. Therefore, the whole expressions results in

$$\mathbf{A}\times\mathbf{p} + \mathbf{A}\times\mathbf{p} = \frac{\hbar}{\imath}(\boldsymbol{\nabla}\times\mathbf{A}) = \frac{\hbar}{\imath}\mathbf{B}$$

From (6.22), we finally obtain

$$\boxed{\imath\hbar\frac{\partial\varphi}{\partial t} = \underbrace{\left\{\frac{1}{2m}(\mathbf{p}-\frac{e}{c}\mathbf{A})^2 - \frac{e\hbar}{2mc}\boldsymbol{\sigma}\cdot\mathbf{B} + e\phi\right\}}_{=:H_{\text{Pauli}}}\varphi\,.}$$

The newly defined

$$H_{\text{Pauli}} = \frac{1}{2m}(\mathbf{p} - \frac{e}{c}\mathbf{A})^2 - \frac{e\hbar}{2mc}\boldsymbol{\sigma} \cdot \mathbf{B} + e\phi \tag{6.23}$$

is the Hamiltonian of the **Pauli equation**, the non-relativistic equation for an electron (spin 1/2) described by a 2-spinor φ.

Proof:
Let $\mathbf{B} = \nabla \times \mathbf{A}$ be a homogeneous magnetic field, i.e. $\mathbf{B}(\mathbf{x}) \equiv \mathbf{B} = \text{const}$. Furthermore, we choose $\mathbf{A} = \frac{1}{2}(\mathbf{B} \times \mathbf{r})$.

We make the control calculation

$$\begin{aligned}
\textbf{rot } \mathbf{A} = \nabla \times \mathbf{A} &= \frac{1}{2}\nabla \times (\mathbf{B} \times \mathbf{r}) \\
&= \frac{1}{2}\nabla \times \begin{pmatrix} B_y z - B_z y \\ B_z x - B_x z \\ B_x y - B_y x \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} \partial_y(B_x y - B_y x) - \partial_z(B_z x - B_x z) \\ \partial_z(B_y z - B_z y) - \partial_x(B_x y - B_y x) \\ \partial_x(B_z x - B_x z) - \partial_y(B_y z - B_z y) \end{pmatrix} \\
&= \frac{1}{2}\begin{pmatrix} 2B_x \\ 2B_y \\ 2B_z \end{pmatrix} = \begin{pmatrix} B_x \\ B_y \\ B_z \end{pmatrix} = \mathbf{B}\,.
\end{aligned}$$

Considering the quadratic term of (6.23), we have

$$\frac{1}{2m}\left(\mathbf{p} - \frac{e}{c}\mathbf{A}\right)^2 = \frac{p^2}{2m} - \frac{e}{2mc}\left(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}\right) + \frac{e^2}{2mc^2}\mathbf{A}^2$$

where for the middle term we find

$$\begin{aligned}
\left(\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p}\right)\varphi &= \mathbf{p} \cdot (\mathbf{A}\varphi) + \mathbf{A} \cdot (\mathbf{p}\varphi) \\
&= \underbrace{(\mathbf{p} \cdot \mathbf{A})}_{\substack{= \frac{\hbar}{i}\nabla\cdot\mathbf{A} = 0, \\ \text{Coulomb gauge}}} \varphi + \mathbf{A} \cdot (\mathbf{p}\,\varphi) + \mathbf{A} \cdot (\mathbf{p}\,\varphi) \\
&= 2\mathbf{A} \cdot \mathbf{p}\,\varphi\,.
\end{aligned}$$

Therefore we can calculate further

$$\begin{aligned}
\mathbf{p} \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{p} = 2\mathbf{A} \cdot \mathbf{p} &= (\mathbf{B} \times \mathbf{r}) \cdot \mathbf{p} \\
&= \epsilon_{ijk} B_i x_j p_k \\
&= \epsilon_{jki} x_j p_k B_i \\
&= (\mathbf{r} \times \mathbf{p}) \cdot \mathbf{B} \\
&= \mathbf{L} \cdot \mathbf{B}\,,
\end{aligned}$$

where we introduced the *orbital angular momentum*

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}\,.$$

By also introducing the *spin angular momentum*

$$\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma} \,,$$

Eq. (6.23) takes the form

$$\boxed{H_{\text{Pauli}} = \frac{p^2}{2m} - \underbrace{\frac{e}{2mc}(\mathbf{L}+2\mathbf{S})}_{\substack{=:\boldsymbol{\mu},\text{ magnetic moment}\\ \text{of the electron}}} \cdot \mathbf{B} + \frac{e^2}{2mc^2}A^2 + e\phi \,.}$$

So the magnetic moment consists of two parts

$$\boldsymbol{\mu} = \boldsymbol{\mu}_{\text{orbit}} + \boldsymbol{\mu}_{\text{spin}}$$

where

$$\boldsymbol{\mu}_{\text{spin}} = g\,\frac{e}{2mc}\mathbf{S} \,,$$

with the gyromagnetic ratio (or Landé factor)

$$g = 2 \,.$$

QED finds g slightly larger than 2, and can predict a precise value of g with high precision (10 digits).

6.3.3 Relativistic corrections to the Pauli equation

To derive the **relativistic correction of the Pauli equation**, we again consider the Dirac Equation (6.19) in the formulation with the Dirac Hamiltonian:

$$\imath\hbar\frac{\partial\psi}{\partial t} = H_{\text{Dirac}}\psi \,,$$

with

$$H_{\text{Dirac}} = c\boldsymbol{\alpha}\cdot\boldsymbol{\pi} + \beta mc^2 + e\phi \,, \qquad \text{and} \quad \boldsymbol{\pi} = \mathbf{p} - \frac{e}{c}\mathbf{A} \,.$$

Taking the stationary equation, $\boxed{H_{\text{Dirac}}\psi = E\psi}$, we choose the ansatz: $\psi = \begin{pmatrix}\varphi\\ \chi\end{pmatrix}$.

Then,

$$E\begin{pmatrix}\varphi\\ \chi\end{pmatrix} = c\begin{pmatrix}0 & \boldsymbol{\sigma}\cdot\boldsymbol{\pi}\\ \boldsymbol{\sigma}\cdot\boldsymbol{\pi} & 0\end{pmatrix}\begin{pmatrix}\varphi\\ \chi\end{pmatrix} + \begin{pmatrix}mc^2+e\phi & 0\\ 0 & -mc^2+e\phi\end{pmatrix}\begin{pmatrix}\varphi\\ \chi\end{pmatrix}$$

or,

$$(E-e\phi)\varphi - c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\chi = mc^2\varphi \tag{6.24a}$$

$$(E-e\phi)\chi - c\boldsymbol{\sigma}\cdot\boldsymbol{\pi}\varphi = -mc^2\chi \tag{6.24b}$$

For simplicity consider the case $\mathbf{A} = 0$, i.e. $\boldsymbol{\pi} = \mathbf{p}$. Then (6.24b) yields:

$$\begin{aligned}
\chi &= (E + mc^2 - e\phi)^{-1} c(\boldsymbol{\sigma}\cdot\mathbf{p})\varphi \\
&= \left(\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc} - \frac{1}{2mc}(E - mc^2 - e\phi)\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc^2}\right)\varphi
\end{aligned}$$

$$\left(\text{b.c. } \frac{1}{E+mc^2-e\phi} = \frac{1}{2mc^2+(E-mc^2-e\phi)} = \frac{1}{2mc^2}\frac{1}{1+\frac{E-mc^2-e\phi}{2mc^2}} \approx \frac{1}{2mc^2}\left(1 - \frac{E-mc^2-e\phi}{2mc^2}\right)\right)$$

Inserting this in (6.24a) gives

$$\begin{aligned}
E\,\varphi &= (e\phi + mc^2)\,\varphi + c(\boldsymbol{\sigma}\cdot\mathbf{p})\left(\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc} - \frac{1}{2mc}(E - mc^2 - e\phi)\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc^2}\right)\varphi \\
&= \left\{\underbrace{\frac{(\boldsymbol{\sigma}\cdot\mathbf{p})^2}{2m}}_{=p^2/2m} + e\phi + mc^2 - \frac{(\boldsymbol{\sigma}\cdot\mathbf{p})}{2mc}\,\frac{E - mc^2 - e\phi}{2mc}\,\boldsymbol{\sigma}\cdot\mathbf{p}\right\}\varphi \\
&=: \mathcal{H}_2\,\varphi
\end{aligned} \tag{6.25}$$

To leading order $\chi = \frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc}\varphi = \mathcal{O}(v/c)$, therefore neglecting smaller terms, we find that the Dirac spinor $\psi = \begin{pmatrix}\varphi\\ \chi\end{pmatrix}$ is correctly normalized to 1, if we instead of φ choose the rescaled spinor $\bar{\varphi} = (1 + p^2/8m^2c^2)\,\varphi$.

Proof:

$$\begin{aligned}
1 = \int d\mathbf{r}\,\bar{\psi}\psi = \int d\mathbf{r}\begin{pmatrix}\varphi^\dagger & \chi^\dagger\end{pmatrix}\gamma^0\begin{pmatrix}\varphi\\ \chi\end{pmatrix} &= \int d\mathbf{r}\,\left(\varphi^\dagger\varphi - \chi^\dagger\chi\right) \\
&= \int d\mathbf{r}\,\varphi^\dagger\left(1 - \left(\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{2mc}\right)^2\right)\varphi\,,
\end{aligned}$$

i.e. with

$$\bar{\varphi} = \left(1 - \frac{p^2}{4m^2c^2}\right)^{-1/2}\varphi \approx \underbrace{\left(1 + \frac{p^2}{8m^2c^2}\right)}_{=:\Omega}\varphi$$

$\psi = \begin{pmatrix}\bar{\varphi}\\ \chi\end{pmatrix}$ is correctly normalized.

We will now rewrite (6.25), $\mathcal{H}_2\,\varphi = E\,\varphi$, using $\bar{\varphi}$:

$$\varphi = \Omega^{-1}\bar{\varphi} = \left(1 + \frac{p^2}{8m^2c^2}\right)^{-1}\varphi \approx \left(1 - \frac{p^2}{8m^2c^2}\right)\bar{\varphi}\,.$$

Therefore (6.25) becomes

$$\begin{aligned}
&(E - mc^2)\Omega^{-1}\bar{\varphi} = (\mathcal{H}_2 - mc^2)\Omega^{-1}\,\bar{\varphi} \\
\overset{\Omega^{-1}\cdots}{\Rightarrow}\quad &\Omega^{-2}E'\,\bar{\varphi} = \Omega^{-1}(\mathcal{H}_2 - mc^2)\Omega^{-1}\bar{\varphi} \qquad \text{where } E' := E - mc^2\,.
\end{aligned}$$

Inserting the definition of Ω yields

$$\left(1-\frac{p^2}{4m^2c^2}\right)E'\,\bar\varphi = \left\{\left(1-\frac{p^2}{8m^2c^2}\right)\left(\frac{p^2}{2m}+e\phi-\frac{\boldsymbol\sigma\cdot\mathbf p}{2mc}\,\frac{E'-e\phi}{2mc}\,\boldsymbol\sigma\cdot\mathbf p\right)\left(1-\frac{p^2}{8m^2c^2}\right)\right\}\bar\varphi$$
$$\approx\left\{\frac{p^2}{2m}+e\phi-\frac{\boldsymbol\sigma\cdot\mathbf p}{2mc}\,\frac{E'-e\phi}{2mc}\,\boldsymbol\sigma\cdot\mathbf p-\frac{p^2}{8m^2c^2}\left(\frac{p^2}{2m}+e\phi\right)-\left(\frac{p^2}{2m}+e\phi\right)\frac{p^2}{8m^2c^2}\right\}\bar\varphi$$

$$\Rightarrow\quad E'\,\bar\varphi=\left\{\frac{p^2}{2m}+e\phi-\frac{p^4}{8m^3c^2}+\underbrace{\frac{p^2}{4m^2c^2}E'-\frac{p^2}{8m^2c^2}e\phi-e\phi\frac{p^2}{8m^2c^2}}_{=\frac{p^2}{8m^2c^2}(E'-e\phi)+(E'-e\phi)\frac{p^2}{8m^2c^2}}-\frac{\boldsymbol\sigma\cdot\mathbf p}{2mc}\,\frac{E'-e\phi}{2mc}\,\boldsymbol\sigma\cdot\mathbf p\right\}\bar\varphi$$

Because $(\boldsymbol\sigma\cdot\mathbf p)^2=p^2$ one is able to write

$$E'\,\bar\varphi=\left\{\frac{p^2}{2m}+e\phi-\frac{p^4}{8m^3c^2}+\underbrace{\left(\frac{\boldsymbol\sigma\cdot\mathbf p}{2mc}\right)^2\frac{E'-e\phi}{2}+\frac{E'-e\phi}{2}\left(\frac{\boldsymbol\sigma\cdot\mathbf p}{2mc}\right)^2-2\overbrace{\frac{\boldsymbol\sigma\cdot\mathbf p}{2mc}}^{=:A}\overbrace{\frac{E'-e\phi}{2}}^{=:B}\frac{\boldsymbol\sigma\cdot\mathbf p}{2mc}}_{(***)}\right\}\bar\varphi$$

$$\begin{aligned}(***)&=A^2B+BA^2-2ABA\\&=A(AB-BA)-(AB-BA)A=[A,\,[A,B]]\\&=\frac{1}{8m^2c^2}\Big[\boldsymbol\sigma\cdot\mathbf p,\,\underbrace{[\boldsymbol\sigma\cdot\mathbf p,\,E'-e\phi]}_{=\imath e\hbar\boldsymbol\sigma\cdot\nabla\phi}\Big]\\&=\frac{\imath e\hbar}{8m^2c^2}\underbrace{[\boldsymbol\sigma\cdot\mathbf p,\,\boldsymbol\sigma\cdot\nabla\phi]}_{\substack{=\sigma_i\sigma_j[p_i,\,\nabla\phi_j]+\sigma_i\cancel{[p_i,\,\sigma_j]}\nabla\phi_j\\+\sigma_j\cancel{[\sigma_i,\,\nabla\phi_j]}p_i+[\sigma_i,\sigma_j]\,\nabla\phi_j p_i\\=-\imath\hbar\Delta\phi-2\imath\boldsymbol\sigma\cdot(\nabla\phi\times\mathbf p)}}\end{aligned}$$

where on the left side, following relations were used:

$$[p_i,\nabla\phi_j]=\frac{\hbar}{\imath}[\partial_i,\partial_j\phi]$$
$$=\frac{\hbar}{\imath}\partial_i\partial_j\phi=\frac{\hbar}{\imath}\partial_j\partial_i\phi$$

$$\sigma_i\sigma_j=\begin{cases}-\sigma_j\sigma_i\,, & \text{for } i\neq j\\ 1\,, & \text{for } i=j\end{cases}$$

$$[\sigma_i,\sigma_j]=2\imath\varepsilon_{ijk}\sigma_k$$

$$\boxed{E'\,\bar\varphi=\left\{\frac{p^2}{2m}+e\phi-\underbrace{\frac{p^4}{8m^3c^2}}_{p^4\text{-term}}+\underbrace{\frac{e\hbar^2}{8m^2c^2}\Delta\phi}_{\text{Darwin-term}}+\underbrace{\frac{e\hbar}{4m^2c^2}\boldsymbol\sigma\cdot(\nabla\phi\times\mathbf p)}_{\text{LS coupling}}\right\}\bar\varphi}$$

These are the leading relativistic corrections of the Pauli equation. Corrections of higher order in v/c can systematically be calculated by using the **Foldy-Wouthuysen transformation**.

If $\mathbf A\neq 0$ one has to replace $\mathbf p$ through $\mathbf p-e\mathbf A$ as well as adding the additional term $g_s\frac{e}{2mc}\mathbf S$ to the Hamiltonian.

The meanings and implications of each of the additional terms have already been discussed in Quantum Mechanics I:

- The **Darwin term** only has an effect for s-states when considering a Coulomb potential, because $\Delta\frac{1}{r} = 4\pi\delta(\mathbf{r})$.
- The $\mathbf{p^4}$**-term** follows from

$$E = mc^2\sqrt{1+\frac{p^2}{m^2c^2}} \approx mc^2\left(1+\frac{p^2}{2m^2}-\frac{1}{8}\left(\frac{p^2}{m^2c^2}\right)^2\right) = mc^2+\frac{p^2}{2m}-\frac{p^4}{8m^3c^2}$$

- **LS coupling** refers to spin-orbit coupling: For a central potential we have $\nabla\phi = \frac{\mathbf{r}}{r}\phi'$, therefore:

$$\begin{aligned}\frac{e\hbar}{4m^2c^2}\boldsymbol{\sigma}\cdot(\nabla\phi\times\mathbf{p}) &= \frac{\hbar}{4m^2c^2}\,\frac{1}{r}e\phi'(\mathbf{r})\boldsymbol{\sigma}\cdot(\mathbf{r}\times\mathbf{p})\\ &= \frac{\hbar}{4m^2c^2}\,\frac{e\phi'}{r}\boldsymbol{\sigma}\cdot\mathbf{L}\,, \qquad \mathbf{L}: \text{Orbital angular momentum}\end{aligned}$$

6.4 Lorentz covariance of the Dirac equation

Lorentz covariance and the transformation of spinors

The *principle of relativity* states that the laws of nature are identical in every inertial reference frame.
We consider two inertial frames I and I' with the space-time coordinates x and x'. Let the wave function of a particle in these two frames be ψ and ψ', respectively. We write the Poincaré transformation between I and I' as

$$x' = \Lambda x + a\,. \tag{6.26}$$

It must be possible to construct the wave function ψ' from ψ. This means that there must be a local relationship between ψ' and ψ:

$$\psi'(x') = F(\psi(x)) = F(\psi(\Lambda^{-1}(x'-a)))\,. \tag{6.27}$$

The principle of relativity together with the functional relation (6.27) necessarily leads to the requirement of *Lorentz covariance*: The Dirac equation in I is transformed by (6.26) and (6.27) into a Dirac equation in I'. (The Dirac equation is form invariant with respect to Poincaré transformations.) In order that both ψ and ψ' may satisfy the linear Dirac equation, their functional relationship must be linear, i.e.

$$\psi'(x') = S(\Lambda)\psi(x) = S(\Lambda)\psi(\Lambda^{-1}(x'-a))\,. \tag{6.28a}$$

Here, $S(\Lambda)$ is a 4×4-matrix, with which the spinor ψ is to be multiplied. We will determine $S(\Lambda)$ below. In components, the transformation reads:

$$\psi'_\alpha(x') = \sum_{\beta=1}^{4} S_{\alpha\beta}(\Lambda)\psi_\beta(\Lambda^{-1}(x'-a))\,. \tag{6.28b}$$

The Lorentz covariance of the Dirac equation requires that ψ' obey the equation

$$(-\imath\gamma^{\mu}\partial'_{\mu} + m)\,\psi'(x') = 0\,, \qquad (c = 1,\, \hbar = 1) \tag{6.29}$$

where

$$\partial'_{\mu} = \frac{\partial}{\partial x'^{\mu}}\,.$$

The γ-matrices are unchanged under the Lorentz transformations. In order to determine S, we need to convert the Dirac equation in the primed and unprimed coordinate system into one another. The Dirac equation in the unprimed coordinate system

$$(-\imath\gamma^{\mu}\partial_{\mu} + m)\,\psi(x) = 0 \tag{6.30}$$

can by means of the relation

$$\frac{\partial}{\partial x^{\mu}} = \frac{\partial x'^{\nu}}{\partial x^{\mu}}\frac{\partial}{\partial x'^{\nu}} = \Lambda^{\nu}{}_{\mu}\partial'_{\nu}$$

and

$$S^{-1}\psi'(x') = \psi(x)\,,$$

be brought into the form

$$(-\imath\gamma^{\mu}\Lambda^{\nu}{}_{\mu}\partial'_{\nu} + m)\,S^{-1}(\Lambda)\,\psi'(x') = 0\,. \tag{6.31a}$$

After multiplying from the left by S, one obtains

$$-\imath S\Lambda^{\nu}{}_{\mu}\gamma^{\mu}S^{-1}\partial'_{\nu}\psi'(x') + m\psi'(x') = 0\,. \tag{6.31b}$$

From a comparison of (6.31b) with (6.29), it follows that the Dirac equation is form invariant under Lorentz transformations, provided $S(\Lambda)$ satisfies the following condition:

$$S(\Lambda)^{-1}\gamma^{\nu}S(\Lambda) = \Lambda^{\nu}{}_{\mu}\gamma^{\mu}\,. \tag{6.32}$$

It is possible to show (see next section) that this equation has nonsingular solutions for $S(\Lambda)$. A wave function that transforms under a Lorentz transformation according to $\psi' = S\psi$ is known as a *four-component Lorentz spinor*.

Determination of the representation $S(\Lambda)$

Infinitesimal Lorentz transformations

We first consider *infinitesimal (proper, orthochronous) Lorentz transformations*

$$\Lambda^\nu{}_\mu = g^\nu{}_\mu + \Delta\omega^\nu{}_\mu \tag{6.33a}$$

with infinitesimal and antisymmetric $\Delta\omega^{\nu\mu}$

$$\Delta\omega^{\nu\mu} = -\Delta\omega^{\mu\nu}\,. \tag{6.33b}$$

This equation implies that $\Delta\omega^{\nu\mu}$ can have only 6 independent nonvanishing elements. These transformations satisfy the defining relation for Lorentz transformations

$$\Lambda^\lambda{}_\mu g^{\mu\nu}\Lambda^\rho{}_\nu = g^{\lambda\rho}\,, \tag{6.34}$$

as can be seen by inserting (6.33) into this equation:

$$g^\lambda{}_\mu g^{\mu\nu} g^\rho{}_\nu + \Delta\omega^{\lambda\rho} + \Delta\omega^{\rho\lambda} + \mathcal{O}((\Delta\omega)^2) = g^{\lambda\rho}\,. \tag{6.35}$$

Each of the 6 independent elements of $\Delta\omega^{\mu\nu}$ generates an infinitesimal Lorentz transformation. First we consider two typical special cases – rotations and Lorentz boosts:

$$\Delta\omega^0{}_1 = -\Delta\omega^{01} = -\Delta\xi : \quad \text{Transformation to a coordinate system moving with velocity } c\Delta\xi \text{ in the } x \text{ direction} \tag{6.36}$$

$$\Delta\omega^1{}_2 = -\Delta\omega^{12} = \Delta\vartheta : \quad \text{Transformation to a coordinate system that is rotated by an angle } \Delta\vartheta \text{ about the z axis (see Fig. 6.1).} \tag{6.37}$$

Rotation around the z axis

The spatial components transform like (note that only the x and y coordinates are transformed):

$$\begin{aligned}\Lambda &= \begin{pmatrix} 1 & & & \\ & \cos\vartheta & \sin\vartheta & \\ & -\sin\vartheta & \cos\vartheta & \\ & & & 1 \end{pmatrix} \\ &= 1 + \vartheta \begin{pmatrix} 0 & & & \\ & 0 & 1 & \\ & -1 & 0 & \\ & & & 0 \end{pmatrix} + \mathcal{O}(\vartheta^2)\end{aligned}$$

for infinitesimal ϑ. Expressed as single components one finds

$$\Lambda^\nu{}_\mu = \delta^\nu_\mu + \vartheta\Delta^\nu{}_\mu\,, \qquad \text{where} \quad \Delta^1{}_2 = -\Delta^2{}_1 = 1, \;\; \text{all other } 0\,.$$

It must be possible to expand S as a power series in $\Delta^\nu{}_\mu$. We write

$$S = \mathbb{1} + \tau\,, \qquad S^{-1} = \mathbb{1} - \tau\,, \tag{6.38}$$

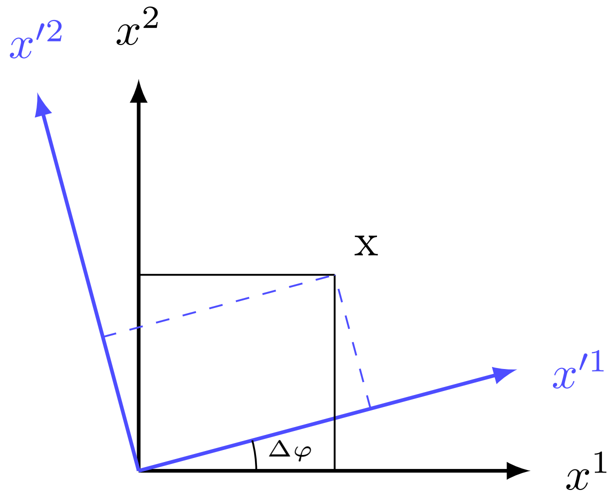


Figure 6.1: Infinitesimal rotation, passive transformation

where $\tau \equiv \tau(\vartheta)$ is likewise infinitesimal. We insert (6.38) into the equation for S, namely $S^{-1}\gamma^\nu S = \Lambda^\nu{}_\mu \gamma^\mu$, and get

$$\begin{aligned}(\mathbb{1}-\tau)\gamma^\nu(\mathbb{1}+\tau) &= \gamma^\nu + \gamma^\nu\tau - \tau\gamma^\nu + \mathcal{O}(\tau^2)\\ &\overset{!}{=} \gamma^\mu(\delta^\nu_\mu + \vartheta\,\Delta^\nu{}_\mu) + \mathcal{O}(\vartheta^2)\,,\end{aligned}$$

from which the equation determining τ follows as

$$\Rightarrow \quad \gamma^\nu\tau - \tau\gamma^\nu \overset{!}{=} \vartheta\gamma^\mu\Delta^\nu{}_\mu\,.$$

$$\begin{aligned}\text{or} \quad \gamma^1\tau - \tau\gamma^1 &= \vartheta\gamma^2\Delta^1{}_2 = \vartheta\gamma^2\\ \gamma^2\tau - \tau\gamma^2 &= \vartheta\gamma^1\Delta^2{}_1 = -\vartheta\gamma^1\end{aligned}$$

what yields the solution

$$\tau = \imath\frac{\vartheta}{2}\begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix}.$$

Proof:

$$\begin{aligned}\gamma^1\tau - \tau\gamma^1 &= \imath\frac{\vartheta}{2}\left\{\begin{pmatrix}0 & \sigma^1\\ -\sigma^1 & 0\end{pmatrix}\begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix} - \begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix}\begin{pmatrix}0 & \sigma^1\\ -\sigma^1 & 0\end{pmatrix}\right\}\\ &= \imath\frac{\vartheta}{2}\begin{pmatrix}0 & \sigma^1\sigma^3 - \sigma^3\sigma^1\\ -\sigma^1\sigma^3 + \sigma^3\sigma^1 & 0\end{pmatrix}\\ &\overset{\sigma^1\sigma^3 = -\imath\sigma^2}{=} \imath\frac{\vartheta}{2}\begin{pmatrix}0 & -2\imath\sigma^2\\ 2\imath\sigma^2 & 0\end{pmatrix} = \vartheta\gamma^2\end{aligned}$$

$$
\begin{aligned}
\gamma^2\tau - \tau\gamma^2 &= \imath\frac{\vartheta}{2}\left\{\begin{pmatrix}0 & \sigma^2\\ -\sigma^2 & 0\end{pmatrix}\begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix} - \begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix}\begin{pmatrix}0 & \sigma^2\\ -\sigma^2 & 0\end{pmatrix}\right\}\\
&= \imath\frac{\vartheta}{2}\begin{pmatrix}0 & \sigma^2\sigma^3 - \sigma^3\sigma^2\\ -\sigma^2\sigma^3 + \sigma^3\sigma^2 & 0\end{pmatrix}\\
&\overset{\sigma^2\sigma^3=\imath\sigma^1}{=} \imath\frac{\vartheta}{2}\begin{pmatrix}0 & 2\imath\sigma^1\\ -2\imath\sigma^1 & 0\end{pmatrix} = -\vartheta\gamma^1
\end{aligned}
$$

To within an additive multiple of $\mathbb{1}$, this unambiguously determines τ. If there were two solutions, then the difference between them would commute with all γ^μ, and thus be proportional to $\mathbb{1}$.

By a succession of infinitesimal rotations we can construct the transformation matrix S for a *finite rotation* through an angle ϑ. This is achieved by decomposing the finite rotation into a sequence of N steps ϑ/N:

$$
\begin{aligned}
S &= \lim_{N\to\infty}\left(1 + \tau(\vartheta/N)\right)^N\\
&= \lim_{N\to\infty}\left(1 + \imath\frac{\vartheta}{2N}\begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix}\right)^N\\
&= \exp\left(\imath\frac{\vartheta}{2}\begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix}\right)\\
&= \cos\frac{\vartheta}{2}\,\mathbb{1} + \imath\sin\frac{\vartheta}{2}\begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix}.
\end{aligned}
\tag{6.39}
$$

Note that in the arguments of cos and sin we find $\vartheta/2$, which results in

$$
S(2\pi) = -\mathbb{1} \qquad \text{and} \qquad S(4\pi) = +\mathbb{1}\,.
$$

This means that spinors do not regain their initial value after a rotation through 2π, but only after a rotation through 4π, a fact that is also confirmed by neutron scattering experiments. Also note that $S(\vartheta)$ does not mix the upper and lower components of a 4-spinor ψ. Therefore the upper two components transform exactly like Pauli (2-)spinors with respect to rotations:

$$
\varphi = \begin{pmatrix}a\\ b\end{pmatrix} \qquad\qquad \varphi'(x') = e^{\imath\frac{\vartheta}{2}\sigma^3}\,\varphi(x)\,.
$$

For a rotation through an angle ϑ about an *arbitrary* axis $\mathbf{n} = (n_1,\, n_2,\, n_3)^{\mathcal{T}}$, one has:

$$
\begin{aligned}
S &= \exp\left\{\imath\frac{\vartheta}{2}\mathbf{n}\cdot\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix}\right\}\\
&= \exp\left\{\imath\frac{\vartheta}{2}\left[n_1\begin{pmatrix}\sigma^1 & 0\\ 0 & \sigma^1\end{pmatrix} + n_2\begin{pmatrix}\sigma^2 & 0\\ 0 & \sigma^2\end{pmatrix} + n_3\begin{pmatrix}\sigma^3 & 0\\ 0 & \sigma^3\end{pmatrix}\right]\right\}.
\end{aligned}
\tag{6.40}
$$

Boost in x direction

As second example we want to consider a Lorentz boost in x direction. With the definition $\tanh\xi = v/c$ we find the matrix representation of Λ is given by (see Sec. B.2):

$$\Lambda = \left(\begin{array}{cc|cc} \cosh\xi & -\sinh\xi & 0 & 0 \\ -\sinh\xi & \cosh\xi & 0 & 0 \\ \hline 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right)$$
$$= \mathbb{1} + \xi \left(\begin{array}{cc|cc} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array}\right) + \mathcal{O}(\xi^2)\,,$$

where to derive the second representation we assumed ξ as infinitesimal. This yields the equation

$$\Lambda^\nu{}_\mu = 1 + \xi\Delta^\nu{}_\mu\,, \quad \text{where } \Delta^0{}_1 = \Delta^1{}_0 = -1\,, \text{ all other } 0$$

for the single components of the transformation matrix. Analogous to the previous example of a rotation, we take

$$S = 1 + \tau\,, \qquad S^{-1} = 1 - \tau\,,$$

where $\tau \equiv \tau(\xi)$ is assumed infinitesimal. τ is determined through

$$\begin{aligned} S^{-1}\gamma^\nu S &= (1-\tau)\gamma^\nu(1+\tau) \\ &= \gamma^\nu + \gamma^\nu\tau - \tau\gamma^\nu + \mathcal{O}(\tau^2) \\ &\stackrel{!}{=} \gamma^\mu(\delta^\nu_\mu + \xi\Delta^\nu{}_\mu) + \mathcal{O}(\xi^2)\,, \end{aligned}$$

which leads to the equations

$$\begin{aligned} \Rightarrow \quad & \gamma^\nu\tau - \tau\gamma^\nu \stackrel{!}{=} \xi\gamma^\mu\Delta^\nu{}_\mu \\ \text{or} \quad & \gamma^0\tau - \tau\gamma^0 = \xi\gamma^1\Delta^0{}_1 = -\xi\gamma^1 \\ & \gamma^1\tau - \tau\gamma^1 = \xi\gamma^0\Delta^1{}_0 = -\xi\gamma^0\,, \end{aligned}$$

which are solved by

$$\tau = -\frac{1}{2}\xi\gamma^0\gamma^1 = -\frac{1}{2}\xi\alpha^1 = -\frac{1}{2}\begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}\,.$$

Proof:

$$\gamma^0\tau - \tau\gamma^0 = -\frac{1}{2}\xi(\underbrace{\gamma^0\gamma^0}_{=\mathbb{1}}\gamma^1 - \underbrace{\gamma^0\gamma^1\gamma^0}_{=-\gamma^1}) = -\xi\gamma^1$$

$$\gamma^1\tau - \tau\gamma^1 = -\frac{1}{2}\xi(\underbrace{\gamma^1\gamma^0\gamma^1}_{\substack{=-\gamma^1\gamma^1\gamma^0 \\ =-(-\mathbb{1})\gamma^0=\gamma^0}} - \gamma^0\underbrace{\gamma^1\gamma^1}_{=-\mathbb{1}}) = -\xi\gamma^0$$

By a sequence of infinitesimal boosts, we can construct the transformation matrix S of a finite boost with the parameter $\xi = N \cdot (\xi/N)$, where we assume $N \to \infty$, so that ξ/N is infinitesimal. This yields

$$\begin{aligned} S &= \lim_{N\to\infty} \left(1 - \frac{1}{2}\frac{\xi}{N}\begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}\right)^N \\ &= \exp\left\{-\frac{\xi}{2}\begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix}\right\} \\ &= \cosh\frac{\xi}{2}\,\mathbb{1} - \sinh\frac{\xi}{2}\begin{pmatrix} 0 & \sigma^1 \\ \sigma^1 & 0 \end{pmatrix} \end{aligned}$$

We want to consider now a **general** infinitesimal Lorentz transformation

$$\Lambda^\nu{}_\mu = \delta^\nu_\mu + \Delta\omega^\nu{}_\mu \quad \text{and} \quad (\Lambda^{-1})^\nu{}_\mu = \delta^\nu_\mu - \Delta\omega^\nu{}_\mu \,.$$

To first order the transformation S has the form

$$\begin{aligned} S(\Lambda) &= 1 - \frac{\imath}{4}\sigma_{\mu\nu}\Delta\omega^{\mu\nu} \\ \text{resp.} \quad S(\Lambda)^{-1} &= 1 + \frac{\imath}{4}\sigma_{\mu\nu}\Delta\omega^{\mu\nu}\,, \end{aligned}$$

where the matrix $\sigma_{\mu\nu}$ needs to be determined. Condition (6.32), $\boxed{\gamma^\mu\Lambda^\nu{}_\mu = S^{-1}\gamma^\nu S}$ implies

$$\begin{aligned} \left(1 - \frac{\imath}{4}\sigma_{\alpha\beta}\Delta\omega^{\alpha\beta}\right)\gamma^\mu\left(1 + \frac{\imath}{4}\sigma_{\alpha\beta}\Delta\omega^{\alpha\beta}\right) &= \gamma^\mu + \frac{\imath}{4}[\gamma^\mu,\, \sigma_{\alpha\beta}]\Delta\omega^{\alpha\beta} \\ &\stackrel{!}{=} \gamma^\mu + \Delta\omega^\mu{}_\nu\gamma^\nu \end{aligned}$$

$$\Rightarrow \quad \boxed{\frac{\imath}{4}[\gamma^\mu,\, \sigma_{\alpha\beta}]\Delta\omega^{\alpha\beta} = \Delta\omega^\mu{}_\nu\gamma^\nu}\,. \tag{6.41}$$

The equation (6.41) has the solution

$$\boxed{\sigma_{\alpha\beta} = \frac{1}{2}[\gamma_\alpha,\, \gamma_\beta]\,.} \tag{6.42}$$

Proof:

$$\begin{aligned}
[\gamma^\mu,\, \gamma^\alpha\gamma^\beta] &= \gamma^\mu\gamma^\alpha\gamma^\beta - \gamma^\alpha \underbrace{\gamma^\beta\gamma^\mu}_{=2g^{\beta\mu}-\gamma^\mu\gamma^\beta} \\
&= \underbrace{\gamma^\mu\gamma^\alpha}_{2g^{\alpha\mu}-\gamma^\alpha\gamma^\mu}\gamma^\beta - 2\gamma^\alpha g^{\beta\mu} + \gamma^\alpha\gamma^\mu\gamma^\beta \\
&= 2g^{\alpha\mu}\gamma^\beta - 2g^{\beta\mu}\gamma^\alpha
\end{aligned}$$

$$\Rightarrow \quad \frac{\imath}{2}[\gamma^\mu,\, \gamma_\alpha\gamma_\beta] = \imath(g^\mu{}_\alpha\gamma_\beta - g^\mu{}_\beta\gamma_\alpha)$$

$$\begin{aligned}
\overset{(6.42)}{\Rightarrow} \quad [\gamma^\mu,\, \sigma_{\alpha\beta}] &= [\gamma^\mu,\, \frac{1}{2}(\gamma_\alpha\gamma_\beta - \gamma_\beta\gamma_\alpha)] \\
&= \imath(g^\mu{}_\alpha\gamma_\beta - g^\mu{}_\beta\gamma_\alpha) - \imath(g^\mu{}_\beta\gamma_\alpha - g^\mu{}_\alpha\gamma_\beta) \\
&= 2\imath(g^\mu{}_\alpha\gamma_\beta - g^\mu{}_\beta\gamma_\alpha) \\
\frac{\imath}{4}[\gamma^\mu.\, \sigma_{\alpha\beta}]\Delta\omega^{\alpha\beta} &= -\frac{1}{2}(g^\mu{}_\alpha\gamma_\beta - g^\mu{}_\beta\gamma_\alpha)\,\Delta\omega^{\alpha\beta} \\
&= -\frac{1}{2}(\Delta\omega^{\mu\beta}\gamma_\beta - \underbrace{\Delta\omega^{\alpha\mu}}_{=-\Delta\omega^{\mu\alpha}(*)}\gamma_\alpha) \\
&= -\Delta\omega^{\mu\nu}\gamma_\nu \\
&= \Delta\omega^\mu{}_\nu\gamma^\nu
\end{aligned}$$

(*) Note that we will address the antisymmetry of $\Delta\omega^{\nu\mu}$ later.

To arrive at a finite Lorentz transformation, we again use a sequence of infinitesimal transformations:

$$\begin{aligned}
S(\Lambda(\omega^{\mu\nu})) &= \lim_{N\to\infty}\left(1 - \frac{\imath}{4}\frac{\omega^{\mu\nu}}{N}\sigma_{\mu\nu}\right)^N \\
&= \exp\left\{-\frac{\imath}{4}\sigma_{\mu\nu}\omega^{\mu\nu}\right\}
\end{aligned}$$

As a conclusion, we will test our result on the concrete example of a rotation about the z axis. We have

$$\begin{aligned}
S = 1 + \tau\,, \qquad \text{with} \quad \tau &= -\frac{\imath}{4}\sigma_{\mu\nu}\Delta\omega^{\mu\nu} \\
&= -\frac{\imath}{4}(\sigma_{12}\Delta\omega^{12} + \sigma_{21}\Delta\omega^{21}) \\
&= -\frac{\imath}{2}\sigma_{12}\Delta\omega^{12}\,,
\end{aligned}$$

where the antisymmetry of $\Delta\omega^{12} = -\Delta\omega^{21}$ and $\sigma_{12} = -\sigma_{21}$ were used. With the reminder

$\gamma_\mu = (\gamma^0, -\gamma^1, -\gamma^2, -\gamma^3)$, we further find:

$$\begin{aligned}
\sigma_{12} &= \frac{\imath}{2}[\gamma_1, \gamma_2] \\
&= \frac{\imath}{2}(\gamma_1\gamma_2 - \underbrace{\gamma_2\gamma_1}_{=-\gamma_1\gamma_2}) \\
&= \imath\gamma_1\gamma_2 \\
&= \imath \begin{pmatrix} 0 & -\sigma_1 \\ \sigma_1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -\sigma^2 \\ \sigma^2 & 0 \end{pmatrix} \\
&= \imath \begin{pmatrix} \overbrace{-\sigma^1\sigma^2}^{=-\imath\sigma^3} & 0 \\ 0 & -\sigma_1\sigma_2 \end{pmatrix} \\
&= \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}
\end{aligned}$$

Combining the previous results and using $\Delta\omega^{12} = -\Delta\omega^1{}_2 = -\vartheta\Delta^1{}_2 = -\vartheta$, we finally arrive at

$$\begin{aligned}
S &= 1 - \frac{\imath}{2}\sigma_{12}\overbrace{\Delta\omega^{12}}^{=-\vartheta} \\
&= 1 + \imath\frac{\vartheta}{2}\begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix} \qquad \checkmark
\end{aligned}$$

which corresponds to the expected result. The remaining example of a boost in x direction remains as an exercise for the reader.

Antisymmetry of $\Delta\omega^{\lambda\rho}$

From a group theoretical standpoint we know that a Lorentz transformation $L \in \mathrm{SO}(3,1)$, which implies

$$\Lambda g \Lambda^T = g \tag{6.43a}$$

$$\text{or} \quad \Lambda^\lambda{}_\mu g^{\mu\nu} \Lambda^\rho{}_\nu = g^{\lambda\rho} \tag{6.43b}$$

For an infinitesimal transformation Λ we find

$$\Lambda^\lambda{}_\mu = \delta^\lambda_\mu + \Delta\omega^\lambda{}_\mu\,, \tag{6.44}$$

what inserted in (6.43) leads to:

$$\begin{aligned}
&(\delta^\lambda_\mu + \Delta\omega^\lambda{}_\mu)g^{\mu\nu}(\delta^\rho_\nu + \Delta\omega^\rho{}_\nu) = g^{\lambda\rho} \\
\Rightarrow\quad & g^{\lambda\rho} + \Delta\omega^{\lambda\rho} + \Delta\omega^{\rho\lambda} = g^{\lambda\rho} \\
\Rightarrow\quad & \Delta\omega^{\lambda\rho} = -\Delta\omega^{\rho\lambda}
\end{aligned}$$

Note that for mixed indices, $\Delta\omega^\lambda{}_\rho$ is in general not antisymmetric, e.g.:

$$\begin{aligned}
\Delta\omega^1{}_2 &= -\Delta\omega^{12} = +\Delta\omega^{21} = -\Delta\omega^2{}_1 \qquad &\text{(cf. rotation around } z \text{ axis)} \\
\Delta\omega^0{}_1 &= -\Delta\omega^{01} = +\Delta\omega^{10} = +\Delta\omega^1{}_0 \qquad &\text{(cf. boost in } x \text{ direction)}
\end{aligned}$$

Spatial Reflection, Parity

The Lorentz transformation corresponding to a spatial reflection is represented by

$$\Lambda^{\mu}{}_{\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} . \tag{6.45}$$

The associated S is determined, according to (6.32), from

$$S^{-1}\gamma^{\mu}S = \Lambda^{\mu}{}_{\nu}\gamma^{\nu} = \sum_{\nu=1}^{4} g^{\mu\nu}\gamma^{\nu} = g^{\mu\mu}\gamma^{\mu} , \tag{6.46}$$

where no summation over μ is implied. One immediately sees that the solution of (6.46), which we shall denote in this case by P, is given by

$$S = P \equiv e^{\imath\varphi}\gamma^0 . \tag{6.47}$$

Here, $e^{\imath\varphi}$ is an unobservable phase factor. This is conventionally taken to have one of the four values ± 1, $\pm\imath$; four reflections then yield the identity $\mathbb{1}$. The spinors transform under a spatial reflection according to

$$\psi'(x') \equiv \psi'(\mathbf{x}', t) = \psi'(-\mathbf{x}, t) = e^{\imath\varphi}\gamma^0\psi(x) = e^{\imath\varphi}\gamma^0\psi(-\mathbf{x}', t) . \tag{6.48}$$

The complete spatial reflection (parity) transformation for spinors is denoted by

$$\mathcal{P} = e^{\imath\varphi}\gamma^0\mathcal{P}^{(0)} , \tag{6.48'}$$

where $\mathcal{P}^{(0)}$ causes the spatial reflection $\mathbf{x} \to -\mathbf{x}$.
From the relationship $\gamma^0 \equiv \beta = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}$ one sees in the rest frame of the particle, spinors of positive and negative energy that are eigenstates of P – with opposite eigenvalues, i.e., opposite parity. *This means that the intrinsic parities of particles and antiparticles are opposite.*

Charge conjugation

We revisit the Dirac equation with an electromagnetic field given by (6.18)

$$\left\{\gamma^{\mu}\Big(\imath\hbar\partial_{\mu} - \frac{e}{c}A_{\mu}\Big) - mc\right\}\psi = 0 \tag{6.18}$$

If we take the adjoint (complex conjugation and transposition) of this equation, we find

$$\psi^{\dagger}\left(\underbrace{\gamma^{\mu\dagger}}_{=\gamma^0\gamma^{\mu}\gamma^0}\Big(-\imath\hbar\overleftarrow{\partial}_{\mu}\Big) - \frac{e}{c}\gamma^{\mu\dagger}A_{\mu} - mc\right) = 0$$

$$\Rightarrow \quad \underbrace{\psi^{\dagger}\gamma^0}_{=\bar{\psi}}\Big(\gamma^{\mu}\Big(-\imath\hbar\overleftarrow{\partial}_{\mu}\Big) - \frac{e}{c}\gamma^{\mu}A_{\mu} - mc\Big)\gamma^0 = 0$$

After multiplying this result from the right with γ^0 and taking the transpose, we get

$$\left(\gamma^{\mu\mathrm{T}}\Big(-\imath\hbar\partial_\mu - \frac{e}{c}A_\mu\Big) - mc\right)\bar{\psi}^{\mathrm{T}} = 0 \tag{6.49}$$

We now define the operator

$$C := \imath\gamma^2\gamma^0 = \begin{pmatrix} 0 & -\imath\sigma^2 \\ -\imath\sigma^2 & 0 \end{pmatrix}, \qquad \text{with} \quad C^{-1} = -C\,, \tag{6.50}$$

which applied to the transposed Dirac matrices yields the effect

$$\boxed{C\gamma^{\mu\mathrm{T}}C^{-1} = -\gamma^\mu\,.} \tag{6.51}$$

Examples:

$$\begin{aligned}
\gamma^{0\mathrm{T}} = \gamma^0 \qquad &\Rightarrow \quad C\gamma^{0\mathrm{T}}C^{-1} = \imath\gamma^2\gamma^0\gamma^0(-\imath\gamma^2\gamma^0) \\
&\qquad\qquad\qquad\;\; = \gamma^2\gamma^2\gamma^0 = -\gamma^0 \\
\gamma^{1\mathrm{T}} = -\gamma^1 \qquad &\Rightarrow \quad C\gamma^{1\mathrm{T}}C^{-1} = \imath\gamma^2\gamma^0(-\gamma^1)(-\imath\gamma^2\gamma^0) \\
&\qquad\qquad\qquad\;\; = -\gamma^2\gamma^0\gamma^1\gamma^2\gamma^0 \\
&\qquad\qquad\qquad\;\; = +\gamma^0\gamma^1\gamma^0 = -\gamma^1
\end{aligned}$$

etc.

Applying the operator C to the manipulated Dirac equation (6.49), one finds

$$C\left\{\gamma^{\mu\mathrm{T}}\Big(-\imath\hbar\partial_\mu - \frac{e}{c}A_\mu\Big) - mc\right\} C^{-1}C\bar{\psi}^{\mathrm{T}} = 0$$

$$\left\{-\gamma^{\mu}\Big(-\imath\hbar\partial_\mu - \frac{e}{c}A_\mu\Big) - mc\right\} C\bar{\psi}^{\mathrm{T}} = 0$$

$$\boxed{\left\{\gamma^{\mu}\Big(\imath\hbar\partial_\mu \underbrace{+}_{\text{note } e\to -e!} \frac{e}{c}A_\mu\Big) - mc\right\} \psi^C = 0\,,} \tag{6.52}$$

where we defined the **charge conjugated solution**

$$\boxed{\psi^C := C\bar{\psi}^{\mathrm{T}}\,,} \tag{6.53}$$

which represents a solution to the Dirac equation, where the sign of the charge has been flipped.

We consider the particle at rest as an example case. For negative energies and a spin down ($s_z = -1/2$), one possible solution of the Dirac equation is given by

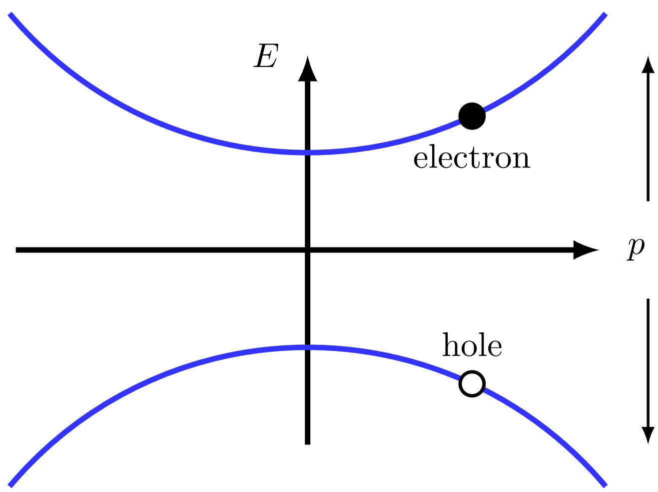
$$\psi_\downarrow^{(-)} = e^{\imath mc^2 t/\hbar}\begin{pmatrix}0\\0\\0\\1\end{pmatrix}.$$

The charge conjugated solution is then

$$\begin{aligned}\psi^C &= C\Big[(\psi^*)^{\mathrm{T}}\gamma^0\Big]^T \\ &= \imath\gamma^2\gamma^0\gamma^{0\mathrm{T}}\psi^* \\ &= e^{-\imath mc^2 t/\hbar}\,(\imath\gamma^2)\begin{pmatrix}0\\0\\0\\1\end{pmatrix} \\ &= e^{-\imath mc^2 t/\hbar}\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = \psi_\uparrow^{(+)}\end{aligned}$$

We find that starting with a solution ψ of *negative* energy and $s_z = -1/2$, the charge conjugated solution gives a solution with *positive* energy and $s_z = +1/2$. Therefore we conclude that to each particle with $E > 0$, $s_z = \pm 1/2$ and charge e belongs a particle with $E < 0$, $s_Z = \mp 1/2$ and charge $-e$. These are linked via charge conjugation.

In 1930, Dirac postulated that in the vacuum (ground state) all states with negative energy are occupied – these build the so called "Dirac sea".



An excitation of an electron in the Dirac sea (with energy $E < 0$) into a state with $E > 0$ leaves behind a "hole" in the Dirac sea with charge $-e$ (e the charge of the electron), what corresponds to the charge difference between the *Dirac sea with hole* and the *Dirac sea without hole*. Respectively the energy $E > 0$ corresponds to the energy difference of the states of the *Dirac sea with hole* and *without hole*.

The described "hole" is the **positron** – the charge conjugated particle of the electron – which was observed in 1932.

Further Properties of S

For the calculation of the transformation of bilinear forms such as $j^\mu(x)$, we need to establish a relationship between the adjoint transformations $S^\dagger$ and S^{-1}.

Assertion:

$$S^\dagger\gamma^0 = b\gamma^0 S^{-1}\,, \tag{6.54a}$$

where

$$b = \pm 1 \qquad \text{for} \qquad \Lambda^{00} \begin{cases} \geq +1 \\ \leq -1 \end{cases} . \tag{6.54b}$$

Proof: We take as our starting point Eq. (6.32)

$$S^{-1}\gamma^\mu S = \Lambda^\mu{}_\nu \gamma^\nu , \quad \Lambda^\mu{}_\nu \quad \text{real,} \tag{6.55}$$

and write the adjoint relation

$$(\Lambda^\mu{}_\nu \gamma^\nu)^\dagger = S^\dagger \gamma^{\mu\dagger} S^{\dagger -1} . \tag{6.56}$$

The hermitian adjoint matrix can be expressed most concisely as

$$\gamma^{\mu\dagger} = \gamma^0 \gamma^\mu \gamma^0 . \tag{6.57}$$

By means of the anticommutation relations, one easily checks that (6.57) is in accord with $\gamma^{0\dagger} = \gamma^0$, $\gamma^{k\dagger} = -\gamma^k$. We insert this into the left- and the right-hand sides of (6.56) and then multiply by γ^0 from the left- and right-hand side to gain

$$\begin{aligned} \gamma^0 \Lambda^\mu{}_\nu \gamma^0 \gamma^\nu \gamma^0 \gamma^0 &= \gamma^0 S^\dagger \gamma^0 \gamma^\mu \gamma^0 S^{\dagger -1} \gamma^0 \\ \Lambda^\mu{}_\nu \gamma^\nu = S^{-1} \gamma^\mu S &= \gamma^0 S^\dagger \gamma^0 \gamma^\mu (\gamma^0 S^\dagger \gamma^0)^{-1} , \end{aligned}$$

since $(\gamma^0)^{-1} = \gamma^0$. Furthermore, on the left-hand side we have made the substitution $\Lambda^\mu{}_\nu \gamma^\nu = S^{-1}\gamma^\mu S$. We now multiply by S and S^{-1}:

$$\gamma^\mu = S\gamma^0 S^\dagger \gamma^0 \gamma^\mu (\gamma^0 S^\dagger \gamma^0)^{-1} S^{-1} \equiv (S\gamma^0 S^\dagger \gamma^0) \gamma^\mu (S\gamma^0 S^\dagger \gamma^0)^{-1} .$$

Thus, $S\gamma^0 S^\dagger \gamma^0$ commutes with all γ^μ and is therefore a multiple of the unit matrix

$$S\gamma^0 S^\dagger \gamma^0 = b\mathbb{1} , \tag{6.58}$$

which also implies that

$$S\gamma^0 S^\dagger = b\gamma^0 \tag{6.59}$$

and yields the relation we are seeking [1]

$$S^\dagger \gamma^0 = b(S\gamma^0)^{-1} = b\gamma^0 S^{-1} . \tag{6.54a}$$

Since $(\gamma^0)^\dagger = \gamma^0$ and $S\gamma^0 S^\dagger$ are hermitian, by taking the adjoint of (6.59) one obtains $S\gamma^0 S^\dagger = b^* \gamma^0$, from which it follows that

$$b^* = b \tag{6.60}$$

and thus b is real. Making use of the fact that the normalization of S is fixed by $\det S = 1$, on calculating the determinant of (6.59), one obtains $b^4 = 1$. This, together with (6.60), yields:

$$b = \pm 1 . \tag{6.61}$$

[1] Note: For the Lorentz transformation $L_+^\uparrow$ (restricted L.T. and rotations) and for spatial reflections, one can derive this relation with $b = 1$ from the explicit representations.

The significance of the sign in (6.61) becomes apparent when one considers

$$\begin{aligned} S^\dagger S &= S^\dagger \gamma^0 \gamma^0 S = b\gamma^0 S^{-1}\gamma^0 S = b\gamma^0 \Lambda^0{}_\nu \gamma^\nu \\ &= b\Lambda^0{}_0 \mathbb{1} + \sum_{k=1}^{3} b\Lambda^0{}_k \underbrace{\gamma^0\gamma^k}_{\alpha^k} . \end{aligned} \tag{6.62}$$

$S^\dagger S$ has positive definite eigenvalues, as can be seen from the following. Firstly, $\det S^\dagger S = 1$ is equal to the product of all the eigenvalues, and these must therefore all be nonzero. Furthermore, $S^\dagger S$ is hermitian and its eigenfunctions satisfy $S^\dagger S \psi_a = a\psi_a$, whence

$$a\psi_a^\dagger \psi_a = \psi_a^\dagger S^\dagger S \psi_a = (S\psi_a)^\dagger S\psi_a > 0$$

and thus $a > 0$. Since the trace of $S^\dagger S$ is equal to the sum of all the eigenvalues, we have, in view of (6.62) and using $\operatorname{Tr}\alpha^k = 0$,

$$0 < \operatorname{Tr}(S^\dagger S) = 4b\Lambda^0{}_0 .$$

Thus $b\Lambda^0{}_0 > 0$. Hence, we have the following relationship between the signs of Λ^{00} and b:

$$\begin{aligned} \Lambda^{00} &\geqslant 1 \quad \text{for} \quad b = 1 \\ \Lambda^{00} &\leqslant -1 \quad \text{for} \quad b = -1 . \end{aligned} \tag{6.54b}$$

For Lorentz transformations that do not change the direction of time, we have $b = 1$; while those that do cause time reversal have $b = -1$.

Transformation of Bilinear Forms

The *adjoint* spinor is defined by

$$\bar{\psi} = \psi^\dagger \gamma^0 . \tag{6.63}$$

We recall that $\psi^\dagger$ is referred to as a hermitian adjoint spinor. The additional introduction of $\bar{\psi}$ is useful because it allows quantities such as the current density to be written in a concise form. We obtain the following transformation behaviour under a Lorentz transformation:

$$\psi' = S\psi \Longrightarrow \psi'^\dagger = \psi^\dagger S^\dagger \Longrightarrow \bar{\psi}' = \psi^\dagger S^\dagger \gamma^0 = b\psi^\dagger \gamma^0 S^{-1} , \tag{6.64}$$

thus,

$$\bar{\psi}' = b\bar{\psi} S^{-1} . \tag{6.65}$$

Given the above definition, the current density reads:

$$j^\mu = c\psi^\dagger \gamma^0 \gamma^\mu \psi = c\bar{\psi}\gamma^\mu \psi \tag{6.66}$$

and thus transforms as

$$j^{\mu'} = cb\bar{\psi} S^{-1} \gamma^\mu S\psi = cb\bar{\psi}\Lambda^\mu{}_\nu \gamma^\nu \psi = b\Lambda^\mu{}_\nu j^\nu . \tag{6.67}$$

Hence, j^μ transforms in the same way as a vector for Lorentz transformations without time reflection. In the same way one immediately sees, using (6.28a) and (6.65), that $\bar{\psi}(x)\psi(x)$ transforms as a scalar:

$$\begin{aligned} \bar{\psi}'(x')\psi'(x') &= b\bar{\psi}(x')S^{-1}S\psi(x') \\ &= b\bar{\psi}(x)\psi(x)\,. \end{aligned} \tag{6.68a}$$

We now summarize the transformation behaviour of the most important bilinear quantities under *orthochronous Lorentz transformations*, i.e., transformations that *do not reverse the direction of time*:

$$\bar{\psi}'(x')\psi'(x') = \bar{\psi}(x)\psi(x) \qquad \text{scalar} \tag{6.68a}$$
$$\bar{\psi}'(x')\gamma^\mu\psi'(x') = \Lambda^\mu{}_\nu\bar{\psi}(x)\gamma^\mu\psi(x) \qquad \text{vector} \tag{6.68b}$$
$$\bar{\psi}'(x')\sigma^{\mu\nu}\psi'(x') = \Lambda^\mu{}_\rho\Lambda^\nu{}_\sigma\bar{\psi}(x)\sigma^{\rho\sigma}\psi(x) \qquad \text{antisymmetric tensor} \tag{6.68c}$$
$$\bar{\psi}'(x')\gamma_5\gamma^\mu\psi'(x') = (\det\Lambda)\Lambda^\mu{}_\nu\bar{\psi}(x)\gamma_5\gamma^\nu\psi(x) \qquad \text{pseudovector} \tag{6.68d}$$
$$\bar{\psi}'(x')\gamma_5\psi'(x') = (\det\Lambda)\bar{\psi}(x)\gamma_5\psi(x) \qquad \text{pseudoscalar}\,, \tag{6.68e}$$

where $\gamma_5 = \imath\gamma^0\gamma^1\gamma^2\gamma^3$. We recall that $\det\Lambda = \pm 1$; for spatial reflections the sign is -1.

Chapter 7

Quantization of the Klein-Gordon and the Dirac fields

7.1 Canonical quantization of a scalar field

Important quantization procedures:

a) *Canonical quantization*: Canonical quantization is strongly oriented along the development of quantum mechanics. Suitable canonically conjugated variables (of the fields) are sought and then replaced by operators, where the Poisson bracket of classical physics turn into the commutator. A problem with this method is that time is treated as a distinct coordinate and so, inter alia, the Lorentz invariance of the quantized theory is not guaranteed. However, it has the great advantage that only physical states exist, because only physical modes are quantized. In addition, the procedure is simple, but its application can become very complicated, as in the case of non-Abelian gauge theories, for example.

b) *Path integral quantization*: This procedure is very elegant and fairly general. It is a very intuitive formulation that is also related to many other quantization methods. However, it has the disadvantage that the occurring functional integrals can be mathematically tricky.

c) *Gupta–Bleuler quantization*: This method is also known as *covariant quantization*. In contrast to canonical quantization, it preserves the Lorentz invariance of the classical theory. However, unphysical states with a negative norm, so-called "ghosts", are often generated.

d) *BRST quantization*: This method is named after physicists Becchi, Rouet, Stora and Tyupin. It is the most important quantization method for gauge theories, however, it also generates "ghost" states. There is a close connection with the path integral quantization.

The most physically relevant example of a quantized field is surely the electromagnetic (EM) field. However, as a preliminary we want to start with the quantization of the simple Klein-Gordon field. The insights gained in this way will benefit us later. The EM field is a vector field which satisfies the Klein-Gordon equation.

We consider a real scalar field ϕ satisfying the free Klein-Gordon (KG) equation

$$\left(\Box + \frac{m^2c^2}{\hbar^2}\right)\phi(x) = 0\,, \tag{7.1}$$

with $\Box = \partial_\mu \partial^\mu = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2$ and four-position x. Equation (7.1) describes for a real-valued ϕ a neutral particle with spin 0. The case of a complex wave function, describing charged particles, contains additional difficulties and will be considered elsewhere. Let's remind the Lorentz invariance of the KG equation: the wave function transforms according to $\phi'(x') = \phi(x)$ under Lorentz transformations $x' = \Lambda x$.

In the following we set $\hbar = c = 1$ and the free KG equation reads as

$$\boxed{\left(\Box + m^2\right)\phi(x) = 0\,.}$$

In case of $\nabla^2\phi = 0$, the KG equation reduces to the equation of a harmonic oscillator

$$\frac{\partial^2 \phi}{\partial t^2} = -m^2 \phi\,.$$

In the following, we interpret the field $\phi(x) = \phi(\mathbf{r}, t)$ as a displacement of a vibrating string at a position $\mathbf{r}$ and a time t. In addition, we consider the field to be in a volume $V = L^3$ with periodic boundary conditions and perform a spatial Fourier expansion

$$\phi(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{\imath \mathbf{k}\cdot\mathbf{r}} q_{\mathbf{k}}(t) \tag{7.2}$$

with Fourier coefficients $q^*_{\mathbf{k}} = q_{-\mathbf{k}}$, because ϕ is real-valued, and wave vectors $\mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$ with $n_{x,y,z} = 0, \pm 1, \pm 2, \ldots$, due to periodicity of ϕ. We end up with an equation of motion for the normal modes

$$\boxed{\ddot{q}_{\mathbf{k}} + \left(\mathbf{k}^2 + m^2\right) q_{\mathbf{k}} = 0}$$

or

$$\boxed{\ddot{q}_k + \omega_k^2 q_k = 0}$$

with the definition $\omega_k = \sqrt{\mathbf{k}^2 + m^2}$.
We move on to the Hamiltonian formulation and set

$$\dot{q}_k = p_{-k} \quad \text{and} \quad \dot{p}_{-k} = -\omega_k^2 q_k\,.$$

Hamilton's equations read as

$$\dot{q}_k = \frac{\partial H}{\partial p_k} \quad \text{and} \quad \dot{p}_{-k} = -\frac{\partial H}{\partial q_{-k}}$$

and we obtain the energy (Hamiltonian) of the scalar field

$$H = \sum_k \frac{1}{2}\left(p_k p_{-k} + \omega_k^2 q_k q_{-k}\right)\,.$$

Next, we introduce the transformation

$$b_k = \frac{1}{\sqrt{2\omega_k}}\left[\omega_k q_k + \imath p_{-k}\right] \quad \text{and} \quad b^*_k = \frac{1}{\sqrt{2\omega_k}}\left[\omega_k q_{-k} - \imath p_k\right]$$

and rewrite the canonical coordinates and impulses as

$$q_k = \frac{1}{\sqrt{2\omega_k}}\left(b_k + b^*_{-k}\right) \quad \text{and} \quad p_{-k} = -\imath\sqrt{\frac{\omega_k}{2}}\left(b_k - b^*_{-k}\right)\,. \tag{7.3}$$

Inserting this into the Hamiltonian leads to

$$\begin{aligned} H &= \sum_k \frac{1}{2}\left[-\frac{\omega_k}{2}\left(b_k - b^*_{-k}\right)\left(b_{-k} - b^*_k\right) + \frac{\omega_k}{2}\left(b_k + b^*_{-k}\right)\left(b_{-k} + b^*_k\right)\right] \\ &= \sum_k \frac{\omega_k}{2}\left[b_k b^*_k + b^*_{-k} b_{-k}\right] \\ &= \sum_k \omega_k b^*_k b_k \,. \end{aligned}$$

The quantization is carried out in analogy to the quantization of harmonic oscillator: canonically conjugated variables q_k and p_k become operators $\hat{q}_k$ and $\hat{p}_k$, and the Poisson bracket is replaced by the commutator:

$$[\hat{q}_k, \hat{p}_{k'}] = \imath\delta_{k,k'}\,, \quad [\hat{q}_k, \hat{q}_{k'}] = [\hat{p}_k, \hat{p}_{k'}] = 0$$

and using the new coordinates b_k and b^*_k we obtain the following commutation relations:

$$\left[\hat{b}_k, \hat{b}^\dagger_{k'}\right] = \delta_{k,k'}\,, \quad \left[\hat{b}_k, \hat{b}_{k'}\right] = \left[\hat{b}^\dagger_k, \hat{b}^\dagger_{k'}\right] = 0\,.$$

Thus, inserting the quantized version of (7.3) into (7.2) leads to the field operator

$$\begin{aligned} \hat{\phi}(\mathbf{r}, t) &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} e^{\imath\mathbf{k}\cdot\mathbf{r}} \frac{1}{\sqrt{2\omega_k}}\left[\hat{b}_k(t) + \hat{b}^\dagger_{-k}(t)\right] \\ &= \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_k}}\left[e^{\imath\mathbf{k}\cdot\mathbf{r}}\hat{b}_k(t) + e^{-\imath\mathbf{k}\cdot\mathbf{r}}\hat{b}^\dagger_k(t)\right]\,. \end{aligned}$$

The Heisenberg picture yields the time dependence of the operator

$$\hat{b}_k(t) = e^{\imath\hat{H}t}\hat{b}_k(0)e^{-\imath\hat{H}t}\,,$$

from which follows that

$$\imath\frac{\partial\hat{b}_k}{\partial t} = \left[\hat{b}_k, \hat{H}\right] = \omega_k\left[\hat{b}_k, \hat{b}^\dagger_k\hat{b}_k\right] = \omega_k\hat{b}_k\,.$$

The solution of this simple differential equation is

$$\hat{b}_k(t) = \hat{b}_k(0)e^{-\imath\omega_k t} = \hat{b}_k e^{-\imath\omega_k t}$$

and analog to

$$\hat{b}^\dagger_k(t) = \hat{b}^\dagger_k(0)e^{\imath\omega_k t} = \hat{b}^\dagger_k e^{\imath\omega_k t}\,.$$

And the new representation of the field operator is

$$\boxed{\hat{\phi}(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} \frac{1}{\sqrt{2\omega_k}}\left[e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\hat{b}_k + e^{-\imath(\mathbf{k}\cdot\mathbf{r}-\omega_k t)}\hat{b}^\dagger_k\right]}\,. \tag{7.4}$$

Vacuum expectation values are:

$$\langle 0|\hat{\phi}|0\rangle = 0$$

$$\langle 0|\hat{\phi}^2|0\rangle \to \frac{1}{(2\pi)^3}\int \frac{\mathrm{d}^3 k}{2\sqrt{k^2+m^2}} \quad \text{diverges!}$$

When quantizing a classical Hamiltonian there is some freedom how to choose the operator order, and different choices lead to different ground state energies. We have used the normal order, i.e., all creation operators are to the left of all annihilation operators in the product. We denote $:\hat{O}:$ as the normal ordered form of $\hat{O}$. It can be seen that when normally ordered operators, such as

$$:\hat{b}_k \hat{b}^\dagger_{k'}: = \hat{b}^\dagger_{k'} \hat{b}_k \,, \quad :\hat{b}^\dagger_{k'} \hat{b}_k: = \hat{b}^\dagger_{k'} \hat{b}_k \,, \quad \text{etc} \,,$$

are applied to the vacuum, many contributions of expectation values disappear.

About micro-causality:

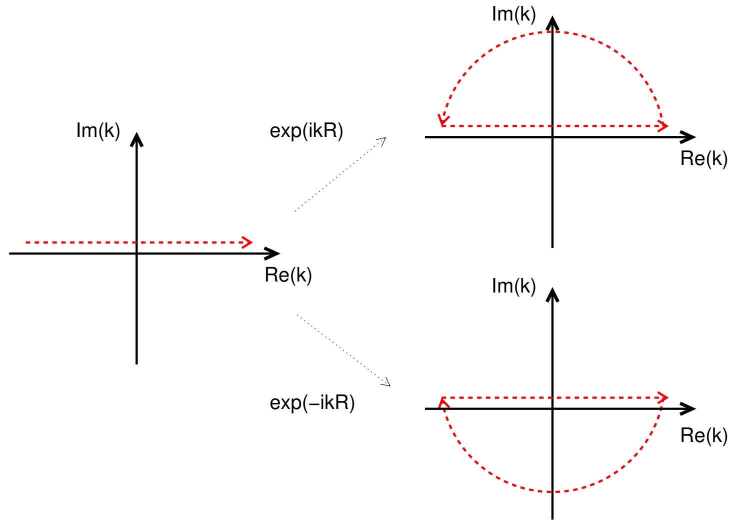
$$\begin{aligned}
[\hat{\phi}(\mathbf{r},t), \hat{\phi}(\mathbf{r}',t')] &= \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}'} \frac{1}{2\sqrt{\omega_\mathbf{k}\omega_{\mathbf{k}'}}} \underbrace{[\hat{b}_\mathbf{k} e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_\mathbf{k} t)} + \hat{b}^\dagger_\mathbf{k} e^{-\imath(\mathbf{k}\cdot\mathbf{r}-\omega_\mathbf{k} t)}, \hat{b}_{\mathbf{k}'} e^{\imath(\mathbf{k}'\cdot\mathbf{r}'-\omega_{\mathbf{k}'} t')} + \hat{b}^\dagger_{\mathbf{k}'} e^{-\imath(\mathbf{k}'\cdot\mathbf{r}'-\omega_{\mathbf{k}'} t')}]}_{=\underbrace{[\hat{b}_\mathbf{k}, \hat{b}^\dagger_{\mathbf{k}'}]}_{=\delta_{\mathbf{k},\mathbf{k}'}} e^{\imath(\mathbf{k}\cdot\mathbf{r}-\omega_\mathbf{k} t)} e^{-\imath(\mathbf{k}'\cdot\mathbf{r}'-\omega_{\mathbf{k}'} t')} + \underbrace{[\hat{b}^\dagger_\mathbf{k}, \hat{b}_{\mathbf{k}'}]}_{=-\delta_{\mathbf{k},\mathbf{k}'}} e^{-\imath(\mathbf{k}\cdot\mathbf{r}-\omega_\mathbf{k} t)} e^{\imath(\mathbf{k}'\cdot\mathbf{r}'-\omega_{\mathbf{k}'} t')}} \\
&= \frac{1}{V} \sum_\mathbf{k} \frac{1}{2\omega_\mathbf{k}} \underbrace{\left(e^{\imath\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')-\imath\omega_\mathbf{k}(t-t')} - e^{-\imath\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')+\imath\omega_\mathbf{k}(t-t')} \right)}_{2\imath \mathrm{Im}\left(e^{\imath\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}')-\imath\omega_\mathbf{k}(t-t')}\right)} \\
&= 2\imath \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \frac{1}{2\omega_\mathbf{k}} \mathrm{Im}\left(e^{\imath\mathbf{k}\cdot\mathbf{R}-\imath\omega_\mathbf{k} T} \right)
\end{aligned}$$

with $\mathbf{R} = \mathbf{r} - \mathbf{r}'$ and $T = t - t'$.

$$\begin{aligned}
[\hat{\phi}(\mathbf{r},t), \hat{\phi}(\mathbf{r}',t')] &= \frac{2\imath}{(2\pi)^3} \mathrm{Im} \int_0^\infty \frac{k^2 dk}{2\omega_\mathbf{k}} e^{-\imath\omega_\mathbf{k} T} \underbrace{\int d\Omega e^{\imath\mathbf{k}\cdot\mathbf{R}}}_{\substack{= 2\pi \int_0^\pi d\theta \sin\theta e^{\imath kR\cos\theta} = 2\pi \int_{-1}^1 d\eta e^{\imath kR\eta} \\ = 2\pi \frac{e^{\imath kR} - e^{-\imath kR}}{\imath KR} = \frac{4\pi}{kR} \sin kR}} \\
&= \frac{\imath}{2\pi^2 R} \underbrace{\int_0^\infty}_{=\frac{1}{2}\int_{-\infty}^{+\infty}} \frac{kdk}{\omega_\mathbf{k}} \sin(kR) \underbrace{\mathrm{Im} e^{-\imath\omega_\mathbf{k} T}}_{=-\sin(\omega_\mathbf{k} T)} \\
&= -\frac{\imath}{4\pi^2 R} \int_{-\infty}^{+\infty} \frac{kdk}{\omega_\mathbf{k}} \sin(kR) \sin(\omega_\mathbf{k} T) \\
&= -\frac{1}{8\pi^2 R} \int_{-\infty}^{+\infty} \frac{kdk}{\sqrt{k^2+m^2}} \sin(\sqrt{k^2+m^2} T) \left(e^{\imath kR} - e^{-\imath kR} \right) .
\end{aligned} \tag{7.5}$$

Close integration contour and use residue theorem. The first term goes to $e^{\pm\imath kT} e^{\imath kR}$ when $|k| \to \infty$. We get: $e^{-\mathrm{Im}k(\pm T+R)+\imath\mathrm{Re}k(\pm T+R)}$ which gives zero for $R > |T|$ for $\mathrm{Re}k > 0$. With these conditions,

$$\left| \int_\mathcal{C} dk e^{\imath \overbrace{k(\pm T+R)}^{=\varepsilon>0}} \right| = \left| \int_0^\pi d\varphi e^{\imath\varepsilon\rho(\cos\varphi + \imath\sin\varphi)} \right| \le \int_0^\pi d\varphi \left| e^{-\varepsilon\rho\sin\varphi} \right| \left| e^{\imath\varepsilon\rho\cos\varphi} \right| = \int_0^\pi d\varphi \underbrace{e^{-\varepsilon\rho\sin\varphi}}_{\to 0 \text{ when } \rho\to\infty} .$$



Thus

$$\left[\hat{\phi}(\mathbf{r},t),\hat{\phi}(\mathbf{r}',t')\right]=0 \quad \text{for } |\mathbf{r}-\mathbf{r}'|>|t-t'|$$

and

$$\left[\hat{\phi}(\mathbf{r},t),\hat{\phi}(\mathbf{r}',t')\right]\neq 0 \quad \text{for } |\mathbf{r}-\mathbf{r}'|\leq|t-t'|\,.$$

This result can be interpreted as follows. The field amplitude $\hat{\phi}(\mathbf{r},t)$ is a physical quantity. If the commutator vanishes then both quantities are compatible with each other: if $\hat{\phi}(\mathbf{r},t)$ is precisely measurable then also $\hat{\phi}(\mathbf{r}',t')$. This is only possible for $|\mathbf{r}-\mathbf{r}'|>|t-t'|$, i.e., only for distances $|\mathbf{r}-\mathbf{r}'|$ which can not be connected via a signal within $|t-t'|$. Thus, the fact that the commutator vanishes for spacelike distances between events $(\mathbf{r},t)$ and $(\mathbf{r}',t')$ is closely related to causality.

Now we can justify why we have choosen bosonic creation and annihilation operators during quantization of the KG field. If we would consider fermions and thus use anti-commutation relation $\left\{\hat{b}_k,\hat{b}^\dagger_{k'}\right\}=\delta_{k,k'}$ etc., instead of $\left[\hat{b}_k,\hat{b}^\dagger_{k'}\right]=\delta_{k,k'}$ etc., then $\left[\hat{\phi}(\mathbf{r},t),\hat{\phi}(\mathbf{r}',t')\right]\neq 0$ for all $(\mathbf{r},t)$ and $(\mathbf{r}',t')$, and causality would not be satisfied.

We see that Fermi statistics is incompatible with the causality requirement of the Klein-Gordon equation. This is an essential building block for the spin-statistics theorem. In general one can say that for Klein-Gordon-like equations for particles with integer spins (0, 1, 2, ...) the Bose statistics is enforced by the causality.

Now we want to estimate the momentum $\hat{\mathbf{p}}$ of the quantized field $\hat{\phi}(\mathbf{r})$. For that we have to examine the behavior of ϕ under translation

$$T(\mathbf{a})\hat{\phi}(\mathbf{r})T^{-1}(\mathbf{a})=\hat{\phi}(\mathbf{r}+\mathbf{a}) \quad \text{with} \quad T(\mathbf{a})=e^{-\imath\hat{\mathbf{p}}\cdot\mathbf{a}}\,.$$

If $\mathbf{a}$ is infinitesimal then $T(\mathbf{a})=1-\imath\hat{\mathbf{p}}\cdot\mathbf{a}$. With the Taylor expansion of $\hat{\phi}(\mathbf{r}+\mathbf{a})$ up to first order we get

$$(1-\imath\hat{\mathbf{p}}\cdot\mathbf{a})\,\hat{\phi}(\mathbf{r})\,(1+\imath\hat{\mathbf{p}}\cdot\mathbf{a})=\hat{\phi}(\mathbf{r})+\nabla\hat{\phi}(\mathbf{r})\cdot\mathbf{a}+\mathcal{O}(a^2)$$

and thus

$$-\imath\left[\hat{\mathbf{p}},\hat{\phi}(\mathbf{r})\right]=\nabla\hat{\phi}(\mathbf{r})\,.$$

Using the expression for the quantized field (7.4) we obtain

$$\left[\hat{\mathbf{p}},\hat{b}_{\mathbf{k}}\right]=\mathbf{k}\hat{b}_{\mathbf{k}}\,.$$

This determines the form of the momentum operator up to an additive constant

$$\boxed{\hat{\mathbf{p}} = \sum_{\mathbf{k}} \mathbf{k} \hat{b}^\dagger_{\mathbf{k}} \hat{b}_{\mathbf{k}}} .$$

7.2 Alternative quantization of a scalar field

A classical observable of a neutral meson wave is a real-valued scalar field

$$\psi(x) = \psi^*(x) ,$$

which obeys the Klein-Gordon equation

$$(\Box + m^2)\psi(x) = 0 .$$

There are two types of solutions

$$\psi_+(x) = e^{\imath(\omega t - \mathbf{kx})} \quad \text{and} \quad \psi_-(x) = e^{-\imath(\omega t - \mathbf{kx})}$$

with $\omega = \sqrt{m^2 + \mathbf{k}^2}$.
Ansatz for a general solution is

$$\psi(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{1}{2\omega} \left(e^{\imath kx} \alpha^*(\mathbf{k}) + e^{-\imath kx} \alpha(\mathbf{k}) \right) \tag{7.6}$$

with $k = (\omega, \mathbf{k})$ and $kx = k^\mu x_\mu = \omega t - \mathbf{k} \cdot \mathbf{x}$.
Quantization: The meson field $\psi(x) = \langle \text{state} | \hat{\Phi}(x) | \text{state} \rangle$ is an observable corresponding to an expectation value of a field operator $\hat{\Phi}(x)$.

1st assumption

$$\hat{\Phi}(x) \text{ is Hermitian, thus } \hat{\Phi}(x) = \hat{\Phi}^\dagger(x)$$
$$\hat{\Phi}(x) \text{ fulfills KG equation } \left(\Box + m^2 \right) \hat{\Phi}(x) = 0$$

Momentum and energy are observables and thus correspond to Hermitian operators $\hat{\mathbf{p}}$ and $\hat{H}$, respectively. Due to relativistic invariance they are combined into a four-operator

$$\hat{p} = (\hat{p}^\mu) = (\hat{H}, \hat{\mathbf{p}})$$

and $\hat{p}^\mu$ is time-independent because of energy-momentum conservation.
In the Heisenberg picture any operator $\hat{A}(t, \mathbf{x})$ obeys

$$\begin{aligned} \frac{\partial}{\partial t} \hat{A}(t, \mathbf{x}) &= \imath \left[\hat{H}, \hat{A}(t, \mathbf{x}) \right] \\ \frac{\partial}{\partial x^j} \hat{A}(t, \mathbf{x}) &= -\imath \left[\hat{p}^j, \hat{A}(t, \mathbf{x}) \right] \quad \text{for} \quad j = 1, 2, 3 . \end{aligned}$$

2nd assumption

$$\frac{\partial}{\partial x^\mu} \hat{\Phi}(x) = \imath \left[\hat{p}_\mu, \hat{\Phi}(x) \right] \tag{7.7}$$

1st and 2nd assumption lead to a particle interpretations of the meson field.
In analogy to (7.6) the general form of the field operator is

$$\hat{\Phi}(x) = \int \frac{\mathrm{d}^3 k}{(2\pi)^3} \frac{1}{2\omega} \left(e^{\imath kx} \hat{a}^\dagger(\mathbf{k}) + e^{-\imath kx} \hat{a}(\mathbf{k}) \right) .$$

The operator $\hat{a}^\dagger(\mathbf{k})$ denotes the Hermitian conjugate of $\hat{a}(\mathbf{k})$.
From (7.7) follows that

$$\int \frac{d^3 k}{(2\pi)^3} \frac{1}{2\omega} \left(e^{\imath kx} \imath k_\mu \hat{a}^\dagger(\mathbf{k}) + e^{-\imath kx} (-\imath k_\mu) \hat{a}(\mathbf{k}) \right) = \imath \int \frac{d^3 k}{(2\pi)^3} \frac{1}{2\omega} \left(e^{\imath kx} \left[\hat{p}_\mu,\, \hat{a}^\dagger(\mathbf{k}) \right] + e^{-\imath kx} \left[\hat{p}_\mu,\, \hat{a}(\mathbf{k}) \right] \right)$$

and thus

$$\left[\hat{p}_\mu,\, \hat{a}^\dagger(\mathbf{k}) \right] = k_\mu \hat{a}^\dagger(\mathbf{k}) \quad \text{and} \quad \left[\hat{p}_\mu,\, \hat{a}(\mathbf{k}) \right] = -k_\mu \hat{a}(\mathbf{k}) . \tag{7.8}$$

We define $|0\rangle$ as a vacuum state (no particle exists), which is normalized as $\langle 0|0\rangle = 1$.

It is $\hat{p}_\mu |0\rangle = 0$ and thus

$$\left[\hat{p}_\mu,\, \hat{a}^\dagger(\mathbf{k}) \right] |0\rangle = k_\mu \hat{a}^\dagger(\mathbf{k}) |0\rangle \quad \Rightarrow \quad \hat{p}_\mu \hat{a}^\dagger(\mathbf{k}) |0\rangle = k_\mu \hat{a}^\dagger(\mathbf{k}) |0\rangle .$$

Thus $|\mathbf{k}\rangle = \hat{a}^+(\mathbf{k}) |0\rangle$ is the eigenstate of the energy and momentum operator with eigenvalue $k_\mu = (\omega,\, \mathbf{k})$. We identify this state as a **one-meson-state** with a sharp energy ω and a sharp momentum $\mathbf{k}$.

Due to $\hat{p}_\mu \hat{a}(\mathbf{k}) |0\rangle = -k_\mu \hat{a}(\mathbf{k}) |0\rangle$ the state $\hat{a}(\mathbf{k}) |0\rangle$ would correspond to a state with negative energy. Thus we demand

$$\hat{a}(\mathbf{k}) |0\rangle = 0 \qquad \forall \mathbf{k} .$$

Similarly, for a state $|p\rangle$ with $\hat{p}^\mu |p\rangle = p^\mu |p\rangle$, i.e., the eigenstate of the four-momentum, follows with (7.8) that

$$\begin{aligned} \hat{p}^\mu \hat{a}^\dagger(\mathbf{k}) |p\rangle &= (p^\mu + k^\mu)\, \hat{a}^\dagger(\mathbf{k}) |p\rangle \\ \hat{p}^\mu \hat{a}(\mathbf{k}) |p\rangle &= (p^\mu - k^\mu)\, \hat{a}(\mathbf{k}) |p\rangle . \end{aligned}$$

And we obtain

$$\hat{p}^\mu \hat{a}^\dagger(\mathbf{k}_1) \hat{a}^\dagger(\mathbf{k}_2) |0\rangle = (k_1^\mu + k_2^\mu) \underbrace{\hat{a}^\dagger(\mathbf{k}_1) \hat{a}^\dagger(\mathbf{k}_2) |0\rangle}_{\text{two-meson-state}}$$

and in a similar way one constructs a n-meson-state.
We can interpret $\hat{a}^\dagger$ as creation operator and $\hat{a}$ as annihilation operator.

We do not know yet anything about the norm of states with one or more mesons. We need an additional physical assumption. Consider a measurement of the meson field at two different space-time points $x = (t, \mathbf{x})$ and $y = (t', \mathbf{y})$. For $(x-y)^2 < 0$, x is outside the future light cone of y and vice versa. Thus, no signal from the measurement at point x can reach y and vice versa.

3rd assumption

Microcausality: $\left[\hat{\Phi}(x),\, \hat{\Phi}(y) \right] = 0$ for $(x-y)^2 < 0$

That means

$$\left[\hat{\Phi}(t,\mathbf{x}),\ \hat{\Phi}(t',\mathbf{y})\right] = 0 \text{ for } |t'-t| < |\mathbf{x}-\mathbf{y}| \neq 0$$

and, in particular, for $\mathbf{x} \neq \mathbf{y}$

$$\left[\hat{\Phi}(t,\mathbf{x}),\ \hat{\Phi}(t,\mathbf{y})\right] = 0$$
$$\left[\hat{\Phi}(t,\mathbf{x}),\ \frac{\partial}{\partial t}\hat{\Phi}(t,\mathbf{y})\right] = 0\,.$$

In the following we want to show that the Bose character of mesons follows from microcausality. The general form of the field operator and its time derivative reads as

$$\hat{\Phi}(t,\mathbf{x}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{1}{2\omega}e^{-\imath\mathbf{k}\cdot\mathbf{x}}\left(e^{\imath\omega t}\hat{a}^\dagger(\mathbf{k}) + e^{-\imath\omega t}\hat{a}(-\mathbf{k})\right)$$
$$\frac{\partial}{\partial t}\hat{\Phi}(t,\mathbf{x}) = \int \frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\imath}{2}e^{-\imath\mathbf{k}\cdot\mathbf{x}}\left(e^{\imath\omega t}\hat{a}^\dagger(\mathbf{k}) - e^{-\imath\omega t}\hat{a}(-\mathbf{k})\right)\,.$$

The inverse Fourier transformation gives

$$e^{\imath\omega t}\hat{a}^\dagger(\mathbf{k}) + e^{-\imath\omega t}\hat{a}(-\mathbf{k}) = 2\omega\int d^3\mathbf{x}\, e^{-\imath\mathbf{k}\cdot\mathbf{x}}\hat{\Phi}(t,\mathbf{x}) \tag{7.9}$$
$$e^{\imath\omega t}\hat{a}^\dagger(\mathbf{k}) - e^{-\imath\omega t}\hat{a}(-\mathbf{k}) = -2\imath\int d^3\mathbf{x}\, e^{-\imath\mathbf{k}\cdot\mathbf{x}}\frac{\partial}{\partial t}\hat{\Phi}(t,\mathbf{x})\,. \tag{7.10}$$

Thus from (7.9) follows that

$$\left[e^{\imath\omega_1 t}\hat{a}^\dagger(\mathbf{k}_1) + e^{-\imath\omega_1 t}\hat{a}(-\mathbf{k}_1),\ e^{\imath\omega_2 t}\hat{a}^\dagger(\mathbf{k}_2) + e^{-\imath\omega_2 t}\hat{a}(-\mathbf{k}_2)\right]$$
$$= 2\omega_1 2\omega_2\int \mathrm{d}^3x\mathrm{d}^3y\, e^{-\imath\mathbf{k}_1\cdot\mathbf{x}}e^{-\imath\mathbf{k}_2\cdot\mathbf{y}}\underbrace{\left[\hat{\Phi}(t,\mathbf{x}),\ \hat{\Phi}(t,\mathbf{y})\right]}_{\substack{=0\\ \text{microcausality}}}$$

and

$$e^{+\imath(\omega_1+\omega_2)t}\left[\hat{a}^\dagger(\mathbf{k}_1),\ \hat{a}^\dagger(\mathbf{k}_2)\right] + e^{-\imath(\omega_1+\omega_2)t}\left[\hat{a}(-\mathbf{k}_1),\ \hat{a}(-\mathbf{k}_2)\right]$$
$$+ e^{+\imath(\omega_1-\omega_2)t}\left[\hat{a}^\dagger(\mathbf{k}_1),\ \hat{a}(-\mathbf{k}_2)\right] + e^{-\imath(\omega_1-\omega_2)t}\left[\hat{a}(-\mathbf{k}_1),\ \hat{a}^\dagger(\mathbf{k}_2)\right] = 0\,.$$

To ensure that this is always true, the following must hold

$$\left[\hat{a}^\dagger(\mathbf{k}_1),\ \hat{a}^\dagger(\mathbf{k}_2)\right] = 0 \quad\text{and}\quad \left[\hat{a}(\mathbf{k}_1),\ \hat{a}(\mathbf{k}_2)\right] = 0 \qquad \forall\, \mathbf{k}_1,\ \mathbf{k}_2\,. \tag{7.11}$$

This means that mesons have Bose character.

The relation between microcausality and the Bose character of mesons does not only apply to free fields considered here. In general, microcausality determines the Bose-character of all particles with integer spin (Pauli 1936, 1940).

Next, we want to compute the commutator of $\hat{a}$ and $\hat{a}^\dagger$. If we solve for $\hat{a}$ and $\hat{a}^\dagger$ from (7.9) and (7.10) , respectively, we obtain the following:

Eqs. (7.9)+(7.10) gives

$$\hat{a}^\dagger(\mathbf{k})e^{\imath\omega t} = \int d^3\mathbf{x} e^{-\imath\mathbf{k}\cdot\mathbf{x}} \left[\omega\hat{\Phi}(t,\mathbf{x}) - \imath\frac{\partial}{\partial t}\hat{\Phi}(t,\mathbf{x})\right],$$

and Eqs. (7.9)−(7.10) gives

$$\hat{a}(\mathbf{k})e^{-\imath\omega t} = \int d^3\mathbf{x} e^{\imath\mathbf{k}\cdot\mathbf{x}} \left[\omega\hat{\Phi}(t,\mathbf{x}) + \imath\frac{\partial}{\partial t}\hat{\Phi}(t,\mathbf{x})\right].$$

Therefore,

$$\begin{aligned}
[\hat{a}(\mathbf{k_1}),\hat{a}^\dagger(\mathbf{k_2})] &= \left[e^{-\imath\omega_1 t}\int d^3\mathbf{x} e^{\imath\mathbf{k_1}\cdot\mathbf{x}}\left[\omega_1\hat{\Phi}(t,\mathbf{x}) + \imath\partial_t\hat{\Phi}(t,\mathbf{x})\right], e^{\imath\omega_2 t} d^3\mathbf{y} e^{-\imath\mathbf{k_2}\cdot\mathbf{y}}\left[\omega_2\hat{\Phi}(t,\mathbf{y}) - \imath\partial_t\hat{\Phi}(t,\mathbf{y})\right]\right] \\
&= e^{\imath(\omega_1-\omega_2)t}\int d^3\mathbf{x}\int d^3\mathbf{y} e^{\imath\mathbf{k_1}\cdot\mathbf{x} - \imath\mathbf{k_2}\cdot\mathbf{y}} \underbrace{[\omega_1\hat{\Phi}(t,\mathbf{x}) + \imath\partial_t\hat{\Phi}(t,\mathbf{x}), \omega_2\hat{\Phi}(t,\mathbf{y}) - \imath\partial_t\hat{\Phi}(t,\mathbf{y})]}_{\imath\omega_2 \underbrace{[\partial_t\hat{\Phi}(\mathbf{x},t),\hat{\Phi}(\mathbf{y},t)]}_{=0 \text{ for } \mathbf{x}\neq\mathbf{y}} - \imath\omega_1 \underbrace{[\hat{\Phi}(\mathbf{x},t),\partial_t\hat{\Phi}(\mathbf{y},t)]}_{=0 \text{ for } \mathbf{x}\neq\mathbf{y}}}
\end{aligned}$$

The integrand vanishes for $\mathbf{x} \neq \mathbf{y}$ and contains a δ contribution for $\mathbf{x} = \mathbf{y}$, otherwise all creation operators would commute with all annihilation operators and therefore all states obtained by applying creation operators onto the vacuum state would equal the zero vector. Therefore, we make an ansatz for the canonical commutation relation as

$$\left[\hat{\Phi}(t,\mathbf{x}), \frac{\partial}{\partial t}\hat{\Phi}(t,\mathbf{y})\right] = \imath\delta^3(\mathbf{x}-\mathbf{y})$$

and obtain

$$\begin{aligned}
[\hat{a}(\mathbf{k_1}),\hat{a}^\dagger(\mathbf{k_2})] &= e^{\imath(\omega_1-\omega_2)t}\underbrace{\int d^3\mathbf{x} e^{\imath(\mathbf{k_1}-\mathbf{k_2})\cdot\mathbf{x}}}_{=(2\pi)^3\delta^3(\mathbf{k_1}-\mathbf{k_2})}(\omega_1+\omega_2) \\
&= 2\omega_1(2\pi)^3\delta^3(\mathbf{k_1}-\mathbf{k_2}),
\end{aligned}$$

since $\omega_1 = \omega_2$ if $\mathbf{k_1} = \mathbf{k_2}$.

7.3 Lagrangian formalism and canonical quantization

Lagrangian density $\mathcal{L}(\Phi,\partial_\mu\Phi)$ for scalar fields:

$$\boxed{\mathcal{L} = \frac{1}{2}\left[\partial_\mu\Phi\partial^\mu\Phi - m^2\Phi^2\right]} \tag{7.12}$$

which gives the Lagrange function:

$$L(x^0) = \int d^3\mathbf{x}\mathcal{L}(\Phi,\partial_\mu\Phi).$$

The action is

$$S[\Phi] = \int dx\mathcal{L}(\Phi,\partial_\mu\Phi) = \int dx^0 L(x^0).$$

Hamiltion principle gives the Klein-Gordon equation

$$\delta S[\Phi] = 0 \quad \Rightarrow \quad \partial_\nu\partial^\nu\Phi + m^2\Phi = 0.$$

Proof:

$$\begin{aligned}\delta S &= \int_\Omega dx \left[\frac{\partial \mathcal{L}}{\partial \Phi}\delta\Phi + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} \underbrace{\delta(\partial_\mu \Phi)}_{=\frac{\partial}{\partial x^\mu}\delta\Phi}\right] \\ &= \int_\Omega dx \left[\frac{\partial \mathcal{L}}{\partial \Phi} - \frac{\partial}{\partial x^\mu}\frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)}\right]\delta\Phi + \underbrace{\int_\Omega dx \frac{\partial}{\partial x^\mu}\left[\frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)}\delta\Phi\right]}_{=\int_{\partial\Omega} d\sigma \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)}\delta\Phi = 0}\end{aligned}$$

$\delta S = 0$ then gives the Euler-Lagrange equation:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \Phi} - \frac{\partial}{\partial x^\mu}\frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} = 0}.$$

We have for Eq. (7.12)

$$\frac{\partial \mathcal{L}}{\partial \Phi} = -m^2\Phi \qquad \text{and} \qquad \frac{\partial \mathcal{L}}{\partial(\partial_\mu \Phi)} = \partial^\mu \Phi,$$

which yields to the KG equation:

$$-m^2\Phi - \frac{\partial}{\partial x^\mu}\partial^\mu\Phi = 0 \quad \Rightarrow \quad \partial_\mu\partial^\mu\Phi + m^2\Phi = 0.$$

Definition: canonical conjugate momentum:

$$\boxed{\Pi = \frac{\partial L}{\partial \dot{\Phi}} = \frac{\partial \mathcal{L}}{\partial \dot{\Phi}} = \frac{\partial \mathcal{L}}{\partial(\partial_0 \Phi)}}.$$

Definition: Hamilton-function:

$$\boxed{H(\Phi, \Pi) = \int d^3\mathbf{x} \left[\Pi\dot{\Phi} - \mathcal{L}(\Phi, \partial_\mu \Phi)\right]},$$

for the Hamilton-density

$$\mathcal{H}(\Phi, \Pi) = \Pi\dot{\Phi} - \mathcal{L}(\Phi, \partial_\mu \Phi).$$

Since $\Pi = \dot{\Phi}$,

$$\begin{aligned}\mathcal{H}(\Phi, \Pi) &= \Pi^2 - \frac{1}{2}\left[\underbrace{\partial_0\Phi\partial^0\Phi}_{=\Pi^2} + \underbrace{\partial_i\Phi\partial^i\Phi}_{=(\nabla\Phi)^2} - m^2\Phi^2\right] \\ &= \frac{1}{2}\left[\Pi^2 + (\nabla\Phi)^2 + m^2\Phi^2\right].\end{aligned}$$

Canonical quantization:
Since Φ and Π are canaonical conjugate fields (due to the definition $\Pi = \frac{\partial L}{\partial \dot{\Phi}}$), one postulates "Canonical commutation relations" (as in basic quantum mechanics):

$$\boxed{\begin{aligned}[\hat{\Phi}(\mathbf{r}, t), \hat{\Pi}(\mathbf{r}', t)] &= \imath\delta(\mathbf{r} - \mathbf{r}'), \\ [\hat{\Phi}(\mathbf{r}, t), \hat{\Phi}(\mathbf{r}', t)] &= [\hat{\Pi}(\mathbf{r}, t), \hat{\Pi}(\mathbf{r}', t)] = 0.\end{aligned}}$$

This procedure is called *canonical quantization.* For KG-field: $\hat{\Pi} = \partial_t \hat{\Phi}$,

$$\left[\hat{\Phi}(\mathbf{r},t), \frac{\partial}{\partial t}\hat{\Phi}(\mathbf{r}',t)\right] = \imath\delta(\mathbf{r}-\mathbf{r}').$$

For the free scalar field with a Lagrangian density (7.12) the canonical quantization yields the same quantized field as obtained in the previous chapters and the Hamiltonian reads as

$$\hat{H} = \frac{1}{2}\int d^3\mathbf{x}\,\left[(\partial_t\hat{\Phi})^2 + (\nabla\hat{\Phi})^2 + m^2\hat{\Phi}^2\right].$$

Remark: For the gauge theories that dominate particle physics today, the canonical quantization can only be carried out for special gauges (cf. quantization of the electromagnetic field).

7.4 Quantization of the Dirac Field

First we recapitulate the derivation of the calculation of the Dirac spinor. The Dirac equation is

$$(-\imath\gamma^\mu\partial_\mu + m)\psi = 0.$$

Ansatz (plane wave with positive energy):

$$\psi = ue^{-\imath kx}.$$

The equation for the spinor u is

$$(k_\mu\gamma^\mu - m)u = 0.$$

Since

$$(k_\mu\gamma^\mu - m)(k_\nu\gamma^\nu + m) = k_\mu k_\nu \underbrace{\gamma^\mu\gamma^\nu}_{=\frac{1}{2}\{\gamma^\mu,\gamma^\nu\}=g^{\mu\nu}} - m^2 = k_\mu k^\mu - m^2 = 0,$$

we have

$$u_r(k) = \mathcal{N}(k_\mu\gamma^\mu + m)u_r(0).$$

Normalization:

$$u_r(0) = (\chi_r, 0) \qquad \text{and} \qquad \bar{u}_r u_s = \delta_{rs}.$$

$$\Rightarrow \qquad \boxed{u_r(k) = \frac{1}{\sqrt{2m(m+E)}}(k_\mu\gamma^\mu + m)u_r(0)}.$$

$$u_r(k) = \frac{1}{\sqrt{2m(m+E)}}\begin{pmatrix} E+m & -\mathbf{k}\cdot\boldsymbol{\sigma} \\ \mathbf{k}\cdot\boldsymbol{\sigma} & -E+m\end{pmatrix}\begin{pmatrix}\chi_r \\ 0\end{pmatrix} = \begin{pmatrix}\sqrt{\frac{E+m}{2m}}\chi_r \\ \frac{\mathbf{k}\cdot\boldsymbol{\sigma}}{\sqrt{2m(m+E)}}\chi_r\end{pmatrix} = \sqrt{\frac{E+m}{2m}}\begin{pmatrix}\chi_r \\ \frac{\mathbf{k}\cdot\boldsymbol{\sigma}}{m+E}\chi_r\end{pmatrix}.$$

Note $\gamma^{\mu\dagger} = \gamma^0\gamma^\mu\gamma^0$ and

$$\begin{aligned}\bar{u} = u^\dagger\gamma^0 &= \mathcal{N}\left[(k_\mu\gamma^\mu + m)u(0)\right]^\dagger\gamma^0 \\ &= \mathcal{N}u(0)^T(k_\mu\gamma^{\mu\dagger} + m)\gamma^0 = \mathcal{N}u(0)^T\gamma^0(k_\mu\gamma^\mu + m) \\ &= \frac{1}{\sqrt{2m(m+E)}}\bar{u}(0)(k_\mu\gamma^\mu + m).\end{aligned}$$

Analogously for plane wave with negative energy:

$$\psi = ve^{+\imath kx},$$

the equation for the spinor v is

$$(k_\mu\gamma^\mu + m)v = 0.$$

We can write

$$\boxed{v_r(k) = -\frac{1}{\sqrt{2m(m+E)}}(k_\mu\gamma^\mu - m)v_r(0)}.$$

$$v_r(k) = \frac{1}{\sqrt{2m(m+E)}}\begin{pmatrix} -E+m & \mathbf{k}\cdot\boldsymbol{\sigma} \\ -\mathbf{k}\cdot\boldsymbol{\sigma} & E+m \end{pmatrix}\begin{pmatrix} 0 \\ \chi_r \end{pmatrix} = \begin{pmatrix} \frac{\mathbf{k}\cdot\boldsymbol{\sigma}}{\sqrt{2m(m+E)}}\chi_r \\ \sqrt{\frac{E+m}{2m}}\chi_r \end{pmatrix} = \sqrt{\frac{E+m}{2m}}\begin{pmatrix} \frac{\mathbf{k}\cdot\boldsymbol{\sigma}}{m+E}\chi_r \\ \chi_r \end{pmatrix},$$

and

$$\bar{v} = \frac{1}{\sqrt{2m(m+E)}}\bar{v}(0)(-k_\mu\gamma^\mu + m).$$

Definition:

$$w_r(k) := \begin{cases} v_2(k) & r=1 \\ -v_1(k) & r=2 \end{cases}$$

is the charge conjugate of u_r. Since then, for C the charge conjugation operator,

$$Cu_r(k) = \imath\gamma^2 u_r^*(k) = w_r(k),$$
$$Cw_r(k) = \imath\gamma^2 w_r^*(k) = u_r(k).$$

Orthogonality relations:

$$\bar{u}_r u_s = \delta_{rs}, \quad \bar{w}_r w_s = -\delta_{rs}, \quad \bar{u}_r w_s = 0, \quad \bar{w}_r u_s = 0,$$
$$\bar{u}_r\gamma^0 u_s = \frac{E}{m}\delta_{rs}, \qquad \bar{w}_r\gamma^0 w_s = \frac{E}{m}\delta_{rs}.$$

The general solution is then now

$$\psi(x) = \sum_{k,r}\sqrt{\frac{m}{VE_k}}\left(b_{rk}u_r(k)e^{-\imath kx} + d_{rk}^* w_r(k)e^{+\imath kx}\right)$$

with $E_k = \sqrt{\mathbf{k}^2 + m^2}$.
Quantization: We consider the Dirac spinor as a field operator. As in the case of the meson field, we expand the field operator in terms of plane waves, where the expansion coefficients become operators, i.e., we replace the Fourier coefficients according to

$$\psi \to \hat{\psi}, \quad b_{rk} \to \hat{b}_{rk} \quad \text{and} \quad d_{rk} \to \hat{d}_{rk} \quad \text{with}$$
$$\{\hat{b}_{rk}, \hat{b}^\dagger_{r'k'}\} = \delta_{rr'}\delta_{kk'}, \qquad \{\hat{d}_{rk}, \hat{d}^\dagger_{r'k'}\} = \delta_{rr'}\delta_{kk'},$$

and all other commutators are zero. The solution of the Dirac equation in the quantized form is thus

$$\boxed{\hat{\psi}(x) = \sum_{k,r}\sqrt{\frac{m}{VE_k}}\left(\hat{b}_{rk}u_r(k)e^{-\imath kx} + \hat{d}^\dagger_{rk}w_r(k)e^{+\imath kx}\right)}.$$

The properties of the operators $\hat{b}$ and $\hat{d}^\dagger$ will be investigated in the following.

We postulate again that the Heisenberg equation is fulfilled:

$$\frac{\partial\hat{\psi}(x)}{\partial x^\mu} = \imath\left[\hat{p}_\mu,\, \hat{\psi}(x)\right] .$$

Thus

$$\left[\hat{p}_\mu,\, \hat{b}^\dagger_{sk}\right] = p_\mu \hat{b}^\dagger_{sk}, \quad \left[\hat{p}_\mu,\, \hat{d}^\dagger_{sk}\right] = p_\mu \hat{d}^\dagger_{sk}, \quad \left[\hat{p}_\mu,\, \hat{b}_{sk}\right] = -p_\mu \hat{b}_{sk}, \quad \left[\hat{p}_\mu,\, \hat{d}_{sk}\right] = -p_\mu \hat{d}_{sk}$$

for $s = \pm\frac{1}{2}$.
Like for the meson field, we require that

$$\hat{b}_{sk}|\,0\,\rangle = \hat{d}_{sk}|\,0\,\rangle = 0\,.$$

Instead of one set of creation operators, we have now four. Accordingly, for each fixed momentum **p**, we can construct four one-particle states:

$$\begin{array}{lll} \text{(a)} & \hat{b}^\dagger_{sk}|\,0\,\rangle, & s = \pm\dfrac{1}{2} \\ \text{(b)} & \hat{d}^\dagger_{sk}|\,0\,\rangle, & s = \pm\dfrac{1}{2} \end{array}$$

The states in (a) correspond to an electron with a fixed momentum **p** and two linearly independent spin-states. If we take the theory seriously, then we have to postulate that an another particle with exactly the same mass exists (Dirac 1930, Oppenheim 1930). This was confirmed by the discovery of the positron (Andersson 1932, 1933). We identify (b) as positrons, and will see that within Dirac's theory electrons and positrons have by default an opposite charge.

Which algebra is valid for the creation and annihilation operators?
In case we would postulate the same commutation relations as for the meson field, namely,

$$\left[\hat{b}_{rk},\, \hat{b}^\dagger_{sk'}\right] = \delta_{rs}\delta_{kk'}$$
$$\left[\hat{d}_{rk},\, \hat{d}^\dagger_{sk'}\right] = \delta_{rs}\delta_{kk'}$$

and all other commutators equal zero, then we would find *nonvanishing commutators for space-like distances*, for example,

$$\left[\hat{\psi}(\mathbf{x},t),\, \bar{\hat{\psi}}(\mathbf{y},t)\right] \neq 0 \quad \text{for } \mathbf{x} \neq \mathbf{y}\,, \tag{7.13}$$

which is in contradiction to microcausality.
One could argue that the Dirac spinor is not directly observable. But (7.13) also implies a violation of the microcausality for bilinear expressions in the Dirac field operator, which we want to identify as observable fields. Thus, electrons cannot be bosons (confirmed experimentally as electrons satisfy the Pauli principle).
The proper commutation relations for the creation and annihilation operators of the Dirac field are anticommutators (Jordan and Wigner 1927, 1928):

$$\left\{\hat{b}_{rk},\, \hat{b}^\dagger_{sk'}\right\} = \delta_{rs}\delta_{kk'}, \quad \left\{\hat{d}_{rk},\, \hat{d}^\dagger_{sk'}\right\} = \delta_{rs}\delta_{kk'}$$
$$\left\{\hat{b}^\dagger_{rk},\, \hat{b}^\dagger_{sk'}\right\} = \left\{\hat{b}_{rk},\, \hat{b}_{sk'}\right\} = \left\{\hat{d}^\dagger_{rk},\, \hat{d}^\dagger_{sk'}\right\} = \left\{\hat{d}_{rk},\, \hat{b}_{sk'}\right\} = \left\{\hat{b}^\dagger_{rk},\, \hat{d}_{sk'}\right\} = \left\{\hat{b}^\dagger_{rk},\, \hat{d}^\dagger_{sk'}\right\} = 0\,.$$

With this we get

$$\left\{\hat{\psi}(\mathbf{x},t),\, \hat{\psi}(\mathbf{y},t)\right\} = \left\{\bar{\hat{\psi}}(\mathbf{x},t),\, \bar{\hat{\psi}}(\mathbf{y},t)\right\} = 0 \tag{7.14}$$

$$\left\{\hat{\psi}(\mathbf{x},t),\, \bar{\hat{\psi}}(\mathbf{y},t)\right\} = \gamma^0\delta(\mathbf{x}-\mathbf{y})\,. \tag{7.15}$$

Proof:

$$\{\hat{\psi}(x),\bar{\hat{\psi}}(y)\} = \frac{1}{V}\sum_{k,k'}\sqrt{\frac{m^2}{E_k E_{k'}}}\sum_{r,r'}\left\{\hat{b}_{rk}u_r(k)e^{-\imath kx} + \hat{d}^\dagger_{rk}w_r(k)e^{\imath kx}, \hat{b}^\dagger_{r'k'}\bar{u}_{r'}(k')e^{\imath k'y} + \hat{d}_{r'k'}\bar{w}_{r'}(k')e^{-\imath k'y}\right\}.$$

Since $\{\hat{b}_{rk},\hat{b}^\dagger_{r'k'}\} = \{\hat{d}_{rk},\hat{d}^\dagger_{r'k'}\} = \delta_{rr'}\delta_{kk'}$ and all other commutators are zero, we obtain

$$\{\hat{\psi}(x),\bar{\hat{\psi}}(y)\} = \frac{1}{V}\sum_k \frac{m}{E_k}\left\{e^{-\imath k(x-y)}\sum_r u_r(k)\bar{u}_r(k) + e^{\imath k(x-y)}\sum_r w_r(k)\bar{w}_r(k)\right\}.$$

We have:

$$\begin{aligned}
\sum_r u_r(k)\bar{u}_r(k) &= \sum_r \mathcal{N}^2(k_\mu\gamma^\mu + m)u_r(0)\bar{u}_r(0)(k_\mu\gamma^\mu+m)\\
&= \mathcal{N}^2(k_\mu\gamma^\mu+m)\underbrace{\sum_r u_r(0)\bar{u}_r(0)}_{=\begin{pmatrix}\mathbb{1} & 0\\ 0 & 0\end{pmatrix}}(k_\mu\gamma^\mu+m)\\
&= \mathcal{N}^2\begin{pmatrix}E+m & -\mathbf{k}\cdot\boldsymbol{\sigma}\\ \mathbf{k}\cdot\boldsymbol{\sigma} & -E+m\end{pmatrix}\begin{pmatrix}\mathbb{1} & 0\\ 0 & 0\end{pmatrix}\begin{pmatrix}E+m & -\mathbf{k}\cdot\boldsymbol{\sigma}\\ \mathbf{k}\cdot\boldsymbol{\sigma} & -E+m\end{pmatrix}\\
&= \mathcal{N}^2\begin{pmatrix}E+m & 0\\ \mathbf{k}\cdot\boldsymbol{\sigma} & 0\end{pmatrix}\begin{pmatrix}E+m & -\mathbf{k}\cdot\boldsymbol{\sigma}\\ \mathbf{k}\cdot\boldsymbol{\sigma} & -E+m\end{pmatrix}\\
&= \frac{1}{2m(E+m)}\begin{pmatrix}(E+m)^2 & -\mathbf{k}\cdot\boldsymbol{\sigma}(E+m)\\ (E+m)\mathbf{k}\cdot\boldsymbol{\sigma} & -\mathbf{k}^2\end{pmatrix}\\
&= \frac{1}{2m}\begin{pmatrix}E+m & -\mathbf{k}\cdot\boldsymbol{\sigma}\\ \mathbf{k}\cdot\boldsymbol{\sigma} & -\frac{\mathbf{k}^2}{E+m}\end{pmatrix}\\
&= \frac{1}{2m}(k_\mu\gamma^\mu+m),
\end{aligned}$$

since $\mathbf{k^2} = (E+m)(E-m)$, and analogously:

$$\sum_r w_r(k)\bar{w}_r(k) = \frac{1}{2m}(k_\mu\gamma^\mu - m).$$

Then

$$\begin{aligned}
\{\hat{\psi}(x),\bar{\hat{\psi}}(y)\} &= \frac{1}{V}\sum_k\frac{m}{E_k}\left\{e^{-\imath k(x-y)}\frac{1}{2m}(k_\mu\gamma^\mu+m) + e^{\imath k(x-y)}\frac{1}{2m}(k_\mu\gamma^\mu-m)\right\}\\
&= \frac{1}{V}\sum_k\frac{1}{2E_k}\left\{(\imath\gamma^\mu\partial_\mu+m)e^{-\imath k(x-y)} - (\imath\gamma^\mu\partial_\mu+m)e^{\imath k(x-y)}\right\}\\
&= (\imath\gamma^\mu\partial_\mu+m)\quad\underbrace{\frac{1}{V}\sum_k\frac{1}{2E_k}\left\{e^{-\imath k(x-y)} - e^{\imath k(x-y)}\right\}}_{=\imath\Delta(x-y)\equiv\frac{1}{V}\sum_k\frac{1}{2\omega_k}\left(e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})-\imath\omega_k(t-t')}+\text{c.c.}\right)}
\end{aligned}$$

As appeared in the proof of the microcausality for the Klein-Gordon field (with Eq. (7.5)), $\Delta(x-y) = 0$ for $(x-y)^2 < 0$, i.e. for space-like distances. Then $\{\hat{\psi}(x), \bar{\hat{\psi}}(y)\} = 0$ for $(x-y)^2 < 0$.

Anti-commutator for equal times (note that $k^0(x_0 - y_0) = E_k(t-t) = 0$):

$$\begin{aligned}
\{\hat{\psi}(t,\mathbf{x}), \bar{\hat{\psi}}(t,\mathbf{y})\} &= \frac{1}{V}\sum_k \frac{1}{2E_k}\left\{e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}(k_\mu\gamma^\mu + m) + e^{-\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}(k_\mu\gamma^\mu - m)\right\} \\
&= \frac{1}{V}\sum_k \frac{1}{2E_k}\left\{e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}(E_k\gamma^0 - \mathbf{k}\cdot\boldsymbol{\gamma} + m) + e^{-\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}(E_k\gamma^0 - \mathbf{k}\cdot\boldsymbol{\gamma} - m)\right\} \\
&= \frac{1}{V}\sum_k \frac{1}{2E_k}\left\{e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}(E_k\gamma^0 - \mathbf{k}\cdot\boldsymbol{\gamma} + m) + e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}(E_k\gamma^0 + \mathbf{k}\cdot\boldsymbol{\gamma} - m)\right\} \\
&= \frac{1}{V}\sum_k \gamma^0 e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \\
&= \gamma^0 \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} = \gamma^0\delta^3(\mathbf{x}-\mathbf{y}).
\end{aligned}$$

Spin-statistic theorem (for fermions):
Consider an observable like $\bar{\hat{\psi}}(x)\hat{\psi}(x)$ and compute the commutator for two space-time coordinates x and y:

$$\begin{aligned}
[\bar{\hat{\psi}}_\alpha(x)\hat{\psi}_\alpha(x), \bar{\hat{\psi}}_\beta(y)\hat{\psi}_\beta(y)] =& \bar{\hat{\psi}}_\alpha(x)[\hat{\psi}_\alpha(x), \bar{\hat{\psi}}_\beta(y)\hat{\psi}_\beta(y)] + [\bar{\hat{\psi}}_\alpha(x), \bar{\hat{\psi}}_\beta(y)\hat{\psi}_\beta(y)]\hat{\psi}_\alpha(x) \\
=& \bar{\hat{\psi}}_\alpha(x)\{\hat{\psi}_\alpha(x), \bar{\hat{\psi}}_\beta(y)\}\hat{\psi}_\beta(y) - \bar{\hat{\psi}}_\alpha(x)\bar{\hat{\psi}}_\beta(y)\{\hat{\psi}_\alpha(x), \hat{\psi}_\beta(y)\} \\
& - \bar{\hat{\psi}}_\beta(y)\{\bar{\hat{\psi}}_\alpha(x), \hat{\psi}_\beta(y)\}\hat{\psi}_\alpha(x) + \{\bar{\hat{\psi}}_\beta(y), \bar{\hat{\psi}}_\alpha(x)\}\hat{\psi}_\beta(y)\hat{\psi}_\alpha(x)
\end{aligned}$$

since $\left[\hat{A}\hat{B},\, \hat{C}\hat{D}\right] = \hat{A}\left\{\hat{B},\, \hat{C}\right\}\hat{D} - \hat{A}\hat{C}\left\{\hat{B},\, \hat{D}\right\} - \hat{C}\left\{\hat{A},\, \hat{D}\right\}\hat{B} + \left\{\hat{C},\, \hat{A}\right\}\hat{D}\hat{B}$.

$$\begin{aligned}
[\bar{\hat{\psi}}_\alpha(x)\hat{\psi}_\alpha(x), \bar{\hat{\psi}}_\beta(y)\hat{\psi}_\beta(y)] &= \bar{\hat{\psi}}_\alpha(x)\{\hat{\psi}_\alpha(x), \bar{\hat{\psi}}_\beta(y)\}\hat{\psi}_\beta(y) - \bar{\hat{\psi}}_\beta(y)\{\bar{\hat{\psi}}_\alpha(x), \hat{\psi}_\beta(y)\}\hat{\psi}_\alpha(x) \\
&= \bar{\hat{\psi}}_\alpha(x)\left[(-\imath\gamma^\mu\partial_\mu + m)_{\alpha\beta}\imath\Delta(x-y)\right]\hat{\psi}_\beta(y) \\
&\quad + \bar{\hat{\psi}}_\beta(y)\left[(-\imath\gamma^\mu\partial_\mu + m)_{\alpha\beta}\imath\Delta(x-y)\right]\hat{\psi}_\alpha(x) \\
&= 0
\end{aligned}$$

for $(x-y)^2 < 0$.
That implies for observable fields $\bar{\hat{\psi}}(x)u\hat{\psi}(x)$, where $u = \bar{u}$ are 4×4 matrices, commutation relations, which are consistent with microcausality. For example, for arbitrary 4×4 matrices u_1 and u_2 we get

$$\left[\bar{\hat{\psi}}(\mathbf{x},t)u_1\hat{\psi}(\mathbf{x},t)),\, \bar{\hat{\psi}}(\mathbf{y},t)u_2\hat{\psi}(\mathbf{y},t)\right] = 0 \quad \text{for} \quad \mathbf{x} \neq \mathbf{y}\,,$$

which follows directly from (7.14) and (7.15).
Single-electron- (or positron) state with a sharp momentum:

$$\begin{aligned}
\left|\mathrm{e}^-(k,s)\right\rangle &= \hat{b}^\dagger_{sk}\,|\,0\,\rangle \\
\left|\mathrm{e}^+(k,s)\right\rangle &= \hat{d}^\dagger_{sk}\,|\,0\,\rangle
\end{aligned}$$

Normalization:

$$\langle \mathrm{e}^-(k',r)|\mathrm{e}^-(k,s)\rangle = \langle\, 0\,|\left\{\hat{b}_{rk'},\, \hat{b}^\dagger_{sk}\right\}|\, 0\,\rangle = \delta_{rs}\delta_{kk'}$$
$$\left\langle \mathrm{e}^+(k',r)|\mathrm{e}^+(k,s)\right\rangle = \langle\, 0\,|\left\{\hat{d}_{rk'},\, \hat{d}^\dagger_{sk}\right\}|\, 0\,\rangle = \delta_{rs}\delta_{kk'}$$

Two-electron-state:

$$\left|\mathrm{e}^-(k,r),\, \mathrm{e}^-(k',s)\right\rangle = \hat{b}^\dagger_{rk}\hat{b}^\dagger_{sk'}\,|\, 0\,\rangle = -\hat{b}^\dagger_{sk'}\hat{b}^\dagger_{rk}\,|\, 0\,\rangle = -\left|\mathrm{e}^-(k',s),\, \mathrm{e}^-(k,r)\right\rangle\,,$$

thus the Pauli principle applies.

What if we would have chosen commutation rules, $[\hat{b}_{rk}, \hat{b}^\dagger_{r'k'}] = [\hat{d}_{rk}, \hat{d}^\dagger_{r'k'}] = \delta_{rr'}\delta_{kk'}$ instead of anti-commutation rules?
Remark that now $[\hat{d}^\dagger_{rk}, \hat{d}_{r'k'}] = -\delta_{rr'}\delta_{kk'}$. Then

$$\begin{aligned}
[\hat{\psi}(x), \bar{\hat{\psi}}(y)] &= \frac{1}{V}\sum_{k,k'}\sqrt{\frac{m^2}{E_k E_{k'}}}\sum_{r,r'}\left[\hat{b}_{rk}u_r(k)e^{-\imath kx} + \hat{d}^\dagger_{rk}w_r(k)e^{+\imath kx}, \hat{b}^\dagger_{r'k'}\bar{u}_{r'}(k')e^{\imath k'y} + \hat{d}_{r'k'}\bar{w}_{r'}(k')e^{-\imath k'y}\right]\\
&= \frac{1}{V}\sum_k \frac{m}{E_k}\left\{e^{-\imath k(x-y)}\sum_r u_r(k)\bar{u}_r(k) - e^{\imath k(x-y)}\sum_r w_r(k)\bar{w}_r(k)\right\}\\
&= (\imath\gamma^\mu\partial_\mu + m)\frac{1}{V}\sum_k \frac{1}{2E_k}\left\{e^{-\imath k(x-y)} + e^{\imath k(x-y)}\right\}\\
&= (\imath\gamma^\mu\partial_\mu + m)\Delta_1(x-y)
\end{aligned}$$

with

$$\begin{aligned}
\Delta_1(x-y) &= \frac{1}{V}\sum_k \frac{1}{2E_k}\left\{e^{-\imath k(x-y)} + e^{\imath k(x-y)}\right\}\\
&= -\frac{\imath}{2\pi^2 R}\int_0^\infty \frac{kdk}{\sqrt{k^2+m^2}}\cos(\sqrt{k^2+m^2}T)\cos(kR)
\end{aligned}$$

with $R = |\mathbf{x}-\mathbf{y}|$ and $T = x^0 - y^0$, from Eq. (7.5).
Now this integrand is an odd function of k for which reason $\int_{-\infty}^0 = -\int_0^\infty$ and therefore the integration cannot be performed from $-\infty$ to $+\infty$ and the residue theorem cannot be applied. Then $\Delta_1(x-y) \neq 0$ also for $(x-y)^2 < 0$ which leads to a contradiction to microcausality.

Chapter 8

Quantum electrodynamics

8.1 Quantization of the electromagnetic field – Lorentz covariant formulation

The four-potential $A^\mu = (\phi, \mathbf{A})$ in Lorenz gauge, $\partial_\mu A^\mu = 0$, and in source-free case, $j^\mu = 0$, obeys the wave equation

$$\Box A_\mu = 0\,.$$

As for mesons, the Fourier expansion of the field operators A_μ reads as

$$A_\mu = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega} \left\{ e^{\imath kx} a_\mu^\dagger(\mathbf{k}) + e^{-\imath kx} a_\mu(\mathbf{k}) \right\}$$

with

$$k = \begin{pmatrix} \omega \\ \mathbf{k} \end{pmatrix}, \quad \omega = |\mathbf{k}|\,, \quad kx = k^\mu x_\mu = \omega t - \mathbf{k}\cdot\mathbf{x}\,.$$

Microcausality leads to Bose commutation relations:

$$\left[a_\mu^\dagger(\mathbf{k}),\ a_\nu^\dagger(\mathbf{k}')\right] = [a_\mu(\mathbf{k}),\ a_\nu(\mathbf{k})] = 0\,,$$
$$\left[a_\mu(\mathbf{k}),\ a_\nu^\dagger(\mathbf{k}')\right] = Z_{\mu\nu}(2\pi)^3 2\omega\, \delta^3(\mathbf{k}-\mathbf{k}')$$

with initially unknown $Z_{\mu\nu}$.

The operators a_μ, $a_\mu^\dagger$ act in the Fock space and its vacuum state is characterized by

$$a_\mu(\mathbf{k})\,|0\rangle = 0 \qquad \forall \mu, \mathbf{k}\,.$$

For an explicit Lorentz covariance of the theory, $Z_{\mu\nu}$ must be a constant second order tensor. The only possible candidate is the metric tensor $g_{\mu\nu}$. We still have a freedom to choose the sign $Z_{\mu\nu} = \pm g_{\mu\nu}$. As it turns out later, the correct choice is

$$\left[a_\mu(\mathbf{k}),\ a_\nu^\dagger(\mathbf{k}')\right] = -g_{\mu\nu}(2\pi)^3 2\omega\, \delta^3(\mathbf{k}-\mathbf{k}')\,,$$

albeit applying the operator $a_0^\dagger$ to the vacuum leads to states with a negative norm (is not a probability density) and $a_j^\dagger$ with $j = 1, 2, 3$ leads to states with a positive norm.

Consider a general state: $|\, f\,\rangle = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3\sqrt{2\omega}} \sum_\mu f_\mu(\mathbf{k}) a^\dagger_\mu(\mathbf{k})\,|\,0\,\rangle$
Inner product:

$$\begin{aligned}\langle\, f\,|\, f\,\rangle &= \int \frac{\mathrm{d}^3\mathbf{k}\,\mathrm{d}^3\mathbf{k}'}{(2\pi)^6\sqrt{2\omega 2\omega'}} \sum_{\mu,\nu} f^*_\nu(\mathbf{k}') f_\mu(\mathbf{k})\,\langle 0|\, a_\nu(\mathbf{k}') a^\dagger_\mu(\mathbf{k})\,|0\rangle \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \left[-|f_0(\mathbf{k})|^2 + |f_1(\mathbf{k})|^2 + |f_2(\mathbf{k})|^2 + |f_3(\mathbf{k})|^2\right] \quad \begin{cases} \geq 0 & \text{for} \quad f_0 = 0 \\ < 0 & \text{for} \quad f_0 > 0,\; f_{1,2,3} = 0 \end{cases}\end{aligned}$$

In addition to states with a negative norm there are states

$$|\mathbf{k}, \varepsilon\rangle = -\varepsilon^\mu a^\dagger_\mu(\mathbf{k})\,|0\rangle$$

with an arbitrary polarization four-vector of the photon ε^μ, such that at a fixed $\mathbf{k}$ we have *four* linearly independent polarization directions instead of just *two* as observed experimentally.

The method of Gupta and Bleuler (1950) guarantees positive norm and gets rid of the two unwanted polarization directions: *states* are constrained to the Lorenz gauge condition.

We declare only a part of the state vectors in the Fock space to be physical, namely those which in a certain way satisfy the Lorenz gauge condition. We take the part of A_μ that just contains annihilation operators:

$$A^{(-)}_\mu(x) := \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\, e^{-\imath kx} a_\mu(\mathbf{k})$$

and postulate for physical state vectors

$$\partial^\mu A^{(-)}_\mu(x)\;|\text{physical state}\rangle = 0$$

or

$$k^\mu a_\mu(\mathbf{k})\;|\text{physical state}\rangle = 0 \qquad \forall\,\mathbf{k}\,.$$

Because of that

$$\langle\text{physical state}|\,\partial^\mu A^{(-)}_\mu(x)\,|\text{physical state}\rangle = 0\,,$$

i.e., the *expectation value* of the divergence of the field A_μ vanishes for any physical state. The subspace $\{|\,\text{physical state}\rangle\}$ is obviously a linear space.

Claim:

$$\langle\text{physical state}\,|\,\text{physical state}\rangle \geq 0\,,$$

i.e., the subspace $\{|\,\text{physical state}\rangle\}$ has a positive semi-definite metric.
Proof:
We choose a new basis for creation and annihilation operators. We consider $a^\dagger_\mu(\mathbf{k})$ at fixed $\mathbf{k}$. We choose two unit vectors $\mathbf{e}_1$, $\mathbf{e}_2 \perp \mathbf{k}$, such that $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3 = \mathbf{k}/|\mathbf{k}|$ form an orthonormal trihedron, i.e., $\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$.
We define operators α_μ as

$$\begin{aligned}\alpha^\dagger_0(\mathbf{k}) &= \frac{1}{\sqrt{2}}\left(a^\dagger_0(\mathbf{k}) - \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k})\right) \\ \alpha^\dagger_1(\mathbf{k}) &= \mathbf{e}_1\cdot\mathbf{a}^\dagger(\mathbf{k}) \\ \alpha^\dagger_2(\mathbf{k}) &= \mathbf{e}_2\cdot\mathbf{a}^\dagger(\mathbf{k}) \\ \alpha^\dagger_3(\mathbf{k}) &= \frac{1}{\sqrt{2}}\left(a^\dagger_0(\mathbf{k}) + \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k})\right)\,,\end{aligned}$$

where $\mathbf{a}^\dagger = \left(a_1^\dagger,\, a_2^\dagger,\, a_3^\dagger\right)$.

Commutation relations are

$$\begin{aligned}\left[\alpha_0(\mathbf{k}),\, \alpha_0^\dagger(\mathbf{k}')\right] &= \frac{1}{2}\left[a_0(\mathbf{k}) - \mathbf{e}_3\cdot\mathbf{a}(\mathbf{k}), a_0^\dagger(\mathbf{k}') - \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k}')\right] \\ &= \frac{1}{2}\left\{\underbrace{\left[a_0(\mathbf{k}), a_0^\dagger(\mathbf{k}')\right]}_{-(2\pi)^3 2\omega\delta_{kk'}} - \underbrace{\mathbf{e}_3\cdot\left[\mathbf{a}(\mathbf{k}), a_0^\dagger(\mathbf{k}')\right]}_{=0} - \underbrace{\left[\mathbf{a}(\mathbf{k}), \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k}')\right]}_{=0} + \left[\mathbf{e}_3\cdot\mathbf{a}(\mathbf{k}), \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k}')\right]\right\}\end{aligned}$$

Now,

$$\begin{aligned}\left[\mathbf{e}_3\cdot\mathbf{a}(\mathbf{k}), \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k}')\right] &= \left[e_3^i a_i(\mathbf{k}), e_3^j a_j^\dagger(\mathbf{k}')\right] \\ &= e_3^i e_3^j \delta_{ij}\left[+(2\pi)^3 2\omega\delta_{\mathbf{kk}'}\right] \\ &= \underbrace{|\mathbf{e}_3|^2}_{=1}(2\pi)^3 2\omega\delta_{\mathbf{kk}'} \\ &= +(2\pi)^3 2\omega\delta_{\mathbf{kk}'}\end{aligned}$$

So,

$$\left[\alpha_0(\mathbf{k}),\, \alpha_0^\dagger(\mathbf{k}')\right] = 0\,,$$

Analogously,

$$\left[\alpha_3(\mathbf{k}),\, \alpha_3^\dagger(\mathbf{k}')\right] = 0$$

Therefore, we obtain

$$\left[\alpha_0(\mathbf{k}),\, \alpha_0^\dagger(\mathbf{k}')\right] = \left[\alpha_3(\mathbf{k}),\, \alpha_3^\dagger(\mathbf{k}')\right] = 0\,. \tag{8.1}$$

Next,

$$\begin{aligned}\left[\alpha_0(\mathbf{k}),\, \alpha_3^\dagger(\mathbf{k}')\right] &= \frac{1}{2}\left[a_0(\mathbf{k}) - \mathbf{e}_3\cdot\mathbf{a}(\mathbf{k}), a_0^\dagger(\mathbf{k}') + \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k}')\right] \\ &= \frac{1}{2}\left\{-(2\pi)^3 2\omega\delta_{kk'} - (2\pi)^3 2\omega\delta_{kk'}\right\} \\ &= -(2\pi)^3 2\omega\delta_{kk'}\end{aligned}$$

$$\begin{aligned}\left[\alpha_3(\mathbf{k}),\, \alpha_0^\dagger(\mathbf{k}')\right] &= \frac{1}{2}\left[a_0(\mathbf{k}) + \mathbf{e}_3\cdot\mathbf{a}(\mathbf{k}), a_0^\dagger(\mathbf{k}') - \mathbf{e}_3\cdot\mathbf{a}^\dagger(\mathbf{k}')\right] \\ &= -(2\pi)^3 2\omega\delta_{kk'}\end{aligned}$$

Therefore, we obtain

$$\left[\alpha_0(\mathbf{k}),\, \alpha_3^\dagger(\mathbf{k}')\right] = \left[\alpha_3(\mathbf{k}),\, \alpha_0^\dagger(\mathbf{k}')\right] = -(2\pi)^3 2\omega\,\delta_{kk'}\,. \tag{8.2}$$

And finally,

$$\begin{aligned}\left[\alpha_1(\mathbf{k}),\, \alpha_1^\dagger(\mathbf{k}')\right] &= \left[\mathbf{e}_1\cdot\mathbf{a}(\mathbf{k}), \mathbf{e}_1\cdot\mathbf{a}^\dagger(\mathbf{k}')\right] \\ &= e_1^i e_1^j \underbrace{\left[a_i(\mathbf{k}), a_j^\dagger(\mathbf{k}')\right]}_{+(2\pi)^3 2\omega\,\delta_{kk'}} \\ &= \underbrace{|\mathbf{e}_1|^2}_{=1}(2\pi)^3 2\omega\,\delta_{kk'} \\ &= +(2\pi)^3 2\omega\,\delta_{kk'}\end{aligned}$$

Analogously,

$$\left[\alpha_2(\mathbf{k}),\, \alpha_2^\dagger(\mathbf{k}')\right] = +(2\pi)^3 2\omega\,\delta_{kk'}\,,$$

and we obtain the final relation as

$$\left[\alpha_1(\mathbf{k}),\, \alpha_1^\dagger(\mathbf{k}')\right] = \left[\alpha_2(\mathbf{k}),\, \alpha_2^\dagger(\mathbf{k}')\right] = +(2\pi)^3 2\omega\,\delta_{kk'} \tag{8.3}$$

For the other relations,

$$\begin{aligned}\left[\alpha_0(\mathbf{k}),\, \alpha_1^\dagger(\mathbf{k}')\right] &= \frac{1}{\sqrt{2}}\left[a_0(\mathbf{k}) - \mathbf{e}_3\cdot\mathbf{a}(\mathbf{k}), \mathbf{e}_1\cdot\mathbf{a}^\dagger(\mathbf{k})\right] \\ &= -\frac{1}{\sqrt{2}} e_3^i e_1^j \underbrace{\left[a_i, a_j^\dagger\right]}_{\propto\delta_{ij}} \propto \mathbf{e}_3\cdot\mathbf{e}_1 = 0\,,\end{aligned}$$

since $\mathbf{e}_3 \perp \mathbf{e}_1$. Analogously, $\left[\alpha_0(\mathbf{k}),\, \alpha_2^\dagger(\mathbf{k}')\right] = 0$.
Now,

$$\begin{aligned}\alpha_0(\mathbf{k})|\text{physical state}\rangle &= \frac{1}{\sqrt{2}}\left(a_0(\mathbf{k}) - \mathbf{e}_3\cdot\mathbf{a}(\mathbf{k})\right)|\text{physical state}\rangle \\ &= \frac{1}{\sqrt{2}}\frac{1}{k_0}\left(k_0 a_0(\mathbf{k}) - \mathbf{k}\cdot\mathbf{a}(\mathbf{k})\right)|\text{physical state}\rangle \\ &= \frac{1}{k_0\sqrt{2}} k^\mu a_\mu(\mathbf{k})|\text{physical state}\rangle\end{aligned}$$

where

$$0 = k^\mu k_\mu = k_0^2 - \mathbf{k}^2 \rightsquigarrow k_0^2 = \mathbf{k}^2 \rightsquigarrow k_0 = |\mathbf{k}|\,.$$

The constraint $k^\mu a_\mu(\mathbf{k})|\text{physical state}\rangle = 0$ reads now as

$$\alpha_0(\mathbf{k})|\text{physical state}\rangle = 0\,. \tag{8.4}$$

Consider the following state vector in the Hilbert space

$$\alpha_1^\dagger(\mathbf{k}_1)\alpha_1^\dagger(\mathbf{k}_2)\cdots\alpha_2^\dagger\cdots\alpha_0^\dagger\cdots\alpha_3^\dagger\cdots|\,0\,\rangle\,, \tag{8.5}$$

i.e. an arbitrary product of creation operators applied to vacuum.

Consider $\alpha_3^\dagger|0\rangle$:

$$\alpha_0\alpha_3^\dagger|0\rangle = \underbrace{\left[\alpha_0, \alpha_3^\dagger\right]}_{\neq 0}|0\rangle + \alpha_3^\dagger \underbrace{\alpha_0|0\rangle}_{=0},$$

which implies that due to commutation relations (8.1-8.3), the constraint (8.4) is only fulfilled if no operator $\alpha_3^\dagger$ occurs or $|\text{physical state}\rangle$ cannot contain $\alpha_3^\dagger$ if (8.4) is fulfilled. For example, from state vectors $\alpha_\mu^\dagger(\mathbf{k})|\,0\,\rangle$ only $\alpha_0^\dagger(\mathbf{k})|\,0\,\rangle$, $\alpha_1^\dagger(\mathbf{k})|\,0\,\rangle$ and $\alpha_2^\dagger(\mathbf{k})|\,0\,\rangle$ are physical. These are orthogonal and their squared lengths are greater than or equal to zero:

$$\begin{aligned}
\langle 0|\,\alpha_0(\mathbf{k})\alpha_0^\dagger(\mathbf{k}')\,|0\rangle &= 0 \\
\langle 0|\,\alpha_1(\mathbf{k})\alpha_1^\dagger(\mathbf{k}')\,|0\rangle &= (2\pi)^3 2\omega\,\delta^3(\mathbf{k}-\mathbf{k}') \\
\langle 0|\,\alpha_2(\mathbf{k})\alpha_2^\dagger(\mathbf{k}')\,|0\rangle &= (2\pi)^3 2\omega\,\delta^3(\mathbf{k}-\mathbf{k}')
\end{aligned} \tag{8.6}$$

An arbitrary physical state vector is a linear combination of state vectors of the form (8.5), which do not contain $\alpha_3^\dagger$. For these it is then easy to show that their squared lengths are greater than or equal to zero. ■

From here it is easy to construct a Hilbert space with a positive-definite metric, which allows a probability interpretation in the sense of quantum mechanics.

Definition: Equivalence relation of state vectors:

$$|\,1\,\rangle \sim |\,2\,\rangle \quad \Longleftrightarrow \quad (\langle\,1\,| - \langle\,2\,|)(|\,1\,\rangle - |\,2\,\rangle) = 0$$

The linear Hilbert space of equivalence classes then has positive-definite metric.

Physical interpretation:
The state of a system of photons is described by a whole class of equivalent state vectors. One can show that the expectation value of observable quantities (like field strength tensor, energy etc.) is identical for equivalent state vectors. In practice, for example, when calculating matrix elements, one can always take any representative of an equivalence class as a state vector.

Due to (8.6) the state vector $\alpha_0^+(\mathbf{k})|\,0\,\rangle$ is equivalent to the zero vector and only linear combinations of

$$\begin{aligned}
|\mathbf{k},\varepsilon_1\rangle &= \alpha_1^\dagger(\mathbf{k})\,|\,0\,\rangle = \mathbf{e}_1\cdot\mathbf{a}^\dagger(\mathbf{k})\;|\,0\,\rangle \\
|\mathbf{k},\varepsilon_2\rangle &= \alpha_2^\dagger(\mathbf{k})\,|\,0\,\rangle = \mathbf{e}_2\cdot\mathbf{a}^\dagger(\mathbf{k})\;|\,0\,\rangle
\end{aligned}$$

with

$$\varepsilon_{1,2} = \begin{pmatrix} 0 \\ \mathbf{e}_{1,2} \end{pmatrix}$$

correspond to physical one-photon-states. This is consistent with experimental findings of two linearly independent one-photon-states for each $\mathbf{k}$.

Physical one-photon-states for fixed $\mathbf{k}$:

$$|\mathbf{k},\varepsilon\rangle = -\varepsilon^\mu a_\mu^\dagger(\mathbf{k})\;|\,0\,\rangle = \boldsymbol{\varepsilon}\cdot\mathbf{a}^\dagger(\mathbf{k})\;|\,0\,\rangle\;, \tag{8.7}$$

where

$$\varepsilon = \begin{pmatrix} 0 \\ \boldsymbol{\varepsilon} \end{pmatrix}$$

satisfy $\varepsilon^0 = 0,\ \boldsymbol{\varepsilon} \cdot \mathbf{k} = 0,\ |\boldsymbol{\varepsilon}| = 1$ and, as a consequence, $\varepsilon^\mu k_\mu = 0$.
This states satisfy the continuum normalization

$$\langle \mathbf{k}', \varepsilon' | \mathbf{k}, \varepsilon \rangle = (\boldsymbol{\varepsilon}'^* \cdot \boldsymbol{\varepsilon})\, (2\pi)^3\, 2\omega\, \delta^3(\mathbf{k} - \mathbf{k}')$$

Remember, linearly polarized photons are described by real polarization vectors $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^*$, right and left circularly polarized photons by

$$\boldsymbol{\varepsilon}_\pm = \mp \frac{1}{\sqrt{2}} (\mathbf{e}_1 \pm \imath \mathbf{e}_2)\,.$$

Why didn't we just focus on state vectors (8.7)? Because the transversality condition on the polarization vector ε is not Lorentz covariant. Consider a Lorentz transformation Λ:

$$k \to k' = \Lambda k \quad \text{and} \quad \varepsilon = \begin{pmatrix} 0 \\ \boldsymbol{\varepsilon} \end{pmatrix} \to \varepsilon' = \Lambda \varepsilon$$

From $\varepsilon^\mu k_\mu = 0$ follows that $\varepsilon'^\mu k'_\mu = 0$, which implies

$$\begin{aligned} \varepsilon'^0 k'_0 - \mathbf{e}' \cdot \mathbf{k}' - \varepsilon'^0 \frac{\mathbf{k}' \cdot \mathbf{k}'}{|\mathbf{k}'|} &= 0 \\ \implies \mathbf{e}' \cdot \mathbf{k}' &= 0 \\ \implies \mathbf{e}' \perp \mathbf{k}' & \end{aligned}$$

and thus

$$\varepsilon' = \begin{pmatrix} \varepsilon'^0 \\ \mathbf{e}' + \varepsilon'^0 \frac{\mathbf{k}'}{|\mathbf{k}'|} \end{pmatrix}.$$

It is $\mathbf{e}' \cdot \frac{\mathbf{k}'}{|\mathbf{k}'|} = 0$ but in general $\varepsilon'^0 \neq 0$.

Comment: However, the corresponding state vector is equivalent to that of a purely transverse photon:

$$\begin{aligned} -\varepsilon'^\mu a^\dagger_\mu(\mathbf{k}')\, |\, 0 \,\rangle &= \left\{ -\varepsilon'^0 a_0^\dagger + \left(\mathbf{e}' + \varepsilon'^0 \frac{\mathbf{k}'}{|\mathbf{k}'|} \right) \mathbf{a}^\dagger(\mathbf{k}') \right\} |\, 0 \,\rangle \\ &= \left\{ \mathbf{e}' \cdot \mathbf{a}^\dagger(\mathbf{k}') - \varepsilon'^0 \left[a_0^\dagger(\mathbf{k}') - \frac{\mathbf{k}'}{|\mathbf{k}'|} \cdot \mathbf{a}^\dagger(\mathbf{k}') \right] \right\} |\, 0 \,\rangle \\ &\sim \mathbf{e}' \cdot \mathbf{a}^\dagger(\mathbf{k}')\, |\, 0 \,\rangle\,. \end{aligned}$$

8.2 Normal and time ordered products

We now want to give the expectation values of some physical observables – $\langle \ldots \rangle$ means the expectation values in any physical state.
Now,

$$A_\mu = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega} \left\{ e^{\imath kx} a_\mu^\dagger(k) + e^{-\imath kx} a_\mu(k) \right\}$$

It is

$$a_0^\dagger = \frac{1}{\sqrt{2}}\left(\alpha_0^\dagger + \alpha_3^\dagger\right) \quad , \quad a_3^\dagger = \frac{1}{\sqrt{2}}\left(\alpha_0^\dagger - \alpha_3^\dagger\right)$$
$$\Longrightarrow a_0^\dagger|\text{physical state}\rangle = 0 \quad , \quad a_3^\dagger|\text{physical state}\rangle = 0\,,$$

since

$$\alpha_0^\dagger|\text{physical state}\rangle = 0$$
$$\alpha_3^\dagger|\text{physical state}\rangle = 0\,.$$

This implies

$$\mathbf{a}^\dagger(\mathbf{k})|\text{physical state}\rangle = \left(\mathbf{e}_1\alpha_1^\dagger(\mathbf{k}) + \mathbf{e}_2\alpha_2^\dagger(\mathbf{k})\right)|\text{physical state}\rangle\,,$$

since

$$\mathbf{e}_1 a^\dagger(\mathbf{k}) = \alpha_1^\dagger(\mathbf{k})$$
$$\mathbf{e}_2 a^\dagger(\mathbf{k}) = \alpha_2^\dagger(\mathbf{k})\,.$$

Therefore,

$$\mathbf{A}|\text{physical state}\rangle = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\left\{e^{\imath kx}\left[\mathbf{e}_1\alpha_1^\dagger(\mathbf{k}) + \mathbf{e}_2\alpha_2^\dagger(\mathbf{k})\right] + e^{-\imath kx}\left[\mathbf{e}_1\alpha_1(\mathbf{k}) + \mathbf{e}_2\alpha_2(\mathbf{k})\right]\right\}|\text{physical state}\rangle\,.$$

Due to $\mathbf{B} = \mathrm{rot}\mathbf{A}$ it is

$$\langle\mathbf{B}(x)\rangle = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\left\{e^{\imath kx}\left\langle -\imath\mathbf{k}\times\left[\mathbf{e}_1\alpha_1^\dagger(\mathbf{k}) + \mathbf{e}_2\alpha_2^\dagger(\mathbf{k})\right]\right\rangle \right.$$
$$\left. + e^{-\imath kx}\left\langle \imath\mathbf{k}\times\left[\mathbf{e}_1\alpha_1(\mathbf{k}) + \mathbf{e}_2\alpha_2(\mathbf{k})\right]\right\rangle\right\}. \quad (8.8)$$

With $\mathbf{E} = -\nabla A_0 - \partial_0\mathbf{A}$ follows $\langle\mathbf{E}\rangle = -\langle\partial_0\mathbf{A}\rangle$ since $\langle\nabla A_0\rangle = 0$ because

$$\langle\text{physical state}|\, a_0^\dagger(\mathbf{k})\,|\text{physical state}\rangle =$$
$$\langle\text{physical state}|\,\frac{1}{\sqrt{2}}\left(\alpha_0^\dagger(\mathbf{k}) + \alpha_3^\dagger(\mathbf{k})\right)|\text{physical state}\rangle = 0\,, \quad (8.9)$$

since $\alpha_0^\dagger\,|\text{physical state}\rangle = 0$ and $\langle\text{physical state}|\,\alpha_3^\dagger = 0$, because $|\text{physical state}\rangle$ does not contain any $\alpha_3^\dagger$. Analogous arguments apply to $\langle\text{physical state}|\,a_0(\mathbf{k})\,|\text{physical state}\rangle = 0$. Thus

$$\langle\mathbf{E}\rangle = -\langle\partial_0\mathbf{A}\rangle$$
$$= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\left\{-\imath\omega e^{\imath kx}\left\langle\mathbf{e}_1\alpha_1^\dagger(\mathbf{k}) + \mathbf{e}_2\alpha_2^\dagger(\mathbf{k})\right\rangle + \imath\omega e^{-\imath kx}\left\langle\mathbf{e}_1\alpha_1(\mathbf{k}) + \mathbf{e}_2\alpha_2(\mathbf{k})\right\rangle\right\}$$

In agreement with the experiment, only the transversal degrees of freedom of the photons contribute.

Classical expressions for the energy p^0 and the momentum $\mathbf{p}$ of the electromagnetic field are

$$p^0 = \int_{t=\text{const.}} \mathrm{d}^3x\,\frac{1}{2}\left[\mathbf{E}(x)^2 + \mathbf{B}(x)^2\right]$$
$$\mathbf{p} = \int_{t=\text{const.}} \mathrm{d}^3x\,\mathbf{E}(x)\times\mathbf{B}(x)\,.$$

If we consider **E** and **B** as field operator then we get for an arbitrary physical state:

$$\begin{aligned}\left\langle p'^0 \right\rangle &= \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\,\omega\cdot\left\langle \sum_{i=1}^{2}\left\{\alpha_i^\dagger(\mathbf{k})\alpha_i(\mathbf{k})+\alpha_i(\mathbf{k})\alpha_i^\dagger(\mathbf{k})\right\}\right\rangle \\ \left\langle \mathbf{p}' \right\rangle &= \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\,\mathbf{k}\cdot\left\langle \sum_{i=1}^{2}\left\{\alpha_i^\dagger(\mathbf{k})\alpha_i(\mathbf{k})+\alpha_i(\mathbf{k})\alpha_i^\dagger(\mathbf{k})\right\}\right\rangle\end{aligned}$$

Again only the physical degrees of freedom of the photons contribute.

There is a new difficulty. Consider vacuum expectation values:

$$\begin{aligned}\langle 0|\, p'^0\, |0\rangle &= \frac{1}{2}\int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\,\omega\cdot\sum_{l=1}^{2}\langle 0|\,\alpha_i(\mathbf{k})\alpha_i^\dagger(\mathbf{k})\,|0\rangle \\ &= \frac{1}{2}\int \mathrm{d}^3\mathbf{k}\,\omega\cdot 2\,\delta^3(0) \\ &= \frac{1}{2}\int \mathrm{d}^3\mathbf{k}\,\omega\cdot 2\,\frac{V}{(2\pi)^3} \qquad (8.10)\\ \langle 0|\,\mathbf{p}'\,|0\rangle &= \frac{1}{2}\int \mathrm{d}^3\mathbf{k}\,\mathbf{k}\cdot 2\,\delta^3(0) \\ &= \frac{1}{2}\int \mathrm{d}^3\mathbf{k}\,\mathbf{k}\cdot 2\,\frac{V}{(2\pi)^3}\,, \qquad (8.11)\end{aligned}$$

where we have used Fermi's trick to replace $(2\pi)^3\delta^3(0)$ by the normalization volume V:

$$\delta^3(\mathbf{k}-\mathbf{k}') = \int \frac{\mathrm{d}^3\mathbf{x}}{(2\pi)^3} e^{\imath(\mathbf{k}-\mathbf{k}')\cdot\mathbf{x}} \quad\Rightarrow\quad (2\pi)^3\delta^3(0) = \int \mathrm{d}^3\mathbf{x} \to V\,,$$

which is true for an integral over a finite volume V.

(8.11) is relatively harmless: symmetrical integration over all momenta gives zero.

(8.10) represents the zero-point energy of the electromagnetic field in a volume V. Only energy differences can be measured and we choose vacuum as the zero point for the energy. The present energy operator is replaced by

$$p^0 = p'^0 - \langle 0|\, p'^0\, |0\rangle$$

and the expectation value for the new operator is

$$\begin{aligned}\left\langle p^0 \right\rangle &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\,\omega\left\langle \frac{1}{2}\sum_{i=1}^{2}\left\{\alpha_i^\dagger(\mathbf{k})\alpha_i(\mathbf{k})+\alpha_i(\mathbf{k})\alpha_i^\dagger(\mathbf{k})-\langle 0|\,\alpha_i(\mathbf{k})\alpha_i^\dagger(\mathbf{k})\,|0\rangle\right\}\right\rangle \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\,\omega\left\langle \frac{1}{2}\sum_{i=1}^{2}\left\{\alpha_i^\dagger(\mathbf{k})\alpha_i(\mathbf{k})+\alpha_i(\mathbf{k})\alpha_i^\dagger(\mathbf{k})-\left[\alpha_i(\mathbf{k}),\,\alpha_i^\dagger(\mathbf{k})\right]\right\}\right\rangle \\ &= \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega}\,\omega\left\langle \sum_{i=1}^{2}\alpha_i^\dagger(\mathbf{k})\alpha_i(\mathbf{k})\right\rangle\end{aligned}$$

Note that, all creation operators are to the left of the annihilation operators and that gives a well-defined operator without divergences.

Mathematically, the divergence problems are caused by products of field operators at the same position such as $\mathbf{E}(x)^2$, which turned out to be too singular. We can achieve the subtraction of the vacuum energy automatically if we introduce a new kind of product of field operators, the so-called *normal ordered product*.
Definition: In the normal product, all creation operators act as if they were to the *left* to all annihilation operators.

$$\begin{aligned} :a^\dagger a'^\dagger: &= a^\dagger a'^\dagger \\ :a^\dagger a': &= a^\dagger a' \\ :a a'^\dagger: &= a'^\dagger a \\ :a a': &= a a' \end{aligned}$$

where a, a' are arbitrary annihilation operators of Bose fields. In the case of fermions, an additional minus sign appears when exchanging operators.

Example:

$$\begin{aligned} \mathbf{E}(x) \sim a^\dagger + a \quad \Longrightarrow \quad :\mathbf{E}^2(x): &\sim \ :\left(a^\dagger + a\right)\left(a^\dagger + a\right): \\ &= \ :\left(a^\dagger a^\dagger + a^\dagger a + a a^\dagger + aa\right): \\ &= \ a^\dagger a^\dagger + 2a^\dagger a + aa \end{aligned}$$

The correct expressions for energy and momentum are

$$\begin{aligned} p^0 &= \int_{t=\text{const}} \mathrm{d}^3\mathbf{x}\, \frac{1}{2} :\left(\mathbf{E}^2(x) + \mathbf{B}^2(x)\right): \\ \mathbf{p} &= \int_{t=\text{const}} \mathrm{d}^3\mathbf{x}\, :\mathbf{E}(x) \times \mathbf{B}(x): \end{aligned}$$

The analogous problem occurs with the Dirac field and can also be solved by the normal product. Note that the Dirac current $\bar{\psi}(x)\gamma^\mu\psi(x)$ transforms like a four-current density. Originally, the Dirac field was considered to be a relativistic probability amplitude of an electron. The zero component of the Dirac current was interpreted as a probability density, because for a Dirac spinor it is $\bar{\psi}(x)\gamma^0\psi(x) = \psi^+(x)\psi(x) > 0$ for $\psi(x) \neq 0$. However, a one-particle interpretation of the Dirac spinor is not tenable and the question arises: What role does the Dirac current play in the theory of the free quantized Dirac field?

Charge and current distribution, i.e. the electromagnetic four-current density $\jmath^\mu(x)$ of a system of electrons and positrons is definitively an observable. We make the ansatz:

$$\jmath^\mu(x) = -e\bar{\psi}(x)\gamma^\mu\psi(x)\,,$$

where $-e$ denotes a negative elementary charge.
Thus the total charge operator is

$$Q' = \int \mathrm{d}^3\mathbf{x}\, \jmath^0(\mathbf{x}, t) = -e \int \mathrm{d}^3\mathbf{x}\, \bar{\psi}(\mathbf{x}, t)\gamma^0\psi(\mathbf{x}, t)\,.$$

Reminder:

$$\psi(x) = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\,\frac{1}{2p^0} \sum_{s=\pm\frac{1}{2}} \left\{ e^{\imath px} v_s(p) b_s^\dagger(\mathbf{p}) + e^{-\imath px} u_s(p) a_s(\mathbf{p}) \right\}$$

Thus

$$Q' = -e \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2p^0} \sum_{s=\pm\frac{1}{2}} \left\{ a_s^\dagger(\mathbf{p}) a_s(\mathbf{p}) + b_s(\mathbf{p}) b_s^\dagger(\mathbf{p}) \right\}$$

and we get

$$\begin{aligned}
\langle 0| Q' |0\rangle &= -e \int \frac{\mathrm{d}^3 \mathbf{p}}{(2\pi)^3 2p^0} \sum_{s=\pm\frac{1}{2}} \langle 0| b_s(\mathbf{p}) b_s^\dagger(\mathbf{p}) |0\rangle \\
&= -e \int \frac{\mathrm{d}^3 \mathbf{p}}{(2\pi)^3 2p^0} \sum_{s=\pm\frac{1}{2}} \langle 0| \left\{ b_s(\mathbf{p}),\, b_s^\dagger(\mathbf{p}) \right\} |0\rangle \\
&= -e \int \frac{\mathrm{d}^3 \mathbf{p}}{(2\pi)^3 2p^0} \sum_{s=\pm\frac{1}{2}} (2\pi)^3 2p^0 \delta(0) \\
&= -e \int \mathrm{d}^3 \mathbf{p}\, 2\delta^3(0) \\
&= \infty \quad \text{for} \quad V \to \infty \,,
\end{aligned}$$

which is a similar problem as with the zero point of the energy. We obtain a “good” charge operator Q, if we choose the total charge of the vacuum as the zero point.

$$\begin{aligned}
Q &= Q' - \langle 0| Q' |0\rangle \\
&= -e \int \frac{\mathrm{d}^3 \mathbf{p}}{(2\pi)^3 2p^0} \sum_{s=\pm\frac{1}{2}} \left(a_s^\dagger(\mathbf{p}) a_s(\mathbf{p}) + b_s(\mathbf{p}) b_s^\dagger(\mathbf{p}) - \left\{ b_s(\mathbf{p}),\, b_s^\dagger(\mathbf{p}) \right\} \right) \\
&= -e \int \frac{\mathrm{d}^3 \mathbf{p}}{(2\pi)^3 2p^0} \sum_{s=\pm\frac{1}{2}} \left(a_s^\dagger(\mathbf{p}) a_s(\mathbf{p}) - b_s^\dagger(\mathbf{p}) b_s(\mathbf{p}) \right)
\end{aligned}$$

Q has positive and negative eigenvalues, electrons have charge $-e$ and positrons $+e$. The infinite self-charge of the vacuum is mathematically again caused by products of two field operators at the same position and can be avoided by *normal order* of the fermionic field operators as in the case bosons.

Definition:

$$:\!a_r(\mathbf{p}) a_s^\dagger(\mathbf{p}')\!: \;=\; -a_s^\dagger(\mathbf{p}') a_r(\mathbf{p})\,,$$

i.e., for every interchange of fermionic field operators we get an additional factor -1 according to anti-commutation relations of fermions.

Thus, we obtain a four-current density with a vanishing total charge of the vacuum as

$$\jmath^\mu(x) = -e :\!\bar{\psi}(x) \gamma^\mu \psi(x)\!: .$$

Note that $:\!\bar{\psi}\gamma^0\psi\!:$ is not anymore positive.

8.3 Electromagnetic coupling and perturbation theory

Lagrangian of EM field:

In the framework of a deductive construction of QED one puts the Lagrangian L of the coupled Maxwell-Dirac system at the top, namely first for the classical fields:

$$L = \int \mathrm{d}^3\mathbf{x}\,\mathcal{L}(\mathbf{x}, t)$$

with the Lagrangian density

$$\mathcal{L}(x) = \mathcal{L}_0(x) + \mathcal{L}_{\text{int}}(x)\,,$$

which consists of terms due to free fields, the electromagnetic and the Dirac field,

$$\mathcal{L}_0(x) = -\frac{1}{4}F_{\mu\nu}(x)F^{\mu\nu}(x) + \bar{\psi}(x)(\imath\gamma^\mu\partial_\mu - m)\psi(x)$$

and the interaction term

$$\begin{aligned} \mathcal{L}_{\text{int}}(x) &= -\jmath^\mu(x)A_\mu(x) \\ &= e\bar{\psi}(x)\gamma^\mu A_\mu(x)\psi(x)\,. \end{aligned}$$

The Lagrangian density of the electromagnetic field is not unique. One can derive the Maxwell equations from

$$\mathcal{L} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu} - \jmath_\mu A^\mu\,, \tag{8.12}$$

with

$$F_{\mu\nu} = A_{\mu,\nu} - A_{\nu,\mu}\,, \quad A_{\mu,\nu} = \frac{\partial A_\mu}{\partial x^\nu}$$

where $F_{\mu\nu}$ is the electromagnetic field tensor.

Euler-Lagrange Equation:

$$\frac{\partial\mathcal{L}}{\partial A_\mu} = \partial_\nu\frac{\partial\mathcal{L}}{\partial A_{\mu,\nu}}$$

From the Lagrangian (8.12) we have

$$\begin{aligned} \partial_\nu\frac{\partial\mathcal{L}}{\partial A_{\mu,\nu}} &= \partial_\nu\left\{\frac{\partial}{\partial A_{\mu,\nu}}\left(-\frac{1}{4}\left(A_{\alpha,\beta} - A_{\beta,\alpha}\right)\left(A^{\alpha,\beta} - A^{\beta,\alpha}\right)\right)\right\} \\ &= -\frac{1}{4}\partial_\nu\left\{\frac{\partial}{\partial A_{\mu,\nu}}\left(A_{\alpha,\beta}A^{\alpha,\beta} - A_{\beta,\alpha}A^{\alpha,\beta} - A_{\alpha,\beta}A^{\beta,\alpha} + A_{\beta,\alpha}A^{\beta,\alpha}\right)\right\} \\ &= -\frac{1}{4}\partial_\nu\left\{2\left(A^{\mu,\nu} - A^{\nu,\mu} + A^{\mu,\nu} - A^{\nu,\mu}\right)\right\} \\ &= -\frac{1}{2}\partial_\nu\left(F^{\mu\nu} - \underbrace{F^{\nu\mu}}_{=-F^{\mu\nu}}\right) \\ &= -\partial_\nu F^{\mu\nu}, \end{aligned}$$

and

$$\frac{\partial \mathcal{L}}{\partial A_\mu} = \frac{\partial}{\partial A_\mu}\left(-\jmath_\mu A^\mu\right) = \frac{\partial}{\partial A_\mu}\left(-\jmath^\mu A_\mu\right) = -\jmath^\mu \,.$$

The Euler-Lagrange equation yields

$$\boxed{\partial_\nu F^{\mu\nu} = \jmath^\mu .}$$

Now, applying ∂_ν to $(A^{\mu,\nu} - A^{\nu,\mu})$, we get

$$\begin{aligned}\partial_\nu\left(A^{\mu,\nu} - A^{\nu,\mu}\right) &= \partial_\nu\left(\partial^\nu A^\mu - \partial^\mu A^\nu\right)\\ &= \Box A^\mu - \partial^\mu \partial_\nu A^\nu\\ &= \jmath^\mu .\end{aligned}$$

For the Lorentz Gauge

$$\partial_\nu A^\nu = 0 \,,$$

we get,

$$\boxed{\Box A^\mu = \jmath^\mu \,,}$$

which is the Maxwell equation for 4-vector potential.

Question: What is $\jmath^\mu$ in the presence of charged particles, *e.g.* electrons, described by the Dirac field ψ?

Answer: $\jmath^\mu = -e\bar{\psi}\gamma^\mu\psi$.

Dirac equation from the Lagrangian density of the Dirac field:

The Lagrangian density for a Dirac field is

$$\mathcal{L}_0 = \bar{\psi}\left(\imath\gamma^\mu\partial_\mu - m\right)\psi$$

Proof:

$$\frac{\partial \mathcal{L}}{\partial \bar{\psi}} = \left(\imath\gamma^\mu\partial_\mu - m\right)\psi$$

$$\partial_\mu \frac{\partial \mathcal{L}}{\partial\left(\partial_\mu \bar{\psi}\right)} = 0.$$

The Euler-Lagrange equation reads

$$\frac{\partial \mathcal{L}}{\partial \bar{\psi}} - \partial_\mu \frac{\partial \mathcal{L}}{\partial\left(\partial_\mu \bar{\psi}\right)} = \underbrace{\left(\imath\gamma^\mu\partial_\mu - m\right)\psi = 0}_{\text{Dirac Equation}} .$$

Analogously,

$$\underbrace{\frac{\partial \mathcal{L}}{\partial \psi}}_{=-m\bar{\psi}} - \partial_\mu \underbrace{\frac{\partial \mathcal{L}}{\partial\left(\partial_\mu \psi\right)}}_{=\partial_\mu\left(\imath\bar{\psi}\gamma^\mu\right)} = \underbrace{-\left(\imath\partial_\mu\bar{\psi}\gamma^\mu + m\bar{\psi}\right) = 0}_{\text{Adjoint Dirac Equation}}$$

Dirac field in the presence of EM field:

We had already derived the form of the coupling term in the context of the interaction between the quantized radiation field and matter. These so-called *minimal coupling* results from $\mathcal{L}_0$ by the substitution

$$\partial_\mu \to \partial_\mu - \imath e A_\mu \,,$$

then,

$$\begin{aligned} \mathcal{L} &= \bar{\psi}\left(\imath\gamma^\mu\left(\partial_\mu - \imath e A_\mu\right) - m\right)\psi \\ &= \bar{\psi}\left(\imath\gamma^\mu\partial_\mu - m\right)\psi + e\bar{\psi}\gamma^\mu A_\mu\psi \\ &= \mathcal{L}_0 - \jmath^\mu A_\mu \,, \end{aligned}$$

with $\jmath^\mu = -e\bar{\psi}\gamma^\mu\psi$. This makes the theory *locally* gauge invariant under $U(1)$.

Why "minimal coupling"?

Dirac-Lagrangian is invariant under a "global" $U(1)$ transformation:

$$\begin{aligned} &\psi \longrightarrow e^{\imath e\Lambda(x)}\psi =: \psi' \quad \text{with} \quad \Lambda = \text{Const.} \\ \rightsquigarrow\ &\bar{\psi} = e^{-\imath e\Lambda(x)}\bar{\psi} =: \bar{\psi}' \end{aligned}$$

Since

$$\begin{aligned} \mathcal{L}_0' &= \bar{\psi}'\left(\imath\partial_\mu\gamma^\mu - m\right)\psi' \\ &= e^{-\imath e\Lambda}\bar{\psi}\left(\imath\partial_\mu\gamma^\mu - m\right)e^{\imath e\Lambda}\psi \\ &= \bar{\psi}\left(\imath\partial_\mu\gamma^\mu - m\right)\psi \\ &= \mathcal{L}_0 \,. \end{aligned}$$

From this global $U(1)$ symmetry follows, in accordance with the Noether-theorem, the conservation of charge

$$Q = -e\int \mathrm{d}^3\mathbf{x}\bar{\psi}\gamma^0\psi \qquad \text{i.e.} \quad \frac{\mathrm{d}}{\mathrm{d}t}Q = 0\,.$$

Proof. We assume the transformation as follows,

$$\psi(\Lambda) = \exp(\imath e\Lambda)\psi(0)$$

Then we get,

$$
\begin{aligned}
0 = \frac{\partial \mathcal{L}}{\partial \Lambda} &= \frac{\partial \mathcal{L}}{\partial \psi}\frac{\partial \psi}{\partial \Lambda} + \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \underbrace{\frac{\partial(\partial_\mu \psi)}{\partial \Lambda}}_{=\partial_\mu \frac{\partial \psi}{\partial \Lambda}} \\
&= \frac{\partial \mathcal{L}}{\partial \psi}\frac{\partial \psi}{\partial \Lambda} + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \frac{\partial \psi}{\partial \Lambda} \right) - \left(\partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \right) \frac{\partial \psi}{\partial \Lambda} \\
&= \underbrace{\left(\frac{\partial \mathcal{L}}{\partial \psi} - \partial_\mu \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \right)}_{=0 \text{ due to Euler-Lagrange}} \frac{\partial \psi}{\partial \Lambda} + \partial_\mu \left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \frac{\partial \psi}{\partial \Lambda} \right) \\
&\implies \partial_\mu \underbrace{\left(\frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \frac{\partial \psi}{\partial \Lambda} \right)}_{=: \jmath^\mu} = 0 \,,
\end{aligned}
$$

which implies that $\jmath^\mu$ is a conserved current, *i.e.*

$$
\begin{aligned}
\partial_0 \jmath^0 = \partial_i \jmath^i \qquad &\text{or, } \frac{\partial}{\partial t}\jmath^0 = \nabla \cdot \jmath \\
\implies \frac{d}{dt} &\underbrace{\int d^3\mathbf{r}\, \jmath^0}_{=:Q \text{ ,the conserved charge}} = 0
\end{aligned}
$$

Now,

$$
\jmath^\mu = \frac{\partial \mathcal{L}}{\partial(\partial_\mu \psi)} \frac{\partial \psi}{\partial \Lambda} = \left(\bar{\psi} \imath \gamma^\mu \right) (\imath e \psi) = -e \bar{\psi} \gamma^\mu \psi
$$

■

$\mathcal{L}_0$ is invariant under $\psi \to e^{\imath e \Lambda}\psi$ with $\Lambda =$ const, i.e., the Lagrange function does not change when the Dirac spinor is multiplied by a constant phase factor. This invariance of the Lagrangian function under a global gauge transformation results, according to the Noether's theorem, in a conservation law and in this case charge is conserved (already proven). Since Λ is constant, the gauge transformation must be the same at every point of space-time, i.e., it is a *global* gauge transformation. This means that if we rotate the phase of the spinor at one point by the angle Λ, we must perform the same rotation at all other points simultaneously.

If one takes this physical interpretation seriously, then one sees that it is impossible to fulfill, since it violates the spirit of relativity, according to which there must be a minimal delay, which corresponds to the time that the light needs to travel from one point in space to another.

To get around this problem, one gives up the requirement that Λ must be a constant and writes the phase factor $\Lambda(x)$ as an arbitrary function of space-time x. This is a *local* gauge transformation, it varies from point to point. It is also called the "gauge transformation of second kind".

The principle of relativity requires that $\mathcal{L}$ should also be invariant under local $U(1)$ transformation:

$$
\psi \longrightarrow e^{\imath e \Lambda(x)} \psi \,, \tag{8.13}
$$

This can be achieved when the derivative ∂_μ is replaced by:

$$\partial_\mu \to \partial_\mu - \imath e A_\mu \,,$$

and the vector potential is transformed as

$$A_\mu \longrightarrow A_\mu + \partial_\mu \Lambda(x) \,, \tag{8.14}$$

which is a gauge transformation.
Then, starting with $\mathcal{L}$ and with the following transformation of ψ as ψ'

$$\mathcal{L} = \bar{\psi} \left[\imath \left(\partial_\mu - \imath e A_\mu\right) \gamma^\mu - m\right] \psi \,, \qquad \psi' = e^{\imath e \Lambda(x)} \psi \,,$$

we get,

$$\begin{aligned}
\mathcal{L}' &= \bar{\psi}' \left[\imath \left(\partial_\mu - \imath e A_\mu\right) \gamma^\mu - m\right] \psi' \\
&= e^{-\imath e \Lambda(x)} \bar{\psi} \left[\imath \left(\partial_\mu - \imath e \left(A_\mu + \partial_\mu \Lambda(x)\right)\right) \gamma^\mu - m\right] e^{\imath e \Lambda(x)} \psi \\
&= \bar{\psi} \left[\imath \left(\partial_\mu - \imath e A_\mu\right) \gamma^\mu - m\right] \psi + e \bar{\psi} \partial_\mu \Lambda(x) \gamma^\mu \psi - e \bar{\psi} \partial_\mu \Lambda(x) \gamma^\mu \psi \\
&= \bar{\psi} \left[\imath \left(\partial_\mu - \imath e A_\mu\right) \gamma^\mu - m\right] \psi = \mathcal{L} \,.
\end{aligned}$$

which is invariant under the given gauge transformation.
Here, the Lagrangian density

$$\begin{aligned}
\mathcal{L} &= \bar{\psi} \left(\imath \left[\partial_\mu - \imath e A_\mu\right] \gamma^\mu - m\right) \psi \\
&= \bar{\psi} \left(\imath \partial_\mu \gamma^\mu - m\right) \psi + \underbrace{e \bar{\psi} \gamma^\mu A_\mu \psi}_{= -\jmath^\mu A_\mu} \\
&= \bar{\psi} \left(\imath \partial_\mu \gamma^\mu - m\right) \psi - e \jmath^\mu A_\mu \,.
\end{aligned}$$

In other words, $\mathcal{L}$ is invariant under the local gauge transformation (8.13) and (8.14). This invariance of the coupled Maxwell-Dirac system, discovered by H. Weyl in 1929, is called nowadays a $U(1)$ gauge symmetry. Gauge symmetries are the cornerstone of modern theories of elementary particles. Both the strong and weak interactions are governed by gauge symmetries, which are a generalization of the gauge symmetry of QED.

If we neglect the coupling term in $\mathcal{L}$, i.e. we set $e = 0$, then we get the free Maxwell and Dirac equations as Euler-Lagrange equations. The quantization of the corresponding fields is done as discussed already. The idea is now to perform a series expansion in e in order to account for the coupling. Such a approach is called perturbation theory.

The interaction or Dirac representation:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{int}}$$

The field operators obey

$$\frac{\mathrm{d}}{\mathrm{d}t} A(t) = \imath \left[\mathcal{H}_0, \, A(t)\right] \quad \Longrightarrow \quad A(t) = e^{\imath \mathcal{H}_0 t} A e^{-\imath \mathcal{H}_0 t}$$

Time-evolution of states due to

$$\imath \frac{\partial}{\partial t} \left|t\right\rangle = \mathcal{H}_{\text{int}}(t) \left|t\right\rangle \quad \Longrightarrow \quad \left|t\right\rangle = T \exp\left(-\imath \int_0^t \mathrm{d}\tau \mathcal{H}_{\text{int}}(\tau)\right) \left|t = 0\right\rangle \tag{8.15}$$

where T is the time-ordering operator.
Since the coupling term $\mathcal{L}_{\text{int}}$ in the Lagrangian density does not contain any time derivatives, the interaction energy $\mathcal{H}_{\text{int}}(t)$ equals $\mathcal{L}_{\text{int}}$ except for a sign:

$$\mathcal{H}_{\text{int}}(t) = -\int \mathrm{d}^3\mathbf{r}\, \mathcal{L}_{\text{int}}(\mathbf{r},t) = \int \mathrm{d}^3\mathbf{r}\, \jmath^\mu(\mathbf{r},t) A_\mu(\mathbf{r},t)\,,$$

this means

$$\mathcal{H}_{\text{int}}(t) = -e \int \mathrm{d}^3\mathbf{r}\ :\bar{\psi}(\mathbf{r},t)\gamma^\mu\psi(\mathbf{r},t):\ A_\mu(\mathbf{r},t)\,. \tag{8.16}$$

The equations (8.15) and (8.16) are the basis for the Feynman rules of QED.

We consider the following physical problem: At time $t \to -\infty$, a certain number of electrons e^-, positrons e^+, and photons γ are present, all widely separated from each other. These particles can over time hit each other, scatter off each other, annihilate each other or create new particles. We ask about the state at time $t \to +\infty$, in particular, about the transition amplitude into a given state with a certain number of electrons, positrons and photons.

$$e^-(p_1) + \ldots + e^+(q_1) + \ldots + \gamma(k_1) + \ldots \quad \longrightarrow \quad e^-(p_1') + \ldots + e^+(q_1') + \ldots + \gamma(k_1') + \ldots$$

8.4 Feynman rules

We start from equation (8.15) and expand in (8.16) $\bar{\psi}$, ψ and A_μ in terms of creation and annihilation operators, where we schematically set $\bar{\psi} \sim b + a^\dagger$, $\psi \sim b^\dagger + a$, $A_\mu \sim \alpha^\dagger + \alpha$.
Reminder:

$$\psi(x) = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3}\frac{1}{2p^0}\sum_{s=\pm 1/2}\left\{e^{\imath px}v_s(p)b_s^\dagger(\mathbf{p}) + e^{-\imath px}u_s(p)a_s(\mathbf{p})\right\}$$

We obtain the following structure for $\mathcal{H}_{\text{int}}$:

$$\begin{aligned}\mathcal{H}_{\text{int}} &\sim\ :\left(b + a^\dagger\right)\left(b^\dagger + a\right):\left(\alpha^\dagger + \alpha\right)\\ &\sim \underbrace{-b^\dagger b\left(\alpha^\dagger + \alpha\right)}_{(a)} + \underbrace{a^\dagger b^\dagger\left(\alpha^\dagger + \alpha\right)}_{(b)} + \underbrace{ba\left(\alpha^\dagger + \alpha\right)}_{(c)} + \underbrace{a^\dagger a\left(\alpha^\dagger + \alpha\right)}_{(d)}\end{aligned}$$

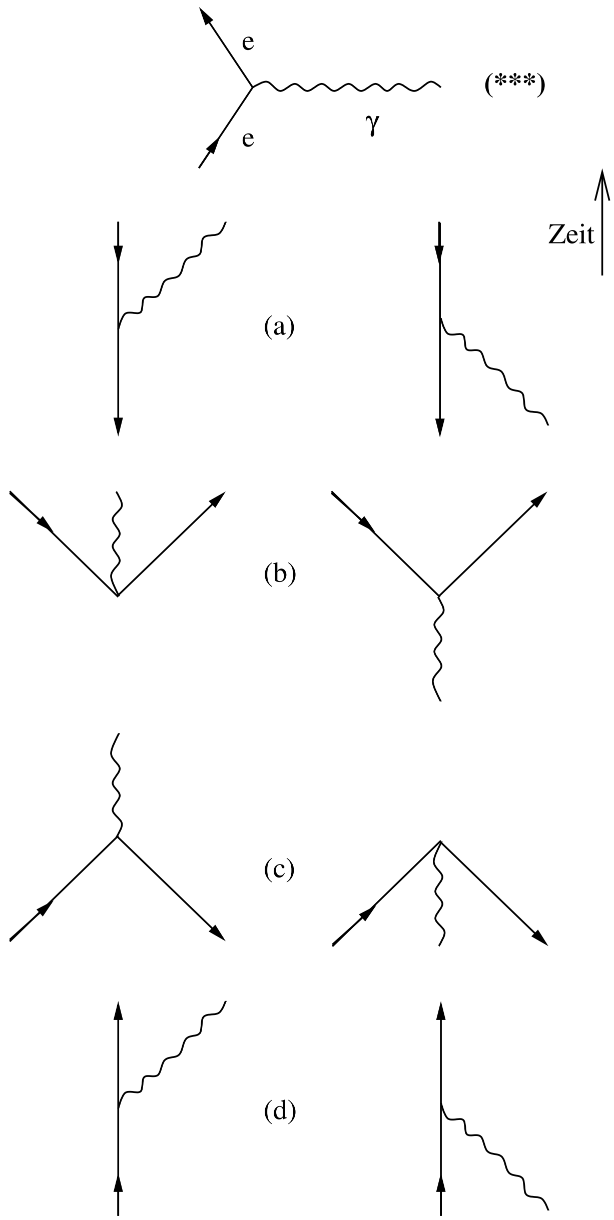
If we apply $\mathcal{H}_{\text{int}}$ to any state then, for example, the term (d) causes the following: By a an electron is annihilated, by $a^\dagger$ an electron with a in general different momentum is re-created. Thereby a photon is either emitted ($\alpha^\dagger$) or absorbed (α).
Diagrammatic illustration:

(a) Emission or absorption of a photon by a positron.

(b) Creation of an electron-positron pair under emission or absorption of a photon.

(c) Annihilation of an electron-positron pair under emission or absorption of a photon.

(d) Emission or absorption of a photon by an electron.



All processes can be represented by a single diagram, see $(***)$, if one defines to symbolize positrons by electron lines running backwards in time.

At the time $t \to \infty$ we have a certain number of electrons, positrons and photons, which we indicate by corresponding lines. According to (8.15) there is a probability per unit time for a transition to an other state, where one of the processes (a)-(d) is possible. This can repeat. According to the rules of quantum mechanics, the transition amplitudes into a certain final state must be added coherently, independent of the intermediate steps leading to this state. The correct superposition results from the formal solution of (8.15):

$$|t\rangle = \left\{ 1 + (-\imath) \int_{-\infty}^{t} \mathrm{d}t' \, \mathcal{H}_{\mathrm{int}}(t') + (-\imath)^2 \int_{-\infty}^{t} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}t'' \, \mathcal{H}_{\mathrm{int}}(t') \mathcal{H}_{\mathrm{int}}(t'') + \dots \right\} |t = -\infty\rangle$$

This results in the $\mathcal{S}$ operator, which describes the time evolution of the states from $t \to -\infty$

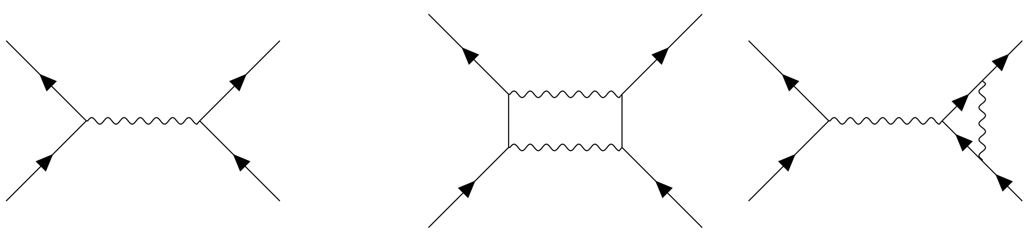
to $t \to +\infty$:

$$
\begin{aligned}
|t = +\infty\rangle &= \mathcal{S}\,|t = -\infty\rangle \\
&= \left\{ 1 + (-\imath) \int_{-\infty}^{\infty} \mathrm{d}t'\, \mathcal{H}_{\text{int}}(t') + (-\imath)^2 \int_{-\infty}^{\infty} \mathrm{d}t' \int_{-\infty}^{t'} \mathrm{d}t''\, \mathcal{H}_{\text{int}}(t')\mathcal{H}_{\text{int}}(t'') + \ldots \right\} |t = -\infty\rangle
\end{aligned}
$$

Using the time ordered product, $\mathcal{S}$ can be written in a bit compact way:

$$
\begin{aligned}
\mathcal{S} &= \sum_{n=0}^{\infty} \frac{(-\imath)^n}{n!} \int_{-\infty}^{\infty} \mathrm{d}t_1 \cdots \int_{-\infty}^{\infty} \mathrm{d}t_n\, T\left(\mathcal{H}_{\text{int}}(t_1) \cdots \mathcal{H}_{\text{int}}(t_n)\right) \\
&= T\left\{ \exp\left[-\imath \int_{-\infty}^{\infty} \mathrm{d}t\, \mathcal{H}_{\text{int}}(t) \right] \right\} \qquad (8.17)
\end{aligned}
$$

Since $\mathcal{H}_{\text{int}}$ is proportional to e, (8.17) is basically an expansion of the $\mathcal{S}$ operator in powers of $e = \sqrt{4\pi\alpha}$, where α is the fine-structure constant.



2nd order in e 4th order in e

Figure 8.1: Some diagrams for the electron-electron scattering.

8.5 Simple reaction: electron-electron scattering

$$e^-\,(p_1,\,r_1) + e^-\,(p_2,\,r_2) \to e^-\,(p_3,\,r_3) + e^-\,(p_4\;r_4) \tag{8.18}$$

Four-momenta in the center-of-mass system:

$$\underbrace{p_1 = \begin{pmatrix} E \\ \mathbf{p} \end{pmatrix}, \quad p_2 = \begin{pmatrix} E \\ -\mathbf{p} \end{pmatrix},}_{\text{Before scattering}} \qquad \underbrace{p_3 = \begin{pmatrix} E \\ \mathbf{p}' \end{pmatrix}, \quad p_4 = \begin{pmatrix} E \\ -\mathbf{p}' \end{pmatrix},}_{\text{After scattering}}$$

where $|\mathbf{p}| = |\mathbf{p}'|$.

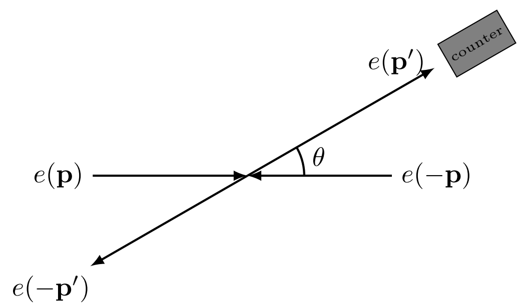


Figure 8.2: Electron-electron scattering in the center-of-mass system.

State before scattering:

$$|t \to -\infty\rangle = a^+_{r_1}(\mathbf{p}_1)a^+_{r_2}(\mathbf{p}_2)|\,0\,\rangle$$

Transition amplitudes for the reaction (8.18):

$$\begin{aligned} S_{fi} &= \langle e\,(p_3,\,r_3)\,e\,(p_4,\,r_4)|\,\mathcal{S}\,|e\,(p_1,\,r_1)\,e\,(p_2,\,r_2)\rangle \\ &= \langle\,0\,|\,a_{r_3}(\mathbf{p}_3)a_{r_4}(\mathbf{p}_4)\,\mathcal{S}\,a^\dagger_{r_1}(\mathbf{p}_1)a^\dagger_{r_2}(\mathbf{p}_2)\,|\,0\,\rangle \end{aligned} \tag{8.19}$$

We truncate the expansion of $\mathcal{S}$ after terms of order e^2:

$$\begin{aligned} &\mathcal{S} = \mathbf{1} && \leftarrow \begin{cases} \text{does not contribute to (8.19) if} \\ {\scriptstyle (p_1,r_1),(p_2,r_2)\neq(p_3,r_3),(p_4,r_4)} \end{cases} \\ &\quad + (-\imath)\int_{-\infty}^{\infty} \mathrm{d}t'\,\mathcal{H}_{\text{int}}(t') && \leftarrow \begin{cases} \text{does not contribute to (8.19), contains only} \\ \text{one photon creation or annihilation operator} \end{cases} \\ &\quad + \frac{(-\imath)^2}{2!}\int_{-\infty}^{\infty}\mathrm{d}t'\int_{-\infty}^{\infty}\mathrm{d}t''\,T(\mathcal{H}_{\text{int}}(t')\mathcal{H}_{\text{int}}(t'')) && \leftarrow \{\ \text{relevant, is of order } e^2 \end{aligned}$$

Thus

$$S_{fi} = \frac{(-\imath)^2}{2!}\int_{-\infty}^{\infty}\mathrm{d}t'\int_{-\infty}^{\infty}\mathrm{d}t''\;\langle e(p_3,r_3)e(p_4,r_4)|\,T(\mathcal{H}(t')\mathcal{H}(t''))\,|e(p_1,r_1)e(p_2,r_2)\rangle$$

Inserting the explicit form of the interaction energy $\mathcal{H}_{\text{int}}(t)$ from (8.16) leads to

$$\begin{aligned} S_{fi} = \frac{(\imath)^2}{2!}e^2 \int \mathrm{d}x'\mathrm{d}x''\,\langle\,0\,|\,a_{r_3}(\mathbf{p}_3)a_{r_4}(\mathbf{p}_4) \\ T\left\{:\bar\psi(x')\gamma^\mu\psi(x'):\ A_\mu(x')\ :\bar\psi(x'')\gamma^\nu\psi(x''):\ A_\nu(x'')\right\} \\ a^\dagger_{r_1}(\mathbf{p}_1)a^\dagger_{r_2}(\mathbf{p}_2)\,|\,0\,\rangle \end{aligned} \tag{8.20}$$

Structure of the matrix element:

$$\langle\, 0\,|\, aa \,:\, (b+a^\dagger)(b^\dagger + a) \,:\, (\alpha+\alpha^\dagger) \,:\, (b+a^\dagger)(b^\dagger+a) \,:\, (\alpha+\alpha^\dagger)\, a^\dagger a^\dagger \,|\, 0\,\rangle$$

Evaluation is made easier by use of *Wick's theorem.*
Reminder:

$$\langle\, 0\,|\, a_i a_j^\dagger \,|\, 0\,\rangle = \langle\, 0\,|\, \{a_i, a_j^\dagger\} - a_j^\dagger a_i \,|\, 0\,\rangle = \{a_i, a_j^\dagger\}$$

thus

$$\begin{aligned}
\langle\, 0\,|\, a_1 a_2^\dagger a_3 a_4^\dagger \,|\, 0\,\rangle &= \langle\, 0\,|\, \left(\left\{a_1, a_2^\dagger\right\} - a_2^\dagger a_1\right)\left(\left\{a_3, a_4^\dagger\right\} - a_3^\dagger a_4\right) |\, 0\,\rangle \\
&= \left\{a_1, a_2^\dagger\right\} \cdot \left\{a_3, a_4^\dagger\right\} \\
&= \langle\, 0\,|\, a_1 a_2^\dagger \,|\, 0\,\rangle \langle\, 0\,|\, a_3 a_4^\dagger \,|\, 0\,\rangle
\end{aligned}$$

Definition: "*Contraction*": $\langle\, 0\,|a_i a_j^\dagger|\, 0\,\rangle = \underbrace{a_i a_j^\dagger}$
That means: $\langle\, 0\,|\, \underbrace{a_1 a_2^\dagger}\underbrace{a_3 a_4^\dagger} \,|\, 0\,\rangle = \underbrace{a_1 a_2^\dagger}\ \underbrace{a_3 a_4^\dagger}$
Consider

$$\begin{aligned}
\langle\, 0\,|\, a_1 a_2 a_3^\dagger a_4^\dagger \,|\, 0\,\rangle &= \langle\, 0\,|\, a_1 \left(\left\{a_2, a_3^\dagger\right\} - a_3^\dagger a_2\right) a_4^\dagger \,|\, 0\,\rangle \\
&= \langle\, 0\,|\, a_1 a_4^\dagger \,|\, 0\,\rangle \left\{a_2, a_3^\dagger\right\} - \langle\, 0\,|\, a_1 a_3^\dagger a_2 a_4^\dagger \,|\, 0\,\rangle \\
&= \langle\, 0\,|\, a_1 a_4^\dagger \,|\, 0\,\rangle \langle\, 0\,|\, a_2 a_3^\dagger \,|\, 0\,\rangle - \langle\, 0\,|\, a_1 a_3^\dagger \,|\, 0\,\rangle \langle\, 0\,|\, a_2 a_4^\dagger \,|\, 0\,\rangle
\end{aligned}$$

i.e.

$$\begin{aligned}
\langle\, 0\,|\, a_1 a_2 a_3^\dagger a_4^\dagger \,|\, 0\,\rangle &= \langle\, 0\,|\, \underbrace{a_1 \underbrace{a_2 a_3^\dagger} a_4^\dagger} \,|\, 0\,\rangle + \langle\, 0\,|\, a_1 a_2 a_3^\dagger a_4^\dagger \,|\, 0\,\rangle \\
&= +\,\underbrace{a_1 a_4^\dagger}\ \underbrace{a_2 a_3^\dagger} \overbrace{\ -\ }^{\text{For fermions!}} \underbrace{a_1 a_3^\dagger}\ \underbrace{a_2 a_4^\dagger}
\end{aligned}$$

Wick's theorem: Vacuum expectation value of a product of creation and annihilation operators is equal to the sum of all contractions.

Regarding S_{fi}: The operators α, $\alpha^\dagger$ from $A_\mu(x')$ can only be contracted with those from $A_\nu(x'')$.

In the case of contraction of Fermi operators, we do not get a contribution if an operator from $\psi(x')$ is connected with one from $\bar{\psi}(x'')$, because then also at least one contraction of an incoming electron operator with an outgoing one occurs, which vanishes because of $(p_1, r_1), (p_2, r_2) \neq (p_3, r_3), (p_4, r_4)$.

Thus, there are only contributions from contraction of incoming and outgoing electrons with the field operators ψ and $\bar{\psi}$, respectively. For example, $a^+_{r_1}(\mathbf{p}_1)$ with $\psi(x')$ and $\psi(x'')$ etc.

$$
\begin{aligned}
&\langle 0 \,|\, a(\mathbf{p}_3)a(\mathbf{p}_4) \;:\; \overline{\psi}(x')\gamma^\mu\psi(x') \;::\; \overline{\psi}(x'')\gamma^\nu\psi(x'') \;:\; a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2) \,|\, 0 \,\rangle \\
&= \quad a(\mathbf{p}_3)a(\mathbf{p}_4) : \overline{\psi}(x')\gamma^\mu\psi(x') :: \overline{\psi}(x'')\gamma^\nu\psi(x'') : a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2) \\
&+ \quad a(\mathbf{p}_3)a(\mathbf{p}_4) : \overline{\psi}(x')\gamma^\mu\psi(x') :: \overline{\psi}(x'')\gamma^\nu\psi(x'') : a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2) \\
&+ \quad a(\mathbf{p}_3)a(\mathbf{p}_4) : \overline{\psi}(x')\gamma^\mu\psi(x') :: \overline{\psi}(x'')\gamma^\nu\psi(x'') : a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2) \\
&+ \quad a(\mathbf{p}_3)a(\mathbf{p}_4) : \overline{\psi}(x')\gamma^\mu\psi(x') :: \overline{\psi}(x'')\gamma^\nu\psi(x'') : a^\dagger(\mathbf{p}_1)a^\dagger(\mathbf{p}_2) \\
&= \quad \Big\{ \bar{u}(p_4)e^{\imath p_4 x'}\gamma^\mu u(p_1)e^{-\imath p_1 x'} \cdot \bar{u}(p_3)e^{\imath p_3 x''}\gamma^\nu u(p_2)e^{-\imath p_2 x''} \\
&\qquad -(1 \leftrightarrow 2) - (3 \leftrightarrow 4) + (1 \leftrightarrow 2, 3 \leftrightarrow 4) \Big\} \,.
\end{aligned}
$$

Because contractions of Fermi operators yield the same for $x'_0 > x''_0$ and $x''_0 > x'_0$, inserting this result into (8.20) leads to thus

$$
\begin{aligned}
S_{fi} = \frac{(\imath e)^2}{2} \int \mathrm{d}x'\,\mathrm{d}x'' \left\{ \theta(x'_0 - x''_0)\, \langle 0|\, A_\mu(x')A_\nu(x'')\, |0\rangle + \theta(x''_0 - x'_0)\, \langle 0|\, A_\nu(x'')A_\mu(x')\, |0\rangle \right\} \\
\cdot \Big\{ \bar{u}(p_4)\gamma^\mu u(p_1)e^{\imath(p_4-p_1)x'} \cdot \bar{u}(p_3)\gamma^\nu u(p_2)e^{\imath(p_3-p_2)x''} - (1 \leftrightarrow 2) - (3 \leftrightarrow 4) + (1 \leftrightarrow 2, 3 \leftrightarrow 4) \Big\} \,.
\end{aligned}
$$

Pooling of terms, which differ only by the name of the integration and summation variables, gives

$$
\begin{aligned}
S_{fi} = (\imath e)^2 \int dx' dx'' \overbrace{\langle 0|\, T(A_\mu(x')A_\nu(x''))\, |0\rangle}^{\text{Photon propagator}} \\
\cdot \Big\{ \bar{u}(p_4)\gamma^\mu u(p_1)\bar{u}(p_3)\gamma^\nu u(p_2)e^{\imath(p_4-p_1)x'}e^{\imath(p_3-p_2)x''} \\
-\bar{u}(p_3)\gamma^\mu u(p_1)\bar{u}(p_4)\gamma^\nu u(p_2)e^{\imath(p_3-p_1)x'}e^{\imath(p_4-p_2)x''} \Big\} \,.
\end{aligned}
$$

With

$$
\langle 0|\, T(A_\mu(x')A_\nu(x''))\, |0\rangle = \int \frac{dk}{(2\pi)^4}\, e^{-\imath k(x'-x'')} \frac{-\imath g_{\mu\nu}}{k^2 + \imath\epsilon} \qquad (\epsilon \to 0)
$$

the integrals over x' and x'' can be easily performed and give δ-functions for the four-momenta. The final result is

$$
S_{fi} = \imath(2\pi)^4 \delta(p_4 + p_3 - p_2 - p_1)\, T_{fi}\,, \tag{8.21}
$$

where

$$
\begin{aligned}
T_{fi} = \frac{1}{\imath} \Big\{ \bar{u}(p_4)(\imath e\gamma^\mu)u(p_1) \frac{-\imath g_{\mu\nu}}{(p_4 - p_1)^2} \bar{u}(p_3)(\imath e\gamma^\nu)u(p_2) \\
-\bar{u}(p_3)(\imath e\gamma^\mu)u(p_1) \frac{-\imath g_{\mu\nu}}{(p_3 - p_1)^2} \bar{u}(p_4)(\imath e\gamma^\nu)u(p_2) \Big\} \,.
\end{aligned}
$$

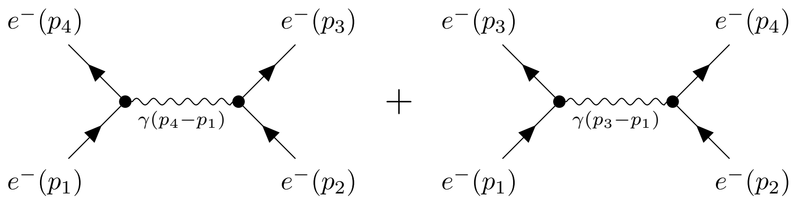


Figure 8.3: Four-momentum conservation applies to every vertex.

8.6 Photon propagator

Field operator of the four-potential A_μ reads as

$$A_\mu = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega} \left\{ e^{\imath kx} \alpha_\mu^\dagger(\mathbf{k}) + e^{-\imath kx} \alpha_\mu(\mathbf{k}) \right\} \tag{8.22}$$

with

$$k = \begin{pmatrix} \omega \\ \mathbf{k} \end{pmatrix}, \quad \omega = |\mathbf{k}|, \quad kx = k^\mu x_\mu = \omega t - \mathbf{k} \cdot \mathbf{x} \,.$$

Vacuum expectation value of an ordinary product of two four-potentials:

$$\langle 0| A_\mu(x) A_\nu(y) |0\rangle = -g_{\mu\nu} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3 2\omega} \, e^{-\imath k(x-y)}$$

Definition of a time-ordered product of two operators A_μ

$$T(A_\mu(x)A_\nu(y)) = \theta(x^0 - y^0)A_\mu(x)A_\nu(y) + \theta(y^0 - x^0)A_\nu(y)A_\mu(x) \,. \tag{8.23}$$

Time-ordered product independent of the reference system due to

$$[A_\mu(x), A_\nu(y)] = 0 \quad \text{for} \quad (x-y)^2 < 0 \,.$$

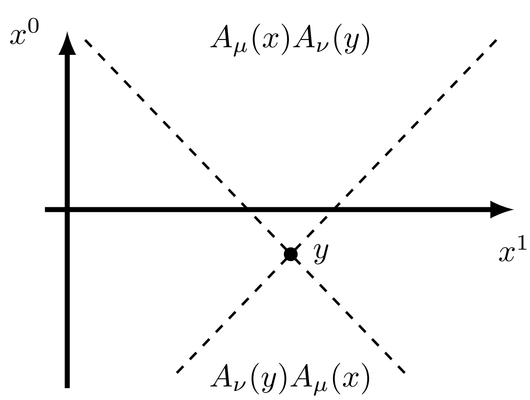


Figure 8.4: Illustration of the definition of the time-ordered product (8.23).

Claim:

$$\langle 0| T(A_\mu(x)A_\nu(y)) |0\rangle = \imath g_{\mu\nu} D_F(x-y) \tag{8.24}$$

with

$$\imath g_{\mu\nu} D_F(x-y) = \lim_{\epsilon\to 0} \int \frac{\mathrm{d}k}{(2\pi)^4}\, e^{-\imath k(x-y)} \frac{-\imath g_{\mu\nu}}{k^2+\imath\epsilon}\,,$$

where

$$\mathrm{d}k = \mathrm{d}k^0 \mathrm{d}k^1 \mathrm{d}k^2 \mathrm{d}k^3\,.$$

Proof:

$$\imath g_{\mu\nu} D_F(x-y) = g_{\mu\nu} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, e^{\imath\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \int_{-\infty}^{\infty} \frac{\mathrm{d}k^0}{2\pi\imath}\, e^{-\imath k^0(x^0-y^0)} \cdot \frac{1}{(k^0)^2-\mathbf{k}^2+\imath\epsilon} \tag{8.25}$$

The poles of integration are at

$$k^0 = \pm\sqrt{\mathbf{k}^2-\imath\epsilon} \longrightarrow \pm|\mathbf{k}|\,,$$

as indicated in the Figure 8.5.

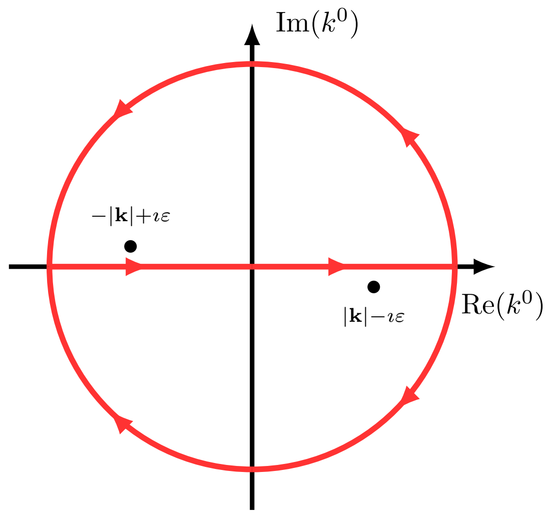


Figure 8.5: Position of the poles and the integration path in the k^0-plane for the integral (8.25)

For $x^0 > y^0$ it is

$$e^{-\imath k^0(x^0-y^0)} \longrightarrow 0 \quad \text{for} \quad \mathrm{Im}\, k^0 \to -\infty\,.$$

We can then add a very large semicircle to the integration path in the lower half of the k^0-plane and apply the residual theorem. We obtain

$$\imath g_{\mu\nu} D_F(x-y) = -g_{\mu\nu} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \frac{e^{-\imath\left[|\mathbf{k}|(x^0-y^0)-\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})\right]}}{2|\mathbf{k}|}$$

and by comparison with (8.22)

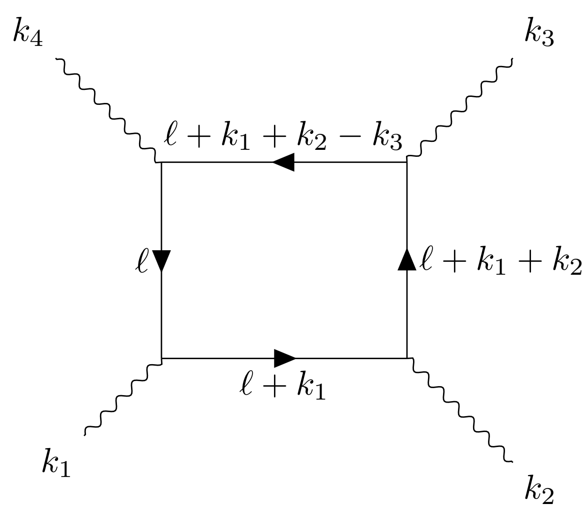
$$\imath g_{\mu\nu} D_F(x-y) = \langle 0| A_\mu(x)A_\nu(y) |0\rangle \quad \text{for} \quad x^0 > y^0\,.$$

For $x^0 < y^0$ we can close the integration path in the upper half-plane and we get

$$\begin{aligned} \imath g_{\mu\nu} D_F(x-y) &= -g_{\mu\nu} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} \frac{e^{-\imath\left[|\mathbf{k}|(y^0-x^0)-\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})\right]}}{2|\mathbf{k}|} \\ &= \langle 0| A_\nu(y) A_\mu(x) |0\rangle \quad \text{for} \quad x^0 < y^0 \,. \end{aligned}$$

With this (8.24) is proven. The function $\imath g_{\mu\nu} D_F(x-y)$ or its Fourier transform $-\imath g_{\mu\nu}/(k^2+\imath\epsilon)$ is called Feynman propagator of the free photon field. It plays a crucial role in the framework of the Feynman rules. The transition amplitude for a designated reaction is given by the sum of all diagrams with predefined incoming and outgoing lines. Within a diagram an arbitrary number of vertices is permitted. At every vertex, the four-momentum conservation is granted, which implies a momentum conservation as a whole ($\sum \text{inc.}\, p = \sum \text{outg.}\, p$).

Example: Photon-photon scattering, $\gamma(k_1) + \gamma(k_2) \to \gamma(k_3) + \gamma(k_4)$

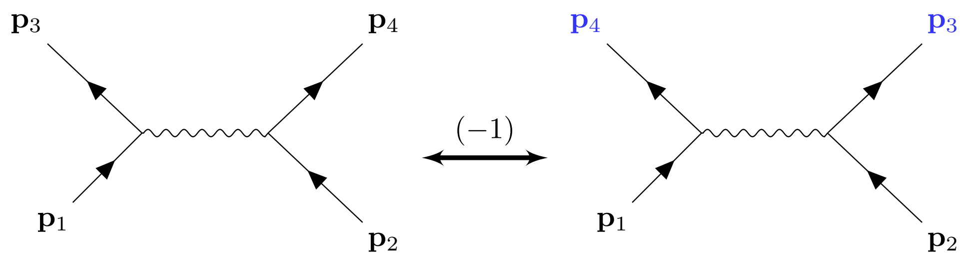


The loop momentum is ℓ. One always has to integrate over it with measure $\int \frac{d\ell}{(2\pi)^4}$.

For the S-matrix element, a factor considering the energy momentum conservation has to be added:

$$(2\pi)^4 \delta\left(\sum_f p_f - \sum_i p_i\right) ,$$

where p_i represent the momenta of the incoming particles and p_f the momenta of the outgoing particles respectively. There is also a factor of (-1) for every closed fermion loop. If a permutation of outer momenta of fermions takes place, there is also an additional factor given by the sign of the permutation, e.g.:



8.7 Electron propagator

The electron propagator is defined in terms of the expectation value of the time-ordered product

$$\langle 0|\mathrm{T}(\psi_\alpha(x)\bar{\psi}'_\alpha(x'))|0\rangle =: \imath S_F^{\alpha\alpha'}(x-x')\,,$$

where the action of the time-ordering operator T is given by

$$\mathrm{T}(\psi_\alpha(x)\bar{\psi}'_\alpha(x')) = \begin{cases} \psi_\alpha(x)\bar{\psi}'_\alpha(x')\,, & \text{for } t > t' \\ -\bar{\psi}'_\alpha(x')\psi_\alpha(x)\,, & \text{for } t < t' \end{cases}.$$

For convenience we will drop the spinor indices α and α' in the following but will keep in mind that $\bar{\psi}\psi \hat{=} \bar{\psi}_{\alpha'}\psi_\alpha$ etc. We calculate

$$\begin{aligned}\langle 0|\psi(x)\bar{\psi}(x')|0\rangle &= \frac{1}{V}\sum_{k,k'}\left(\frac{m^2}{E_k\,E'_k}\right)^{\frac{1}{2}}\sum_{r,\,r'}\langle 0|\left(\hat{b}_{r,k}u_r(k)e^{-\imath kx} + \hat{d}^\dagger_{r,k}w_r(k)e^{\imath kx}\right) \\ &\qquad\cdot\left(\hat{d}_{r',k'}\bar{w}_{r'}(k')e^{-\imath k'x'} + \hat{b}^\dagger_{r',k'}\bar{u}_{r'}(k')e^{\imath kx}\right)|0\rangle \\ &= \frac{1}{V}\sum_k\left(\frac{m}{E_k}\right)\left\{e^{-\imath k(x-x')}\underbrace{\sum_r u_r(k)\bar{u}_r(k)}_{=\frac{1}{2m}(k_\mu\gamma^\mu+m)}\right\} \\ &= \left(\imath\partial_\mu\gamma^\mu + m\right)\underbrace{\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{e^{-\imath k(x-x')}}{2E_k}}_{=:\,\imath\Delta^+(x-x')}\end{aligned}$$

$$\begin{aligned}-\langle 0|\bar{\psi}(x')\psi(x)|0\rangle &= -\frac{1}{V}\sum_k\left(\frac{m}{E_k}\right)\left\{e^{\imath k(x-x')}\underbrace{\sum_r \bar{w}_r(k)w_r(k)}_{=\frac{1}{2m}(k_\mu\gamma^\mu-m)}\right\} \\ &= (\imath\partial_\mu\gamma^\mu + m)\underbrace{\int\frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\frac{e^{\imath k(x-x')}}{2E_k}}_{=:\,\imath\Delta^-(x-x')}\end{aligned}$$

This yields

$$S_F(x) = (\imath\partial_\mu\gamma^\mu + m)\Delta_F(x)\,, \qquad \text{with } \Delta_F(x) = \begin{cases}\Delta^+(x)\,, & t > 0 \\ \Delta^-(x)\,, & t < 0\end{cases}.$$

Claim:

$$\Delta_F(x) = \lim_{\varepsilon\to 0} \int \frac{\mathrm{d}^4 k}{(2\pi)^4} \frac{e^{\imath kx}}{k^2 - m^2 + i\varepsilon}$$

Proof:
We rewrite $k^2 - m^2 + \imath\varepsilon$ as

$$k_0^2 - (\omega_k - \imath\eta)^2 = \underbrace{k_0^2 - \omega_k^2}_{=k^2-m^2} + \underbrace{2\omega_k \imath\eta}_{=:\imath\varepsilon} + \eta^2$$

and using this to express $\Delta_F(x)$ as

$$\Delta_F(x) = \lim_{\eta\to 0} \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} e^{-\imath \mathbf{k}\cdot\mathbf{x}} \times \underbrace{\frac{\imath}{2\pi\imath} \int_{-\infty}^{\infty} \mathrm{d}k_0 \, \frac{e^{-\imath k_0 x^0}}{k_0^2 - (\omega_k - \imath\eta)^2}}_{\substack{\text{evaluate with} \\ \text{residue theorem}}} .$$

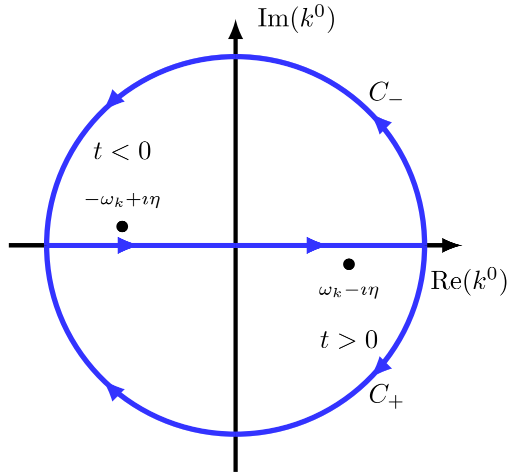
To use the residue theorem we rewrite the denominator of the second integral as

$$\frac{1}{k_0^2 - (\omega_k - \imath\eta)^2} = \frac{1}{2k_0} \left\{ \frac{1}{k_0 - (\omega_k - \imath\eta)} + \frac{1}{k_0 + (\omega_k - \imath\eta)} \right\},$$

which shows that there exists two poles, one at $\omega_k - \imath\eta$, the other at $-(\omega_k - \imath\eta)$.

$$e^{-\imath k_0 x^0} \longrightarrow 0$$

$$\begin{aligned}
&\text{for } t(=x^0) > 0 \qquad \text{if} \quad \operatorname{Im} k_0 < 0 \\
&\qquad\qquad\qquad\qquad\qquad |k_0| \to \infty \\
&\text{for } t(=x^0) < 0 \qquad \text{if} \quad \operatorname{Im} k_0 > 0 \\
&\qquad\qquad\qquad\qquad\qquad |k_0| \to \infty
\end{aligned}$$



$$\begin{aligned}
\Rightarrow \quad & \frac{1}{2\pi\imath} \int_{-\infty}^{\infty} \mathrm{d}k_0 \, \frac{e^{-\imath k_0 x^0}}{k_0^2 - (\omega_k - \imath\eta)^2} \\
= & \underbrace{\frac{1}{2\pi\imath} \int_{-\infty}^{\infty} \frac{\mathrm{d}k_0}{2k_0}}_{= \begin{cases} \int_{C_+} \frac{\mathrm{d}k_0}{2k_0} & \text{for } t > 0 \\ \int_{C_-} \frac{\mathrm{d}k_0}{2k_0} & \text{for } t > 0 \end{cases}} \left\{ \frac{e^{-\imath k_0 x^0}}{k_0 - (\omega_k - \imath\eta)} + \frac{e^{-\imath k_0 x^0}}{k_0 + (\omega_k - \imath\eta)} \right\} \\
= & \begin{cases} \dfrac{e^{-\imath\omega_k t}}{2\omega_k}, & t > 0 \\ \dfrac{e^{+\imath\omega_k t}}{2\omega_k}, & t < 0 \end{cases}
\end{aligned}$$

Note: We used *Cauchy's integral formula* $\frac{1}{2\pi\imath}\oint dz\, \frac{f(z)}{z-z_0} = f(z_0)$ to evaluate the integrals.

This yields the intermediate result

$$\Delta_F(x) = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3} e^{\imath\mathbf{k}\cdot\mathbf{x}} \times \frac{e^{\mp\imath\omega_k t}}{2\omega_k} = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \frac{e^{\mp\imath kx}}{2\omega_k}\,,$$

where in the exponent the "$-$" corresponds to $t > 0$ and the "$+$" to $t < 0$ respectively. Also note that we made use of the fact that $\int d\mathbf{k}\, e^{\imath\mathbf{k}\cdot\mathbf{x}} = \int \mathrm{d}^3\mathbf{k}\, e^{-\imath\mathbf{k}\cdot\mathbf{x}}$.

Coming back to the definition of the propagator, we further calculate

$$\begin{aligned} S_F(x) &= (\imath\partial_\mu\gamma^\mu + m)\int \frac{\mathrm{d}^4k}{(2\pi)^4}\, \frac{e^{-\imath kx}}{k^2 - m^2 + \imath\varepsilon} \\ &= \int \frac{\mathrm{d}^4k}{(2\pi)^4}\, \frac{k_\mu\gamma^\mu + m}{k^2 - m^2 + \imath\varepsilon} e^{-\imath kx} \end{aligned}$$

and the corresponding Fourier transformation

$$\boxed{\tilde{S}_F(k) = \frac{\not{k} + m}{k^2 - m^2 + \imath\varepsilon} = \frac{1}{\not{k} - m + \imath\varepsilon}\,,}$$

since $(\not{k} - m)(\not{k} + m) = k^2 - m^2$.

Remark: He have

$$\frac{1}{V}\sum_k \frac{1}{2E_k} e^{-\imath kx} = \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}\, \frac{1}{2E_k} e^{-\imath kx} = \frac{1}{2}\int \frac{\mathrm{d}^4k}{(2\pi)^3}\, \delta(k^2 - m^2) e^{-\imath kx}$$

is Lorentz invariant since $d^4p = \det\Lambda d^4p'$.

8.8 Feynman Rules of Quantum Electrodynamics

For given initial and final states $|i\rangle$ and $|f\rangle$, the S-matrix element has the form

$$\langle f|S|i\rangle = \delta_{f,i} + \left[(2\pi)^4\,\delta^{(4)}(P_f - P_i)\,\left(\prod_{\substack{\text{ext.}\\ \text{fermions}}}\sqrt{\frac{m}{V\,E}}\right)\left(\prod_{\substack{\text{ext.}\\ \text{photons}}}\sqrt{\frac{1}{2V|k|}}\right)\right]\mathcal{M}\,,$$

where P_i and P_f are the total momenta of the initial and final states. In order to determine $\mathcal{M}$, one draws all topologically distinct diagrams up to the desired order in the interaction and sums over the amplitudes of these diagrams. The amplitude associated with a particular Feynman diagram is itself determined as follows:

1.) One assigns a factor of $-\imath e\gamma^\mu$ to every vertex point.

2.) For every internal photon line one writes a factor $\imath D_{F_{\mu\nu}}(k) = \imath\frac{-g^{\mu\nu}}{k^2+\imath\epsilon}$.

3.) For every internal fermion line one writes $\imath S_F(p) = \imath \frac{1}{\not{p} - m + \imath\epsilon}$.

4.) To the external lines one assigns the following free spinors and polarization vectors:
incoming electron: $u_r(p)$
outgoing electron: $\bar{u}_r(p)$
incoming positron: $\bar{w}_r(p)$
outgoing positron: $w_r(p)$
incoming photon: $\epsilon_{\lambda\mu}(\mathbf{k})$
outgoing photon: $\epsilon_{\lambda\mu}(\mathbf{k})$

5.) The spinor factors (γ matrices, S_F propagators, four-spinors) are ordered for each fermion line such tat reading them from right to left amounts to following the arrows along the fermion lines.

6.) For each closed fermion loop, multiply, multiply by a factor (-1) and take the trace over the spinor indices.

7.) At every vertex, the four-momenta of the three lines that meet at this point satisfy energy and momentum conservation.

8.) It is necessary to integrate over all free momenta (i.e., those not fixed by four-momentum conservation): $\int \frac{\mathrm{d}^4 q}{(2\pi)^4}$.

9.) One multiplies by a phase factor $\delta_p = 1$ (or -1), depending on whether an even or odd number of transpositions is necessary to bring the fermion operators into normal order.

The minus sign for a closed fermion loop has the following origin: proceeding from the T-product part, which gives the closed loop, $T(\ldots \bar{\psi}(x_1)\not{A}(x_1)\psi(x_1)\bar{\psi}(x_2)\not{A}(x_2)\psi(x_2)\ldots\bar{\psi}(x_f)\not{A}(x_f)\psi(x_f)\ldots)$, one has to permute the operator $\psi(x_1)$ with an uneven number of fermion fields and gets the sequence of propagators $\underbrace{\psi(x_1)\overline{\psi}(x_2)}\ldots\underbrace{\psi(x_f)\overline{\psi}(x_1)}$ with a minus sign.

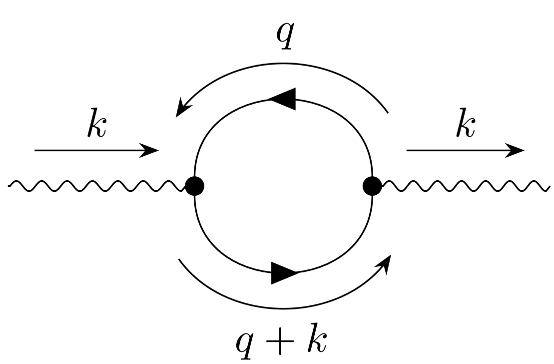


Figure 8.7: Example of a closed fermionic loop.

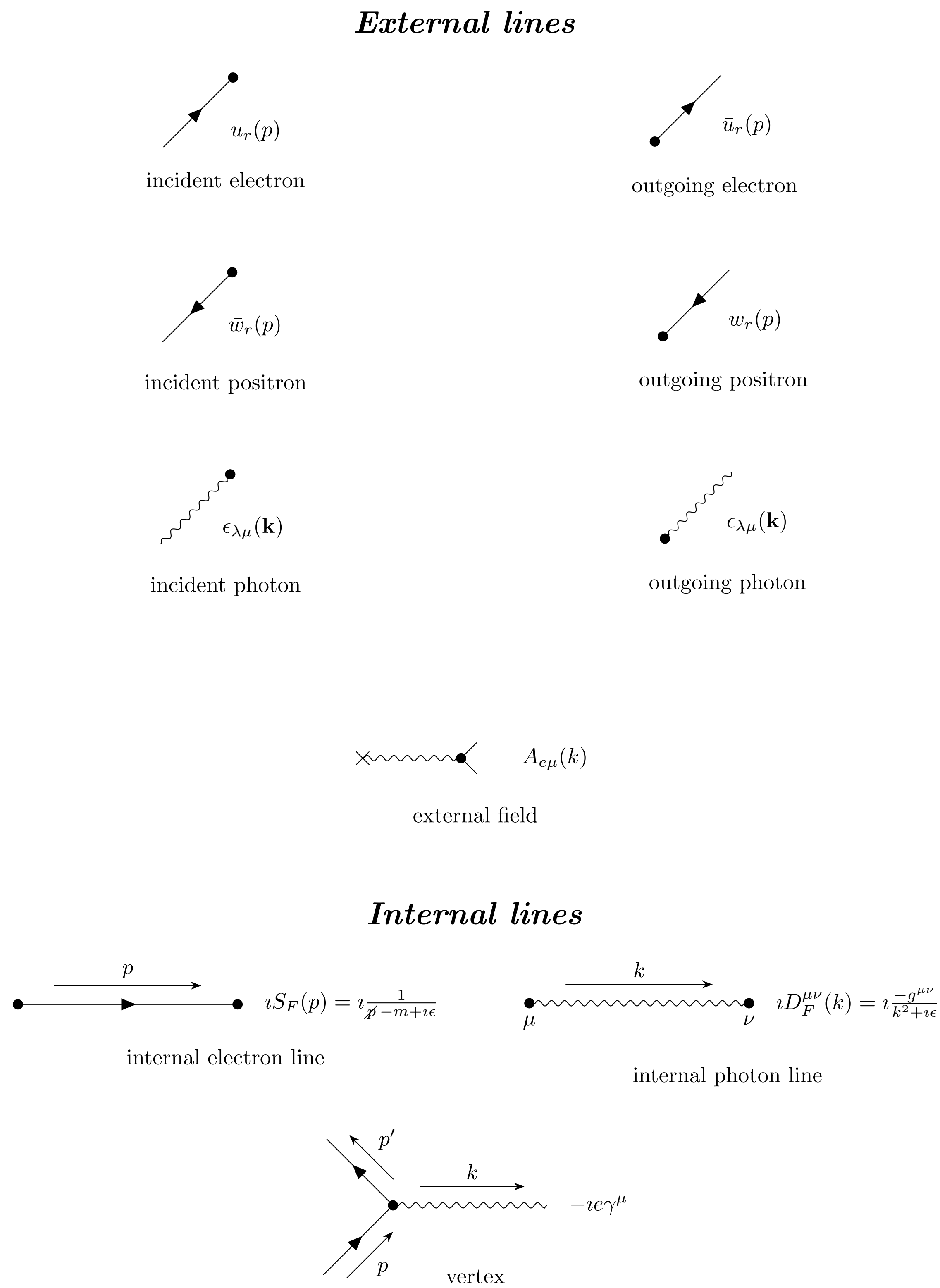


Figure 8.6: Feynman rules of quantum electrodynamics in momentum space.

8.9 Scattering Cross Section

8.9.1 Electron-electron scattering

We come back to the electron-electron scattering process (see 8.5)

$$e^-(p_1, r_1) + e^-(p_2, r_2) \to e^-(p_3, r_3) + e^-(p_4, r_4)\,,$$

where the momenta are given in the center of mass frame as

$$p_1 = \begin{pmatrix} E \\ \mathbf{p} \end{pmatrix}, \quad p_2 = \begin{pmatrix} E \\ -\mathbf{p} \end{pmatrix}, \quad p_3 = \begin{pmatrix} E \\ \mathbf{p}' \end{pmatrix}, \quad p_4 = \begin{pmatrix} E \\ -\mathbf{p}' \end{pmatrix},$$

with $|\mathbf{p}| = |\mathbf{p}'|$.

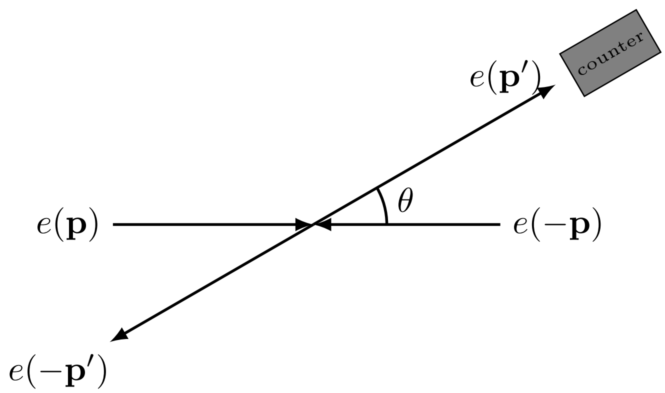


Figure 8.8: Sketch of the electron-electron scattering process.

We now want to calculate the **scattering cross section from the amplitude** of this process.

$$\boxed{d\sigma = \frac{\text{transition rate to } p_3,\, p_4}{\text{flux of incoming particles}} = \frac{dw_{fi}/T}{\phi}}$$

$$dw_{fi} = \underbrace{\frac{1}{2p_1^0\, 2p_2^0}\left(\frac{1}{V}\right)^2}_{\substack{\text{normalization}\\ \text{of the incoming}\\ \text{electron states}}} \cdot \underbrace{\frac{d\mathbf{p}_3\, d\mathbf{p}_4}{(2\pi)^6\, 2p_3^0\, 2p_4^0}}_{\substack{\text{Lorentz invariant}\\ \text{volume element}\\ \text{in } (p_3/p_4)\text{-space}}} \underbrace{\sum_{\text{spins}}{}'}_{\substack{\text{averaging/summation}\\ \text{over the spin direction}\\ \text{of electrons in}\\ \text{the initial/final state}}} \Big[(2\pi)^4\, \delta(p_1 + p_2 - p_3 - p_4)\, |T_{fi}|\Big]^2 \qquad (cf.(8.21))$$

The square of the δ-function can be interpreted with Fermi's trick:

$$\begin{aligned}\Big[(2\pi)^4\, \delta(p_1 + p_2 - p_3 - p_4)\Big]^2 &= \underbrace{\int_{V,T}}_{\substack{\text{large but finite}\\ \text{volume } V/\text{time } T}} \mathrm{d}x\; e^{\imath(p_1+p_2-p_3-p_4)x} (2\pi)^4\, \delta(p_1 + p_2 - p_3 - p_4) \\ &= V \cdot T\, (2\pi)^4\, \delta(p_1 + p_2 - p_3 - p_4)\end{aligned}$$

$$\Rightarrow \frac{dw_{fi}}{T} = \frac{1}{V} \frac{1}{2p_1^0\, 2p_2^0} (2\pi)^4 \delta(p_1 + p_2 - p_3 - p_4) \frac{d\mathbf{p}_3\, d\mathbf{p}_4}{(2\pi)^6\, 2p_3^0\, 2p_4^0} \sum_{\text{spins}}{}' \, |T_{fi}|^2$$

We now have to consider the flux of incoming particles ϕ. We choose the **rest frame of $\mathbf{e_2}$** as reference frame (the final result will be Lorentz invariant). Then

$$\phi = \underbrace{\frac{1}{V}}_{\substack{\text{normalization of}\\ \text{incoming state}}} \underbrace{|v_1|}_{\substack{\text{velocity of}\\ \text{particle 1}}}, \qquad \text{where} \quad |v_1| = \frac{|\mathbf{p}_1|}{p_1^0}, \quad p_1 = \begin{pmatrix} E_1 \\ \mathbf{p}_1 \end{pmatrix}, \quad p_3 = \begin{pmatrix} m_2 \\ m \end{pmatrix},$$

since $|p_1| = \gamma m |v_1|$ and $E_1 = \gamma m c^2$. We define the **center of mass energy** as

$$\begin{aligned} s &:= (p_1 + p_2)^2 \\ &= p_1^2 + 2p_1 p_2 + p_2^2 \\ &= m_1^2 + 2m_2 E_1 + m_2^2 \end{aligned}$$

$$\Rightarrow \quad E_1 = \frac{s - m_1^2 - m_2^2}{2m_2} \qquad (*)$$

Note that in the rest frame of e_2 we have $p_1 = \begin{pmatrix} E_1 \\ \mathbf{p_1} \end{pmatrix}$ and $p_2 = \begin{pmatrix} m_2 \\ 0 \end{pmatrix}$ and therefore $p_1 p_2 = E_1 m_2$. We then find for the absolute value of the momentum of particle 1

$$\begin{aligned} |\mathbf{p}_1| = \sqrt{E_1^2 - m_1^2} &\overset{(*)}{=} \frac{1}{2m_2} \left[(s - m_1^2 - m_2^2)^2 - 4m_1^2 m_2^2 \right]^{\frac{1}{2}} \\ &= \frac{1}{2m_2} \left[s^2 + m_1^4 + m_2^4 - 2sm_1^2 - 2sm_2^2 - 2m_1^2 m_2^2 \right]^{\frac{1}{2}} \\ &=: \frac{1}{\underbrace{2m_2}_{=p_2^0}} w(s, m_1^2, m_2^2), \qquad \text{where} \quad \boxed{w(x,y,z) = \left[x^2 + y^2 + z^2 - 2xy - 2xz - 2yz \right]^{\frac{1}{2}}} \end{aligned}$$

Using above result we find for the flux the expression

$$\Rightarrow \quad \phi = \frac{1}{V} \frac{1}{p_1^0} \frac{w(s, m_1^2, m_2^2)}{2p_2^0}$$

Combining our previous results yields a scattering cross section $d\sigma$ of

$$\Rightarrow \boxed{d\sigma = \frac{1}{2w(s, m_1^2, m_2^2)} \frac{d\mathbf{p}_3\, d\mathbf{p}_4}{(2\pi)^6\, 2p_3^0\, 2p_4^0} (2\pi)^4\, \delta(p_1 + p_2 - p_3 - p_4) \sum_{\text{spins}}{}' |T_{fi}|^2} \qquad (8.26)$$

Now it is for the sum over the matrix elements T_{fi}

$$\begin{aligned}
\sum_{\text{spins}}{}'|T_{fi}|^2 &= \sum_{\text{spins}}{}' T_{fi}^* T_{fi} \\
&= \sum_{\text{spins}}{}' \left\{ \frac{1}{(p_4-p_1)^2}\bar{u}(p_2)\gamma_\mu u(p_3)\bar{u}(p_1)\gamma^\mu u(p_4) - \frac{1}{(p_3-p_1)^2}\bar{u}(p_1)\gamma_\mu u(p_3)\bar{u}(p_2)\gamma^\mu u(p_4)\right\} \\
&\cdot \quad \left\{ \frac{1}{(p_4-p_1)^2}\bar{u}(p_4)\gamma_\nu u(p_1)\bar{u}(p_3)\gamma^\nu u(p_2) - \frac{1}{(p_3-p_1)^2}\bar{u}(p_4)\gamma_\nu u(p_1)\bar{u}(p_3)\gamma^\nu u(p_1)\right\} \\
&= \frac{e^4}{4} \quad \left\{ \frac{1}{u^2}\,\mathrm{Tr}\left[(\not{p}_2+m)\gamma_\mu(\not{p}_3+m)\gamma_\nu\right]\cdot \mathrm{Tr}\left[(\not{p}_1+m)\gamma^\mu(\not{p}_4+m)\gamma^\nu\right]\right. \\
&- \left.\frac{1}{t\,u}\,\mathrm{Tr}\left[(\not{p}_2+m)\gamma_\mu(\not{p}_3+m)\gamma_\nu \not{p}_1+m)\gamma^\mu(\not{p}_4+m)\gamma^\nu\right] \quad + \quad \mathbf{(3\to 4)}\right\},
\end{aligned}$$

where in the last step we used

$$\sum_{s=\pm 1/2} u_s(p)\bar{u}_s(p) = \not{p} + m = p^\mu\gamma_\mu + m$$

and

$$u := (p_4-p_1)^2\,, \quad t := (p_3-p_1)^2\,.$$

We further calculate

$$\mathrm{Tr}\left[(\not{p}_2+m)\gamma_\mu(\not{p}_3+m)\gamma_\nu\right] = 4\Big(g_{\mu\nu}m^2 + p_{2\mu}p_{3\nu} + p_{2\nu}p_{3\mu} - g_{\mu\nu}p_2\cdot p_3\Big)$$

and

$$\begin{aligned}
&\mathrm{Tr}\left[(\not{p}_2+m)\gamma_\mu(\not{p}_3+m)\gamma_\nu(\not{p}_1+m)\gamma^\mu(\not{p}_4+m)\gamma^\nu\right] \\
=&16\Big(-2p_1p_2p_3p_4 + m^2p_1\cdot p_3 + m^2(p_1+p_3)\cdot(p_2+p_4) + m^2p_2\cdot p_4 - 2m^4\Big)\,.
\end{aligned}$$

After a lengthy calculation one finds using the definitions of s, u and t

$$\sum{}'|T_{fi}|^2 = \frac{64\pi^2\alpha^2}{t^2\,u^2}\Big\{(s-2m^2)^2(t^2+u^2) + ut(-4m^2s + 12m^4 + ut)\Big\}\,.$$

Inserting in (8.26) yields in center of mass variables

$$d\sigma = d\Omega\int_0^\infty \mathrm{d}|\mathbf{p}_3|\;|\mathbf{p}_3|^2\int \mathrm{d}\mathbf{p}_4 \frac{1}{2[s(s-4m^2)]^{1/2}}\,\frac{1}{(2\pi)^2}\,\frac{1}{2p_3^0\,2p_4^0}\;\delta(\sqrt{5}-p_3^0-p_4^0)\delta^3(\mathbf{p}_3+\mathbf{p}_4)\;\sum{}'|T_{fi}|^2$$

and finally

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\alpha^2}{st^2u^2}\Big\{(s-2m^2)^2(t^2+u^2) + ut(-4m^2s+12m^4) + ut\Big\}} \qquad \text{(Møller 1932)}$$

where we have

$$E = \sqrt{2}/2\,, \quad t = -4|\mathbf{p}_1|^2\sin^2\frac{\theta}{2}\,, \quad u = -4|\mathbf{p}_1|^2\cos^2\frac{\theta}{2}\,.$$

We will now determine the **kinematic boundaries** of θ, respectively t. Quantum mechanically, both electrons have to be viewed as identical particles in their initial and final states. The question of whether the particle coming from the right or the one coming from the left is hitting a counter placed under an angle of θ is meaningless (see Fig. 8.8). We only can detect that one electron leaves the point of interaction under an angle θ, the other electron under $\pi - \theta$. Therefore the angle range $\boxed{0 \leq \theta \leq \pi/2}$ already captures all **distinct** final states. This ensues $\boxed{0 \geq t \geq -\frac{1}{2}(s - 4m^2)}$.

We find in the **non-relativistic limiting case**, $|\mathbf{p}| \ll m$:

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{\alpha^2 m^2}{16|\mathbf{p}|^4}\left[\underbrace{\frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}}}_{\substack{\hat{=}\,\text{classical Rutherford}\\ \text{scattering}}} - \underbrace{\frac{1}{\sin^2\frac{\theta}{2}\,\cos^2\frac{\theta}{2}}}_{\substack{\text{additional QM term}\\ \text{resulting from the}\\ \text{interference of}\\ \text{both electrons}}}\right]} \qquad \text{(Mott 1930)}$$

The additional term results from the quantum mechanical addition of the amplitudes – which correspond to both of the Feynman diagrams – and the concluding formation of the modulus when calculating the cross section. The minus sign in the interference term results from the Fermi statistics; for bosons one obtains a plus sign.

We can also determine an **ultra relativistic case**, $|\mathbf{p}| \gg m$:

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \frac{\alpha^2}{s}\left\{\frac{1}{\sin^4\frac{\theta}{2}} + \frac{1}{\cos^4\frac{\theta}{2}} + 1\right\} \\ &= \frac{\alpha^2}{s}\frac{(3+\cos^2\theta)^2}{\sin^4\theta} \end{aligned}$$

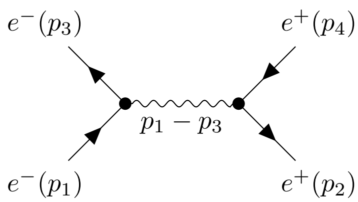
n.b.: $s \cdot \frac{d\sigma}{d\Omega}$ is no longer dependent of s. This **scaling behaviour** of the cross section is interpreted as an indication of the point like nature of the electron. If the electron would possess an finite "extent" $v = 1/\Lambda$, one would expect that $s \cdot \frac{d\sigma}{d\Omega}$ is a nontrivial function of the dimensionless variable s/Λ^2, i.e. $s \cdot \frac{d\sigma}{d\Omega}$ would not be independent of s. Predictions from the theory of electron-electron scattering were throughout verified in experiments.

8.9.2 Electron-positron scattering (Bhabha-Scattering)

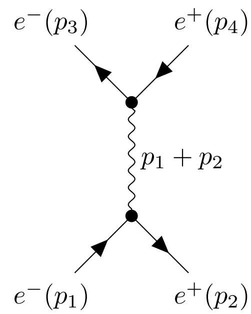
We consider the process

$$e^-(p_1) + e^+(p_2) \to e^-(p_3) + e^+(p_4)\,,$$

which possesses the same kinematic as the previous electron-electron scattering process. The Feynman diagrams of lowest order are given by:



"Scattering"
$(p_1 - p_3)^2 \leq 0$



"Annihilation"
$(p_1 + p_2)^2 \geq 4m^2$

For unpolarized electrons and positrons in the ultra relativistic limiting case, we find in center of mass coordinates

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{\alpha^2}{2}\left\{\frac{1}{2}\,\frac{1+\cos^4\frac{\theta}{2}}{\sin^4\frac{\theta}{2}} + \frac{1}{4}\Big(1+\cos^2\theta\Big) - \frac{\cos^4\frac{\theta}{2}}{\sin^2\frac{\theta}{2}}\right\}\\ &= \frac{\alpha^2}{16s}\,\frac{(3+\cos^2\theta)^2}{\sin^4\frac{\theta}{2}} \qquad \text{for } s \gg 4m^2\,.\end{aligned}$$

We are considering two distinguishable particles in the initial and final states, therefore we have an kinematic range of $0 \leq \theta \leq \pi$.

Bhabha-scattering was studied at the collider PETRA in Hamburg, where the highest center-of-mass energy was $\sqrt{s} \approx 45\,\text{GeV}$. A really good agreement of experiment and theory was found.

If one assumes that quantum electrodynamics needs to be modified from an energy scale Λ on, then for

$$s \ll \Lambda^2 : \qquad \frac{d\sigma}{d\Omega}\Bigg/\frac{d\sigma^{\text{QED}}}{d\Omega} = 1 + \mathcal{O}(s/\Lambda^2)$$

and with an experimental precision of $s \approx 10^3\,\text{GeV}^2$ it follows

$$\frac{s}{\Lambda^2} \lesssim 0.05\,, \quad \text{i.e. } \Lambda \gtrsim 150\,\text{GeV resp. } 1.3\cdot 10^{-16}\,\text{cm}\,.$$

Deviations on this energy scale can thus be explained by the need to extent the QED through the electroweak interaction.

8.9.3 Compton scattering

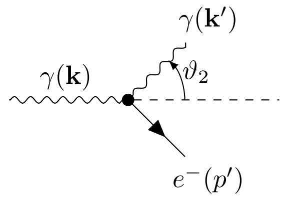


Figure 8.9: The Compton scattering process in the laboratory frame, where the incoming electron rests.

We look at the process

$$\gamma(\mathbf{k}) + e^-(p) \to \gamma(\mathbf{k}') + e^-(p')\,,$$

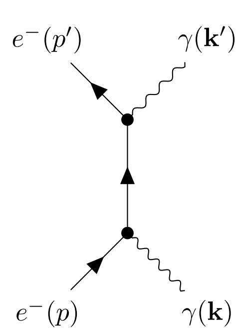
where the incoming electron rests in the laboratory frame. The momenta are therefore described by

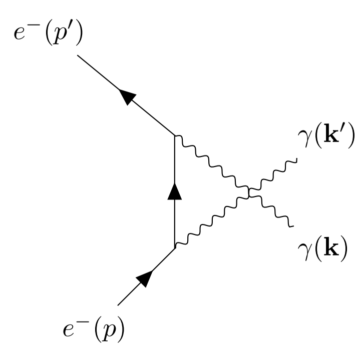
$$p = \begin{pmatrix} m \\ 0 \end{pmatrix}, \qquad p' = \begin{pmatrix} \sqrt{m^2 + \mathbf{p}'^2} \\ \mathbf{p}' \end{pmatrix}$$
$$k = \begin{pmatrix} \omega \\ \mathbf{k} \end{pmatrix}, \qquad k' = \begin{pmatrix} \omega' \\ \mathbf{k}' \end{pmatrix},$$

where $\omega = |\mathbf{k}|$ and $\omega' = |\mathbf{k}'|$. Energy conservation yields

$$\begin{aligned} m + \omega &= \sqrt{m^2 + \mathbf{p}'^2} + \omega' \\ &= \sqrt{m^2 + (\mathbf{k} - \mathbf{k}')^2} + \omega' \\ \Rightarrow \quad \frac{\omega - \omega'}{\omega\omega'} &= \frac{1}{m}\Big(1 - \cos\,\vartheta_2\Big) \\ \text{resp.} \quad \lambda' - \lambda &= \frac{2\pi}{m}\Big(1 - \cos\,\vartheta_2\Big)\,, \end{aligned}$$

where the corresponding wavelength is $3.86 \cdot 10^{-11}$ cm. The Feynman diagram of lowest order for the calculation of the scattering cross section are given below:





For unpolarized electrons and photons, we find the result

$$\frac{d\sigma}{d\Omega_2} = \frac{\alpha^2}{2}\frac{1}{[m + \omega(1 - \cos\,\vartheta_2)]^2} \cdot \left\{ \frac{\omega^2(1 - \cos\,\vartheta_2)^2}{m[m + \omega(1 - \cos\,\vartheta_2)]} + 1 + \cos^2\,\vartheta_2 \right\} \quad \text{(Klein, Nishina 1929)}$$

In the non-relativistic limiting case, $\omega \ll m$, we find

$$\omega' = \omega\,, \qquad \frac{d\sigma}{d\Omega_2} = \frac{\alpha^2}{m^2}\frac{1 + \cos^2\,\vartheta_2}{2}\,, \qquad \sigma_{\text{tot}} = \frac{8\pi}{3}\frac{\alpha^2}{m^2}\,.$$

We also can determine an **ultra relativistic case** with $\omega \gg m$, resp. $\lambda \ll 1/m$:

$$1 - \cos\theta_2 \ll \frac{m}{\omega} \quad \Rightarrow \quad \lambda' \approx \lambda\,, \quad \frac{d\sigma}{d\Omega_2} \approx \frac{\alpha^2}{m^2}$$
$$1 - \cos\theta_2 \gg \frac{m}{\omega} \quad \Rightarrow \quad \lambda' \approx \frac{2\pi}{m}(1-\cos\theta_2)\,, \quad \frac{d\sigma}{d\Omega_2} \approx \frac{\alpha^2}{2m\omega(1-\cos\theta_2)} \propto \frac{1}{\omega}\,,$$

where in the second case the scattered wavelength λ' is independent of the incoming photon.

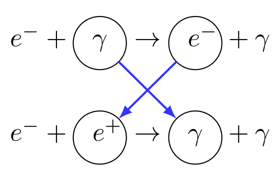
Note: Compton scattering is related by **crossing symmetry** to pair annihilation. Under crossing symmetry one understands that, given a particle interaction, related interactions can be anticipated from the fact that any of the particles can be replaced by its antiparticle on the other side of the interaction. Looking at an arbitrary reaction

$$A + B \to C + D\,,$$

this implies the existence of the following reactions:

$$\begin{aligned} A &\to \overline{B} + C + D \\ A + \overline{C} &\to \overline{B} + D \\ \overline{C} &\to \overline{A} + \overline{B} + D \\ \overline{C} + \overline{D} &\to \overline{A} + \overline{B} \end{aligned}$$

Crossing symmetry applies to all known particles, including the photon, which is its own antiparticle. Considering the Compton process, if the electron on the right side of the process is replaced by its antiparticle – the positron – on the other side of the interaction, as well as the photon on the left wanders to the right, the result represents a pair annihilation, as seen below.



(Compton scattering)

(Pair annihilation)

It could be said that the observation of Compton scattering implies the existence of pair annihilation and predicts that it will produce a pair of photons.

8.10 Problems with external fields

Until now we only considered reactions inside the vacuum, but in reality one often finds predefined external fields (e.g. capacitors, electromagnets, nuclei).
Some examples are

(1) Scattering of an electron at a predefined charge distribution (e.g. a heavy nucleus)

(2) Emission of synchrotron radiation of an electron in an accelerator

(3) Emission of Bremsstrahlung from an electron, which is decelerated in the field of a nucleus (→ generation of X-radiation in a X-ray tube)

(4) Creation of an electron-positron pair via a photon in the field of a heavy nucleus (→ discovery of the positron, Anderson 1932).
Today, this process is usually used in high-energy physics to detect electrons in experiments.

Starting point:

$$\mathcal{H}_{\text{int}}(t) = \int \mathrm{d}^3\mathbf{r}\, \jmath^\mu(\mathbf{r},t)\, A_\mu(\mathbf{r},t)$$

$$A_\mu(\mathbf{r},t) = \underbrace{A'_\mu(\mathbf{r},t)}_{\substack{\text{quantum}\\ \text{field}}} + \underbrace{A_\mu^{\text{ext}}(\mathbf{r},t)}_{\substack{\text{external}\\ \text{potential}}}$$

The sources of A_μ^{ext} are the external charges and currents $\jmath_\mu^{\text{ext}}$, where the following Lorentz conditions are satisfied:

$$\Box A_\mu^{\text{ext}}(x) = \jmath_\mu^{\text{ext}}(x)$$
$$\partial^\mu A_\mu^{\text{ext}}(x) = 0\,.$$

We again employ the Dirac- or interaction-picture: $\imath \frac{\partial}{\partial t} |t\rangle = \mathcal{H}_{\text{int}}(t)\, |t\rangle$.
Let us take a closer look at the structure of $\mathcal{H}_{\text{int}}$:

$$\begin{aligned}\mathcal{H}_{\text{int}} &\sim (\hat{b} + \hat{a}^\dagger)(\hat{b}^\dagger + \hat{a})\, A^{\text{ext}} \\ &\sim \underbrace{-\hat{b}^\dagger \hat{b}\, A^{\text{ext}}}_{(4')} + \underbrace{\hat{a}^\dagger \hat{b}^\dagger\, A^{\text{ext}}}_{(3')} + \underbrace{\hat{b}\hat{a}\, A^{\text{ext}}}_{(2')} + \underbrace{\hat{a}^\dagger \hat{a}\, A^{\text{ext}}}_{(1')}\,,\end{aligned}$$

where the appearing parts have the following interpretation:

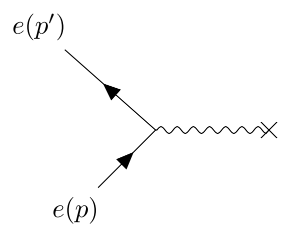
(1') Scattering of an electron at an external potential

(2') Annihilation of an electron-positron pair through an external field

(3') Creation of an electron-positron pair through an external field

(4') Scattering of a potential at an external potential

Diagrammatic visualization:



Feynman rules:

$$\begin{aligned}&\imath e \gamma^\mu \int \mathrm{d}x\, e^{\imath(p'-p)x} A_\mu^{\text{ext}}(x) \\ &= -\imath e \gamma^\mu \frac{1}{(p-p')^2} \int \mathrm{d}x\, e^{\imath(p'-p)y} \cdot \jmath_\mu^{\text{ext}}(x)\end{aligned}$$

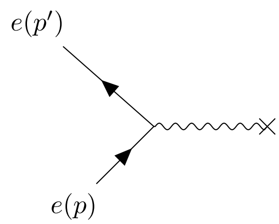
If a vertex of the above kind appears in a diagram, one omits the δ-function of the energy-momentum conservation in the S-matrix element.

8.11 Radiative corrections / Renormalization

Until now, we considered reaction in the QED in *lowest order*, what gives finite results which are in good accordance with experiments. **But** terms of higher order exist in theory and have to be taken into account regarding precision measurements. When calculating higher orders, the so called *radiative corrections*, **infinities** occur. The systematic procedure to calculate terms of higher order with **finite** result is called **renormalization**.

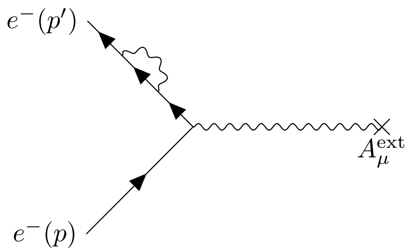
Example: Scattering of an electron at an external potential

Lowest order

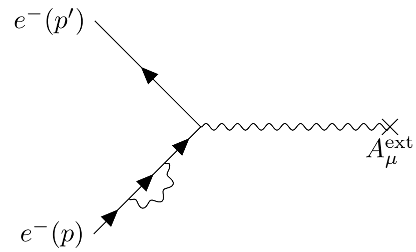


ok ✓

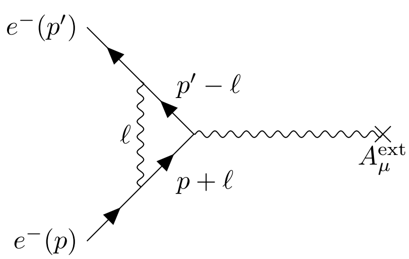
Next higher order:



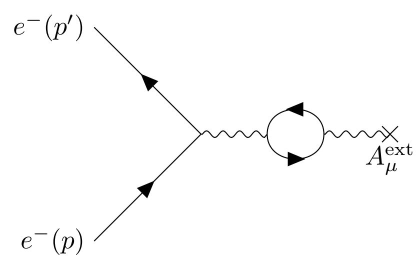
(a)



(b)



(c)



(d)

When we look at diagram (c), the Feynman rules tell us that we have to integrate over the loop-momentum (schematic for the amplitude):

$$A^{(c)} \sim \int \mathrm{d}^4\ell \, \frac{1}{\ell^2} \frac{\not{p} + \not{\ell} + m_e}{p^2 + 2p\ell + \ell^2 - m_e^2} \, \frac{\not{p}' - \not{\ell} + m_e}{p'^2 - 2p'\ell + \ell^2 - m_e^2}$$

The above integral diverges for $\ell \to \infty$ logarithmically ($\int \mathrm{d}^4\ell \frac{1}{\ell^2} \frac{1}{\ell} \frac{1}{\ell}$, note that $d^4\ell$ contains a ℓ^3, hence logarithmic), what leads to the so called "ultraviolet catastrophe". Even for $\ell \to 0$ the

integral diverges. Because of $p^2 = p'^2 = m_e^2$ follows $A^{(c)} \underset{\ell \to 0}{\sim} \int d^4\ell \frac{1}{\ell^2} \frac{1}{p\ell} \frac{1}{p'\ell}$ and we have the so called "infrared catastrophe".
The infrared catastrophe can easily be fixed ("soft photons").

Quantum mechanical considerations regarding the infrared divergence:
What do we observe, when we say a detector measured an electron? We only have a finite energy resolution ΔE, so experimentally it can not be distinguished, if an electron comes in isolated or accompanied by a "soft" photon of energy $\omega \leq \Delta E$.

$$\begin{aligned} \Rightarrow \quad \sigma^{\text{exp}} &= \sigma(1 \text{ electron}) \\ &= \sigma(1 \text{ electron} + 1 \text{ photon of energy } \omega \leq \Delta E) \\ &= \sigma(1 \text{ electron} + 2 \text{ photons of total energy } \omega \leq \Delta E) \\ &= \dots \end{aligned} \qquad (*)$$

Calculations yield

$$\sigma(1 \text{ electron} + 1 \text{ photon of energy } \omega_{\text{min}} \leq \omega \leq \Delta E) \propto \overline{\sigma} \ln \frac{\Delta E}{\omega_{\text{min}}} \underset{\omega_{\text{min}} \to 0}{\longrightarrow} \infty \qquad (**)$$

The theory should give **finite** results for **observable** quantities. This would be the case, if the scattering cross section summed over all final states in $(*)$ is finite. Further calculations show that in every order of α, the infrared divergences of $\sigma(1 \text{ electron})$ of the higher order diagrams and the infrared divergences in $(**)$ cancel each other out.

To avoid problems with divergent integrals in intermediate steps, one introduces a small photon mass which can be set to zero in the final result. This final result also reveals the resolution ΔE of the apparatus.

To overcome the ultraviolet catastrophe is more difficult and subject of the **renormalization theory**. The **basic idea** is that divergent integrals are useless and must be made finite by hand, i.e. must be **regularised**. Different regularisation procedures were proposed, e.g. to abort all divergent integral at a parameter Λ:

$$\int d\ell \frac{1}{\ell^2} \frac{1}{\not{p} + \not{\ell} - m} \frac{1}{\not{p}' - \not{\ell} - m} \quad \longrightarrow \quad \int_{|\ell| \leq \Lambda} d\ell \frac{1}{\ell^2} \frac{1}{\not{p} + \not{\ell} - m} \frac{1}{\not{p}' - \not{\ell} - m} \,.$$

The results then depend logarithmically on Λ. There exist different cutting-off procedures, like the Pauli-Villars or dimensional regularisation, which are of better use for the QED.

After the regularisation one has a theory which is completely finite. The theory makes use of the following parameters for the electron:

$$\underbrace{e_0}_{\substack{\text{charge} \\ \text{parameter}}} \,, \qquad \underbrace{m_0}_{\substack{\text{mass} \\ \text{parameter}}} \,, \qquad \Lambda$$

(similar to the Hamilton function resp. the Feynman rules).

Foundation of the renormalization theory is the assumption, that e_0 and m_0 are <u>not</u> identical with the observable charge e and mass m of the electron.
How can one measure the charge of an electron? One possibility is to use a magnetic field and the formula

$$\mathbf{K} = (-e)\,(\mathbf{v} \times \mathbf{B}) \,, \qquad (***)$$

which, viewed in the context of the QED, corresponds to the scattering of a particle at an external potential. Calculations using the renormalization theory actually result in a force in the shape of $(***)$, but for the charge one finds $e \neq e_0$. It is (with constants a_1, a_2, etc.):

$$e = e_0 \left[1 + a_1 e_0^2 \ln \frac{\Lambda}{m_0} + a_2 e_0^4 \left(\ln \frac{\Lambda}{m_0} \right)^2 + \dots \right] . \tag{8.27}$$

Analogous one finds for the observable mass m (witch constants b_1, b_2, etc.):

$$m = m_0 \left[1 + b_1 e_0^2 \ln \frac{\Lambda}{m_0} + \dots \right] . \tag{8.28}$$

Since in the limit $\Lambda \to \infty$ e and m seem to diverge, they are still meaningless. One way out of this problem is the assumption that e_0 and m_0 only have a *mathematical existence*. When calculating the limit $\Lambda \to \infty$, it is done in such a way that the *observable* quantities e and m are fixed and the mathematical parameters e_0 and m_0 vary with Λ. The original quantities e_0 and m_0 then diverge for $\Lambda \to \infty$, which is irrelevant, because they cannot be observed.

This gives us the following **program** to follow: We calculate a transition amplitude A in the regularised theory with the aid of the known techniques. A will be a function of the "bare" parameters e_0, m_0 and Λ (cutting-off parameter):

$$A = F(e_0, m_0, \Lambda, \underbrace{\dots}_{\text{external momenta and polarisation}}) \tag{8.29}$$

By inversion of (8.27) and (8.28), we express the "bare" parameters via physical ones:

$$e_0 \equiv e_0(e, m, \Lambda)$$
$$m_0 \equiv m_0(e, m, \Lambda)$$

Substitution in (8.29) yields A as a function of the parameters e, m and Λ:

$$A = F\Big(e_0(e, m, \Lambda),\, m_0(e, m, \Lambda),\, \Lambda,\, \dots\Big)$$

We then take $\Lambda \to \infty$, where e and m are now fixed.

Central theorem of the renormalization theory:

> The limit of the expansion with respect to e exists in every order (and after the separation of a suitable scale factor Z, which is not dependent on external momenta).

We define the renormalised Amplitude A' as a function F' of the physical (observable) parameters e and m and of the external variables:

$$\begin{aligned} A' &= \lim_{\Lambda \to \infty} Z(e, m, \Lambda) F\Big(e_0(e, m, \Lambda),\, m_0(e, m, \Lambda),\, \Lambda,\, \dots\Big) \\ &= F'(e,\, m,\, \dots) \end{aligned}$$

The renormalization theory gives an expansion in powers of e of the renormalised amplitudes:

$$F'(e,\, m,\, \dots) = F'_0(m, \dots) + eF'_1(m, \dots) + e^2 F'_2(m, \dots) + \dots\,,$$

where all F'_i are finite. The convergence of the series is not stated though (in most cases not convergent but asymptotic).

The mathematical execution is in most cases tedious. The theory finds excellent confirmation in experiments.

8.12 Principles of Strong Interaction / Quantum Chromodynamics

Hadrons (protons p, neutrons n, pions or π-mesons π^+, π^0 and π^-, as well as Λ, $\Sigma^{+,0,-}$, K, ...) are compound particles – the fundamental particles are **quarks**.

Thereby:
$$\begin{array}{lll} \text{mesons} & \sim q\bar{q} & \text{(quark-antiquark)} \\ \text{baryons} & \sim qqq & \text{(3-quark states)} \end{array}$$

Initially 3 different types of quarks were postulated, so called **quark flavours**

	name	spin	charge	baryon number	strangeness
u	"up"	1/2	2/3	1/3	0
d	"down"	1/2	−1/3	1/3	0
s	"strange"	1/2	−1/3	1/3	−1

E.g. for π- and K-mesons resp. baryons:

$$\begin{array}{r|l} \text{mesons} & \text{baryons} \\ & \\ \pi^+ \sim u\bar{d} & p \sim (uud)_\gamma \\ \pi^0 \sim \frac{1}{\sqrt{2}}(u\bar{u} - d\bar{d}) & n \sim (ddu)_\gamma \\ \pi^- \sim d\bar{u} & \Lambda \sim (uds)_\gamma \\ K^+ \sim u\bar{s} & \\ K^0 \sim d\bar{s} & \end{array}$$

The Ω^--particle (baryon) has spin $-3/2$ and a strangeness of $s = -3$

$$\Omega^-(3/2,\,3/2) \sim \underbrace{\overset{\uparrow\uparrow\uparrow}{sss}}_{\substack{\text{totally}\\ \text{symmetrical}}} \quad \underbrace{\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)}_{\substack{\text{spatial wave function of the 3 quarks,}\\ \text{orbital angular momentum 0}\\ \Rightarrow \text{totally sym.}}}$$

This would give a totally symmetric wave function for a particle with half-integer spin, which is prohibited by the Pauli principle. Therefore an additional quantum number, the **color**, is introduced in 3 different versions,

$$u_1, u_2, u_3\,; \qquad d_1, d_2, d_3\,; \qquad s_1, s_2, s_3\,,$$

which gives for the Ω^--particle

$$\Omega^-(3/2,\,3/2) \sim \underbrace{\overset{\uparrow}{s}_\alpha \overset{\uparrow}{s}_\beta \overset{\uparrow}{s}_\gamma\, \varepsilon_{\alpha\beta\gamma}}_{\substack{\text{totally}\\ \text{anti-symmetrical}}} \; \underbrace{\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)}_{\text{totally sym.}} \qquad \checkmark$$

States are **invariant under rotation inside the color space**,

$$q_\alpha \to \sum_{\beta=1}^{3} \underbrace{q_\beta}_{\in\{u,d,s\}} \mathcal{U}_{\beta\alpha}\,,$$

where $\mathcal{U} \in \mathrm{SU}(3)$ (color-SU(3)) plays a fundamental role in QCD.
E.g. $\quad \pi^+ \sim u_1\bar{d}_1 + u_2\bar{d}_2 + u_3\bar{d}_3 \quad$ is invariant under SU(3).

Experiments showed that, besides the quarks, other flavour-neutral constituents ("partonen") of the nucleons must be present (which carry a part of the total momentum of the nucleon). These particles are responsible for the interaction of the quarks among themselves inside the nucleon. These particles are called **gluons** and follow in a natural way from a SU(3)-gauge theory for the strong interaction of the QCD.

8.12.1 Lagrange density of the QCD: SU(3)-gauge theory

Kinetic term for the quarks:

$$\mathcal{L}_q^0(x) = \sum_{j=1}^{f} \overline{q}^j(x)\Big(\imath\gamma^\mu\partial_\mu - m_j\Big)q^j(x)\,,$$

where $j = 1,\ldots,f$ are the quark flavours and m_j the corresponding mass. We have

$$q^1 = u\,,\quad q^2 = d\,,\quad q^3 = s\,,\quad q^4 = c\,,\ldots$$

The quark fields q^j have three **color**-components each $q^j = \begin{pmatrix} q_1^j \\ q_2^j \\ q_3^j \end{pmatrix}$.

Since the physical bonding states of the quarks (e.g. mesons, baryons) are invariant under SU(3)-rotations in color-space, this should be a consequence of an invariance of the fundamental Lagrange density.

$\mathcal{L}_q^0(x)$ is indeed invariant under $q^j(x) \to \mathcal{U}\cdot q^j(x)\,,\quad (j = 1,\ldots,f)$, where $\mathcal{U}\mathcal{U}^\dagger = \mathbb{1}$, $\det\mathcal{U} = 1$ (i.e. $\mathcal{U} \in \mathrm{SU}(3)$) and $\mathcal{U} \equiv \text{const}$.

The global invariance is – much like the global U(1)-invariance of the Dirac field in the QED – not satisfying from a relativistic standpoint. Therefore one requires a **local** gauge invariance of the theory:

$$\boxed{q^j(x) \to \mathcal{U}(x)\cdot q^j(x)\,,\quad \mathcal{U}(x) \in \mathrm{SU}(3)\,.}$$

Inside the QED framework, this gauge principle is established by the photon. In the QCD it will happen via the introduction of the gluon.

The physical postulate of the invariance under color transformations of the quark field can be understood as the "reason" for the existence of gluons.

Apparently $\mathcal{L}_q^0(x)$ is **not** invariant under $q^j(x) \to \mathcal{U}(x)\cdot q^j(x)$, since

$$\mathcal{L}_q^0(x) \to \sum_{j=1}^{f} \overline{q}^j(x)\Big(\imath\gamma^\mu\partial_\mu - m_j + \imath\gamma^\mu\mathcal{U}^\dagger(x)\partial_\mu\mathcal{U}\Big)q^j(x)\,.$$

In the QED, we needed a photon field A_μ to generate the local gauge invariance according to the number of generators of the gauge group U(1). In the QCD we need 8 gluon fields according to the eight linear independent generators of the SU(3) color-group: $A^a_\mu(x)$ (with $a = 1, \ldots, 8$), 8 gluon four-potentials. We combine these into a 3×3 Hermitian traceless matrix

$$\boxed{\mathbf{A}_\mu(x) = A^a_\mu(x)\,\frac{\lambda_a}{2} = \mathbf{A}^\dagger_\mu(x)\,, \qquad \mathrm{Tr}\ \mathbf{A}_\mu(x) = 0\,,}$$

where the λ_a represent the Gell-Mann-λ matrices, which operate in the color space

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_2 = \begin{pmatrix} 0 & -\imath & 0 \\ \imath & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$
$$\lambda_5 = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ \imath & 0 & 0 \end{pmatrix}, \quad \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\imath \\ 0 & \imath & 0 \end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

$\Big($**n.b.:** infinitesimal transformations in the SU(3): $\mathcal{U} = 1 + \imath\delta\varphi_a \frac{1}{2}\lambda_a \Rightarrow$ finite transformations: $\mathcal{U} = \exp(\imath\delta\varphi_a\frac{1}{2}\lambda_a)\Big)$

The gluons are coupled to the quarks via a **minimal coupling** scheme (analogous to the QED)

$$\boxed{\partial_\mu \to \underbrace{D_\mu}_{\substack{\text{“covariant}\\ \text{derivative”}}} := \partial_\mu + \imath \underbrace{g_s}_{\substack{\text{dimensionless}\\ \text{coupling constant}\\ (\hat{=}\text{charge in QED})}} \mathbf{A}_\mu(x)}$$

With this the Lagrangian becomes

$$\mathcal{L}_q(x) := \sum_{j=1}^{f} \overline{q}^j(x)\Big(\imath\gamma^\mu D_\mu - m_j\Big)q^j(x)\,.$$

$\mathcal{L}_q$ is invariant under local gauge transformations $q^j(x) \to \mathcal{U} \cdot q^j(x)$ if we transform the gluon potential in the following way:

$$\mathbf{A}_\mu(x) \to \mathbf{A}'_\mu(x) = \mathcal{U}(x)\mathbf{A}_\mu(x)\mathcal{U}^\dagger(x) - \frac{\imath}{g_s}\mathcal{U}(x)\partial_\mu\mathcal{U}^\dagger(x) \tag{8.30}$$

$\mathbf{A}'_\mu(x)$ is again Hermitian with a trace of zero for arbitrary $\mathcal{U}(x) \in \mathrm{SU(3)}$:

$$\mathcal{U}(x)\mathcal{U}^\dagger(x) = 1 \quad \Rightarrow \quad \mathcal{U}(x)\Big(\partial_\mu\mathcal{U}^\dagger(x)\Big) + \Big(\partial_\mu\mathcal{U}(x)\Big)\mathcal{U}^\dagger(x) = 0 \quad \Rightarrow \quad \mathbf{A}^\dagger_\mu(x) = \mathbf{A}_\mu(x)$$

$$\text{and} \quad \mathrm{Tr}\Big(\mathcal{U}(x)\partial_\mu\mathcal{U}^\dagger(x)\Big) = 0 \quad \Rightarrow \quad \mathrm{Tr}\ \mathbf{A}'_\mu = \mathrm{Tr}\ \mathbf{A}_\mu - \frac{\imath}{g_s}\ \mathrm{Tr}\Big(\mathcal{U}\partial_\mu\mathcal{U}^\dagger\Big) = 0$$

The gluon field $\mathbf{A}_\mu(x)$ itself must be a dynamical variable. Construction of the part containing the gluon dynamics of the Lagrange density is done analogous to the QED. One defines a **gluon field tensor $\mathbf{F}_{\mu\nu}(x)$**:

$$\mathbf{F}_{\mu\nu}(x) := \partial_\mu \mathbf{A}_\nu(x) - \partial_\nu \mathbf{A}_\mu(x) + \imath g_s \Big[\mathbf{A}_\mu(x),\, \mathbf{A}_\nu(x)\Big] \tag{8.31}$$

For fixed x it represents a Hermitian, traceless matrix, where its components are defined by

$$\mathbf{F}_{\mu\nu}(x) = F^a_{\mu\nu}(x)\,\frac{\lambda_a}{2}\,,$$

where with (8.31) one finds

$$F^a_{\mu\nu}(x) = \partial_\mu A^a_\nu(x) - \partial_\nu A^a_\mu(x) - g_s f^a{}_{bc} A^b_\mu(x) A^c_\nu(x)\,,$$

where f_{abc} represents the structure constants of SU(3). These result from the algebra of the generators by $[\lambda_a,\, \lambda_b] = 2\imath f_{ab}{}^c \lambda_c$.

The term quadratic in the gluon potentials has no analogue in the QED and is typical for the **non-abelian** character of the color group SU(3). This term is necessary to archive a simple transformation behaviour for $\mathbf{F}_{\mu\nu}$ under a gauge transformation, because according to the transformation of the gluon potential (8.30) follows $\mathbf{F}_{\mu\nu} \to \mathcal{U}\mathbf{F}_{\mu\nu}\mathcal{U}^\dagger$. Then the gauge invariant Lagrange density for quarks and gluons is given by

$$\begin{aligned}\mathcal{L}_{\text{QCD}}(x) &= -\frac{1}{2}\,\mathrm{Tr}\Big(\mathbf{F}_{\mu\nu}\mathbf{F}^{\mu\nu}\Big) + \sum_{j=1}^{f} \overline{q}^j(x)\Big(\imath\gamma^\mu D_\mu - m_j\Big) q^j(x) \\ &= -\frac{1}{4}\,F^a_{\mu\nu}(x) F^{a,\mu\nu} + \sum_{j=1}^{f} \overline{q}^j(x)\left[\imath\gamma^\mu\left(\partial_\mu + \imath g_s A^a_\mu(x)\,\frac{\lambda_a}{2}\right) - m_j\right] q^j(x)\end{aligned}$$

Above equation defines the fundamental Lagrange density of the QCD with a similar structure to the QED pendant.

Comparison of QED and QCD

	QED	QCD
quantum number	electrical charge	color
fermions	electrons	quarks (color triplet)
vector bosons	photons (uncharged)	gluons (color octet)
gauge group	U(1) (abelian)	SU(3) (non-abelian)
coupling constant	e, $\alpha = e^2/4\pi$	g_s, $\alpha_s = g_s^2/4\pi$

Appendix A

Correlation Functions, Scattering, and Response

A.1 Scattering and Response

If a time-dependent field $E\, e^{\imath(\mathbf{kr}-\omega t)}$ is applied to many-particle system (solid, liquid, or gas), this induces a "polarization":

$$\underbrace{P(\mathbf{k},\omega)\, e^{(\imath(\mathbf{kr}-\omega t)}}_{\text{periodicity as the applied field}} + \underbrace{P(\mathbf{k},2\omega)\, e^{\imath(\mathbf{kr}-2\omega t)} + P(2\mathbf{k},\omega)\, e^{\imath(2\mathbf{kr}-\omega t)} + \ldots}_{\text{nonlinear effects}}$$

Linear susceptibility is a property of the unperturbed sample:

$$\chi(\mathbf{k},\omega) := \lim_{E\to 0} \frac{P(\mathbf{k},\omega)}{E}$$

Scattering experiments with particles:
The wavelength of the particles must be similar to the scale of the structure that one wants to resolve.
Energy must be comparable to the excitation energies of the quasiparticles.
For example, neutron scattering with thermal neutrons from nuclear reactors.
($\lambda \approx 0.18\, nm$ for $E = 25\, meV \,\widehat{=}\, 290\, K$).

Inelastic scattering cross-section
H_0: Hamiltonian of a many-particle system (sample)
$\mathbf{x}_\alpha$: Coordinates of the particles of the sample (position and other degrees of freedom)
$m, \mathbf{r}, m_s$: mass, position and spin of the incident particle.

$$\boxed{H = H_0 + \frac{\mathbf{p}^2}{2m} + W\left(\{\mathbf{x}_\alpha\}, \mathbf{r}\right)}$$

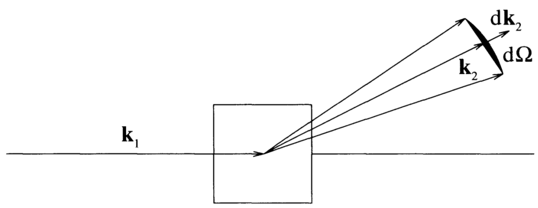
with the kinetic energy of the incident particle $\mathbf{p}^2/2m$ and the interaction between the sample and the incident particle $W\left(\{\mathbf{x}_\alpha\}, \mathbf{r}\right)$.

In second quantization

$$H = H_0 + \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{k}'\mathbf{k}''\sigma'\sigma''} a^\dagger_{\mathbf{k}'\sigma'} a_{\mathbf{k}''\sigma''} \frac{1}{V} \int \mathrm{d}^3\mathbf{r}\, e^{-\imath(\mathbf{k}'-\mathbf{k}'')\mathbf{r}}\, W^{\sigma'\sigma''}(\{\mathbf{x}_\alpha\}, \mathbf{r})$$
$$= H_0 + \frac{\mathbf{p}^2}{2m} + \sum_{\mathbf{k}'\mathbf{k}''\sigma'\sigma''} a^\dagger_{\mathbf{k}'\sigma'} a_{\mathbf{k}''\sigma''} W^{\sigma'\sigma''}_{\mathbf{k}'-\mathbf{k}''}(\{\mathbf{x}_\alpha\})$$

$a^\dagger_{\mathbf{k}'\sigma'}$ creates a incident particle with $\mathbf{k}', \sigma'$
$a_{\mathbf{k}''\sigma''}$ annihilates a incident particle with $\mathbf{k}'', \sigma''$

Eigenstates of H_0: $H_0|n\rangle = E_n|n\rangle$



Inelastic scattering
Momentum transfer: $\mathbf{k} = \mathbf{k}_1 - \mathbf{k}_2$
Energy transfer: $\hbar\omega = \frac{\hbar^2}{2m}(k_1^2 - k_2^2)$

Initial state $|\mathbf{k}_1, m_{s_1}, n_1\rangle$ ($|n_1\rangle$ initial state of the sample)
Final state $|\mathbf{k}_2, m_{s_2}, n_2\rangle$ ($|n_2\rangle$ final state of the sample)

The transition probability per unit time (Fermi's golden rule):

$$\Gamma(\mathbf{k}_1, m_{s_1}, n_1 \to \mathbf{k}_2, m_{s_2}, n_2) = \frac{2\pi}{\hbar} |\langle \mathbf{k}_2, m_{s_2}, n_2 | W | \mathbf{k}_2, m_{s_1}, n_1\rangle|^2\, \delta(E_{n_1} - E_{n_2} + \hbar\omega)$$

where $\langle \mathbf{k}_2, m_{s_2}, n_2 | W | \mathbf{k}_2, m_{s_1}, n_1\rangle = W^{m_{s_1} m_{s_2}}_{\mathbf{k}_2-\mathbf{k}_1}(\{\mathbf{x}_\alpha\})$ and $\hbar\omega = \frac{\hbar^2}{2m}(k_1^2 - k_2^2)$.
The distribution of initial states of the sample $|n_1\rangle$ is $p(n_1) \geq 0$ with $\sum_{n_1} p(n_1) = 1$
The distribution of the spin states of the incident particle m_{s_1} is $p_s(m_{s_1})$ with $\sum_{m_{s_1}} p_s(m_{s1}) = 1$

If only $\mathbf{k}_2$ (and not m_{s_1}) is measured:

$$\Gamma(\mathbf{k}_1 \to \mathbf{k}_2) = \sum_{n_2, n_1} \sum_{m_{s_1}, m_{s_2}} p(n_1)\, p_s(m_{s_1})\, \Gamma(\mathbf{k}_1, m_{s_1}, n_1 \to \mathbf{k}_2, m_{s_2}, n_2)$$

The differential scattering cross-section per atom:

$$\frac{d^2\sigma}{d\Omega d\epsilon}\, d\Omega d\epsilon = \frac{\text{probablility of transition into } d\Omega d\epsilon / s}{\text{number of scatterers} \times \text{flux of incident particles}}$$

The element of the solid angle into which is scattered is $d\Omega$, the flux of incident particles is equal to the magnitude of their current density, the number of scatterers is N, the normalization volume is L^3.

The states of the incident particles are $\psi_{\mathbf{k}_1}(\mathbf{r}) = \frac{1}{L^{3/2}} e^{\imath \mathbf{k}_1 \mathbf{r}}$, thus the current density is $j(\mathbf{r}) = -\frac{\imath\hbar}{2m}(\psi^\star \nabla\psi - (\nabla\psi^\star)\psi) = \frac{\hbar \mathbf{k}_1}{mL^3}$ and $\frac{d^2\sigma}{d\Omega d\epsilon}\, d\Omega d\epsilon = \frac{1}{N}\frac{mL^3}{\hbar k_1}\Gamma(\mathbf{k}_1 \to \mathbf{k}_2)\left(\frac{L}{2\pi}\right)^3 d^3k_2$

The number of final states, i.e., the number of $\mathbf{k}_2$ values in the interval d^3k_2 is $\left(\frac{L}{2\pi}\right)^3 d^3k_2$

Remark: Systems in equilibrium: $p(n_1) = \frac{e^{-\beta E_{n_1}}}{Z}$ (from density matrix $\rho = \frac{e^{-\beta H_0}}{Z}$).

Due to $\delta(\omega) = \int \frac{dt}{2\pi} e^{\imath\omega t}$ the scattering cross-section contains the factor

$$
\begin{aligned}
&\frac{1}{\hbar}\int \frac{dt}{2\pi}\, e^{\imath(E_{n_1}-E_{n_2}+\hbar\omega)t/\hbar}\, \langle n_1|e^{-\imath \mathbf{k}\mathbf{x}_\alpha}|n_2\rangle \\
=&\frac{1}{2\pi\hbar}\int dt\, e^{\imath\omega t}\langle n_1|e^{\imath H_0 t/\hbar} e^{-\imath \mathbf{k}\mathbf{x}_\alpha} e^{-\imath H_0 t/\hbar}|n_2\rangle \\
=&\frac{1}{2\pi\hbar}\int dt\, e^{\imath\omega t}\langle n_1|e^{-\imath \mathbf{k}\mathbf{x}_\alpha(t)}|n_2\rangle
\end{aligned}
$$

$$
\Rightarrow S_{\substack{\text{coh}\\ \text{inc}}}(\mathbf{k},\omega) = \int \frac{dt}{2\pi\hbar}\, e^{\imath\omega t}\, \frac{1}{N}\sum_{\alpha\beta}\langle e^{-\imath \mathbf{k}\mathbf{x}_\alpha(t)} e^{\imath \mathbf{k}\mathbf{x}_\beta(0)}\rangle \begin{pmatrix} 1 \\ \delta_{\alpha\beta}\end{pmatrix}
$$

where the index coh or inc refers to coherent or incoherent dynamical structure function, respectively. Both contain an elastic ($\omega = 0$) and an inelastic ($\omega \neq 0$) component.
The thermal average of an operator O is defined by $\langle O\rangle = \sum_n \frac{e^{-\beta E_n}}{Z}\langle n|O|n\rangle = \mathrm{Tr}(\rho O)$.

Density operator of the target system (sample):

$$
\rho(\mathbf{x},t) = \sum_{\alpha=1}^{N}\delta(\mathbf{x} - \mathbf{x}_\alpha(t))
$$

and its Fourier transform:

$$
\rho_{\mathbf{k}}(t) = \frac{1}{\sqrt{V}}\int d^3x\, e^{-\imath \mathbf{k}\mathbf{x}}\rho(\mathbf{x},t) = \frac{1}{\sqrt{V}}\sum_{\alpha=1}^{N} e^{-\imath \mathbf{k}\mathbf{x}_\alpha(t)}
$$

$$
\Rightarrow S_{coh}(\mathbf{k},\omega) = \int \frac{dt}{2\pi\hbar}\, e^{\imath\omega t}\, \frac{V}{N}\langle \rho_{\mathbf{k}}(t)\, \rho_{-\mathbf{k}}(0)\rangle
$$

with the density-density correlation function $\langle \rho_{\mathbf{k}}(t)\, \rho_{-\mathbf{k}}(0)\rangle$, the momentum $\hbar\mathbf{k}$ and the energy transfer $\hbar\omega$ from the scattered particles to the target system.

Application: scattering from solids to determine the lattice dynamics.

The one-phonon scattering: resonances at $\pm\omega_{t_1}(\mathbf{k})$ and $\pm\omega_{t_2}(\mathbf{k})$ (two transverse phonons), and at $\pm\omega_l(\mathbf{k})$ (longitudinal phonons)

The width of the resonances: lifetime of the phonons.
The background intensity is due to multiphonon scattering.

The intensity of the resonances depends on the scattering geometry via the scalar product of **k** with the polarization vector of the phonons and via the Debye-Waller factor.
Scattering cross-section $\longleftrightarrow$ correlation functions of the many-particle system
In the following: correlation functions $\longleftrightarrow$ response function

With $\epsilon = \frac{\hbar^2 k_2^2}{2m}$, it follows that $d\epsilon = \frac{\hbar^2 k_2}{m}\, dk_2$ and $d^3k_2 = \frac{m}{\hbar^2}\, k_2\, d\epsilon\, d\Omega$

$$\Rightarrow \quad \frac{d^2\sigma}{d\Omega d\epsilon} = \left(\frac{m}{2\pi\hbar^2}\right)^2 \frac{k_2}{k_1}\frac{L^6}{N} \sum_{\substack{n_1,n_2\\ m_{s_1},m_{s_2}}} p(n_1)p(m_{s_1})|\langle \mathbf{k}_1, m_{s_1}, n_1|W|\mathbf{k}_2, m_{s_2}, n_2\rangle|^2\, \delta(E_{n_1} - E_{n_2} + \hbar\omega)$$

Special case: **neutron scattering** (neutral particle)
$\rightsquigarrow$ Scattering solely by nuclei.
The range of the nuclear force: $R \approx 10^{-12}\, cm \;\Rightarrow\; k_1 R \approx 10^{-4} \ll 1 \;\Rightarrow$ only s-wave scattering.

$\Rightarrow$ The interaction can be represented by an effective pseudopotential.

$$W(\mathbf{x}) = \frac{2\pi\hbar^2}{m} \sum_{\alpha=1}^{N} a_\alpha\, \delta(\mathbf{x}_\alpha - \mathbf{x})$$

where a_α is the scattering lengths of the nuclei (Born approximation).
$\rightsquigarrow$ independent of the spin m_{s_1}!

$$\Rightarrow \quad \frac{d^2\sigma}{d\Omega d\epsilon} = \frac{k_2}{k_1}\frac{1}{N}\sum_{n_1 n_2} p(n_1) \left|\sum_{\alpha=1}^{N} a_\alpha \langle n_1|e^{\imath \mathbf{k}\mathbf{x}_\alpha}|n_2\rangle\right|^2 \delta(E_{n_1} - E_{n_2} + \hbar\omega)$$

We have used

$$\begin{aligned}\langle \mathbf{k}_1|\, W\, |\mathbf{k}_2\rangle &= \frac{2\pi\hbar^2}{mL^3}\int d^3x\, e^{-\imath \mathbf{k}_1 \mathbf{x}} \sum_\alpha a_\alpha \delta(\mathbf{x} - \mathbf{x}_\alpha) e^{\imath \mathbf{k}_2 \mathbf{x}} \\ &= \frac{2\pi\hbar^2}{mL^3}\sum_\alpha a_\alpha e^{-\imath(\mathbf{k}_1 - \mathbf{k}_2)\mathbf{x}_\alpha}\end{aligned}$$

and

$$\left|\sum_{\alpha=1}^{N} a_\alpha \langle n_1|e^{\imath \mathbf{k}\mathbf{x}_\alpha}|n_2\rangle\right|^2 = \sum_{\alpha,\beta} a_\alpha a_\beta \langle n_1|e^{-\imath \mathbf{k}\mathbf{x}_\alpha}|n_2\rangle\langle n_2|e^{\imath \mathbf{k}\mathbf{x}_\beta}|n_1\rangle\ \delta(E_{n_1} - E_{n_2} + k\omega)$$

Averaging over the various isotopes with different scattering lengths.
Assumption: positions of the isotopes are randomly distributed:

$$\overline{a_\alpha a_\beta} = \begin{cases}\overline{a}^2 & \text{for } \alpha \neq \beta \\ \overline{a^2} & \text{for } \alpha = \beta\end{cases} \quad \text{with} \quad \overline{a} = \frac{1}{N}\sum_{\alpha=1}^{N} a_\alpha \quad \text{and} \quad \overline{a^2} = \frac{1}{N}\sum_{\alpha=1}^{N} a_\alpha^2$$

$\Rightarrow$ Decomposition of the scattering cross-section into a **coherent** and an **incoherent** part

$$\frac{d^2\sigma}{d\Omega d\epsilon} = A_{\text{coh}}\, S_{\text{coh}}\mathbf{k}, \omega) + A_{\text{inc}}\, S_{\text{inc}}(\mathbf{k}, \omega)$$

With

$$A_{\text{coh}} = \overline{a}^2 \frac{k_2}{k_1} \quad , \quad A_{\text{inc}} = (\overline{a^2} - \overline{a}^2)\frac{k_2}{k_1}$$

$$S_{\text{coh}} = \frac{1}{N}\sum_{\alpha\beta}\sum_{n_1 n_2} p(n_1) \overbrace{\langle n_1|e^{-\imath \mathbf{k}\mathbf{x}_\alpha}|n_2\rangle\langle n_2|e^{\imath \mathbf{k}\mathbf{x}_\beta}|n_1\rangle}^{\text{amplitudes superpose, interference}} \delta(E_{n_1} - E_{n_2} + \hbar\omega)$$

$$S_{\text{inc}} = \frac{1}{N}\sum_{\alpha}\sum_{n_1 n_2} p(n_1) \underbrace{|\langle n_1|e^{-\imath \mathbf{k}\mathbf{x}_\alpha}|n_2\rangle|^2}_{\text{intensities superpose, no interference}} \delta(E_{n_1} - E_{n_2} + \hbar\omega)$$

S_{coh} contains information about the correlations between different atoms.
S_{inc} contains information about the correlation of each atom with itself.

A.2 Correlation and response functions

H_0: time independent Hamiltonian of a many-particle system
Schrodinger equation: $\imath\hbar \frac{\partial}{\partial t}|\psi, t\rangle = H_0 |\psi, t\rangle$
Formal solution:

$$|\psi, t\rangle = \underbrace{e^{-\imath H_0 (t-t_0)/\hbar}}_{=: U(t,t_0)} |\psi, t_0\rangle$$

Heisenberg representation:

State	$\|\psi_H\rangle = \|\psi, t_0\rangle$	is time-independent,
Operator	$A(t) = U_0^\dagger(t,t_0)\, A\, U_0(t,t_0)$	is time-dependent

$$\text{Heisenberg equation of motion} \quad \frac{d}{dt}A(t) = \frac{1}{\hbar}\Big[H_0, A(t)\Big]$$

Density matrix:

$$\rho = \frac{e^{-\beta \hat{H}_0}}{Z} \quad \text{with} \quad Z = \text{Tr}\ e^{-\beta H_0}$$

$$\rho_G = \frac{e^{-\beta(H_0 - \mu N)}}{Z_G} \quad \text{with} \quad Z_G = \text{Tr}\ e^{-\beta(H_0-\mu N)}$$

$$\text{Mean values :} \quad \langle O\rangle = \text{Tr}\,(\rho O)$$

Correlation function:

$$\begin{aligned} C_{AB}(t,t') &:= \langle A(t)\, B(t')\rangle \\ &= \text{Tr}\,(\rho\, e^{\imath H_0 t/\hbar}\, A e^{-\imath H_0 t/\hbar} e^{\imath H_0 t'/\hbar} B e^{-\imath H_0 t'/\hbar}) \\ &= \text{Tr}\,(\rho\, e^{\imath H_0 (t-t')/\hbar}\, A e^{-\imath H_0 (t-t')/\hbar} B) \\ &= C_{AB}(t-t', 0) \quad \Rightarrow \quad \text{temporal translational invariance} \end{aligned}$$

Definition:

$$\left.\begin{aligned} G^{>}_{AB}(t) &:= \langle A(t)\, B(0)\rangle \\ G^{<}_{AB}(t) &:= \langle B(0)\, A(t)\rangle \end{aligned}\right\} \rightsquigarrow \text{ Fourier transform: } \quad G^{\gtrless}_{AB}(\omega) = \int dt\, e^{\imath\omega t}\, G^{\gtrless}_{AB}(t)$$

$$\begin{aligned} \rightsquigarrow G^{>}_{AB}(\omega) &= \int dt\, e^{\imath\omega t}\ \mathrm{Tr}\,(\rho e^{\imath H_0 t/\hbar} A e^{-\imath H_0 t/\hbar} B) \\ &= \int dt\, e^{\imath\omega t} \sum_{n,m} \langle n| \frac{e^{-\beta H_0}}{Z}\, e^{\imath H_0 t/\hbar} A|m\rangle\langle m|e^{-\imath H_0 t/\hbar} B|n\rangle \\ &= \int dt\, e^{\imath\omega t}\, \frac{1}{Z} \sum_{n,m} e^{-\beta E_n} e^{\imath E_n t/\hbar} \langle n|A|m\rangle\, e^{-\imath E_m t/\hbar} \langle m|B|n\rangle \\ &= \frac{1}{Z} \sum_{n,m} e^{-\beta E_n} \langle n|A|m\rangle\langle m|B|n\rangle \int dt\, e^{\imath t(\frac{E_n - E_m}{\hbar} + \omega)} \end{aligned}$$

$$\Rightarrow G^{>}_{AB}(\omega) = \frac{2\pi}{Z} \sum_{n,m} e^{-\beta E_n}\, \langle n|A|m\rangle\langle m|B|n\rangle\ \delta\left(\frac{E_n - E_m}{\hbar} + \omega\right) \tag{A.1}$$

$$\text{and} \qquad G^{<}_{AB}(\omega) = \frac{2\pi}{Z} \sum_{n,m} e^{-\beta E_n}\, \langle n|B|m\rangle\langle m|A|n\rangle\ \delta\left(\frac{E_m - E_n}{\hbar} + \omega\right) \tag{A.2}$$

$$\Rightarrow G^{>}_{AB}(-\omega) = G^{<}_{BA}(\omega)$$

$$G^{<}_{AB}(\omega) = G^{>}_{AB}(\omega)\, e^{-\beta\hbar\omega} \tag{A.3}$$

$$(m \leftrightarrow n) \rightarrow \qquad = \frac{2\pi}{Z} \sum_{n,m} e^{-\beta E_m} \langle m|B|n\rangle\langle n|A|m\rangle\, \delta\left(\frac{E_n - E_m}{\hbar} + \omega\right) \tag{A.4}$$

$$\Rightarrow E_m = E_n + \hbar\omega \tag{A.5}$$

For example:

$$A = \rho_{\mathbf{k}} \quad \text{and} \quad B = \rho_{-\mathbf{k}}$$

with the Fourier transform $\quad \rho_{\mathbf{k}}(r) = \frac{1}{\sqrt{V}} \int d^3\mathbf{r}\, e^{-\imath\mathbf{k}\mathbf{r}}\, \rho(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_{\alpha=1}^{N} e^{-\imath\mathbf{k}\mathbf{r}_\alpha(t)}$

of the density operator $\quad \rho(\mathbf{r}, t) = \sum_{\alpha=1}^{N} \delta(\mathbf{r} - \mathbf{r}_\alpha(r))$

Density-density correlation function $\langle\rho_{\mathbf{k}}(t)\rho_{-\mathbf{k}}(t)\rangle$

Coherent scattering cross-section

$$S_{\mathrm{coh}}(\mathbf{k}, \omega) = \int \frac{dt}{2\pi\hbar}\, e^{\imath\omega t} \frac{V}{N} \langle\rho_{\mathbf{k}}(t)\rho_{-\mathbf{k}}(t)$$

Due to (A.3) follows:

$$\begin{aligned} S_{\mathrm{coh}}(\mathbf{k}, -\omega) &= e^{-\beta\hbar\omega} S_{\mathrm{coh}}(-\mathbf{k}, \omega) \\ &= e^{-\beta\hbar\omega} S_{\mathrm{coh}}(\mathbf{k}, \omega) \quad \text{for systems with inversion symmetry} \end{aligned}$$

$\Rightarrow$ Anti-Stokes lines (energy loss by the sample) are weaker by a factor $e^{-\beta\hbar\omega}$ than the Stokeslines (energy gain).

For $T \to 0 \quad S_{\mathrm{coh}}(\mathbf{k}, \omega < 0) \to 0$
(system is then in the ground cannot transfer any energy to the scattered particle).

A.3 Dynamical Susceptibility

Consider a many-particle system influenced by an external force $F(t)$ which couples to the operator B:

$$H = H_0 + H'(t)\,; \quad H'(t) = -\underbrace{F(t)}_{\mathbb{C}\text{-number}} \cdot B \tag{A.6}$$

For $t \le t_0$: $F(t) = 0$ (the system is in equilibrium).

How does the system response to the perturbation (A.6)?

The mean value of A at time t:

$$\begin{aligned}
\underbrace{\overline{A(t)}}_{=\langle A(t)\rangle} &= \mathrm{Tr}(\rho_S(t)A) = \mathrm{Tr}(U(t,t_0)\,\rho_S(t_0)\,U^\dagger(t,t_0)A) \\
&= \mathrm{Tr}(\rho_S(t_0)\,U^\dagger(t,t_0)\,A\,U(t,t_0)) \\
&= \mathrm{Tr}\left(\frac{e^{-\beta H_0}}{Z} U^\dagger(t,t_0)\,A\,U(t,t_0)\right) \\
&= \langle U^\dagger(t,t_0)\,A\,U(t,t_0)\rangle_0 = e^{-\imath H(t-t_0)/\hbar}
\end{aligned}$$

The system is in equilibrium at t_0, thus $\rho_S(t_0) = e^{-\beta H_0}/Z$.
$U(t,t_0)$ can be determined perturbation theoretically in the interaction representation.
Equation of motion: $\imath\hbar \frac{d}{dt} U(t,t_0) = H\,U(t,t_0)$
Ansatz:

$$\begin{aligned}
U(t,t_0) &= e^{-\imath H_0(t-t_0)/\hbar}\,U'(t,t_0) \\
\Rightarrow \imath\hbar\frac{d}{dt}U'(t,t_0) &= e^{\imath H_0(t-t_0)/\hbar}\,\underbrace{(-H_0+H)}_{=H'(t)}\,U \\
\text{Thus} \quad \imath\hbar\frac{d}{dt}U'(t,t_0) &= H'_I(t)\,U'(t,t_0) \\
H'_I(t) &= e^{\imath H_0(t-t_0)/\hbar} H'(t)\,e^{-\imath H_0(t-t_0)/\hbar}
\end{aligned}$$

"Interaction representation of H'".

$$\begin{aligned}
\Rightarrow \quad U'(t,t_0) &= 1 + \frac{1}{\imath\hbar}\int_{t_0}^{t} dt'\,H'_I(t')\,U'(t',t_0) \\
&= 1 + \frac{1}{\imath\hbar}\int_{t_0}^{t} dt'\,H'_I(t') + \frac{1}{(\imath\hbar)^2}\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\,H'_I(t')\,H'_I(t'') + \dots \qquad \text{(A.7)} \\
&= \mathcal{T}\exp\left\{\frac{1}{\imath\hbar}\int_{t_0}^{t} dt'\,H'_I(t')\right\}
\end{aligned}$$

with the time-ordering operator $\mathcal{T}$.

For the **linear** response, we need only the first two terms in (A.7).

$$\begin{aligned}
\rightsquigarrow \langle A(t)\rangle &= \langle U'^{\dagger}(t,t_0)\, e^{+\imath H_0(t-t_0)/\hbar} A\, e^{-\imath H_0(t-t_0)/\hbar} U'(t,t_0)\rangle_0 \\
&= \left\langle \left(1 - \frac{1}{\imath\hbar}\int_{t_0}^{t} dt' H_I'(t')\right) e^{\imath H_0(t-t_0)/\hbar} A\, e^{-\imath H_0(t-t_0)/\hbar} \left(1 + \frac{1}{\imath\hbar}\int_{t_0}^{t} dt' H_I'(t')\right)\right\rangle_0 \\
&= \underbrace{\langle e^{\imath H_0(t-t_0)/\hbar} A\, e^{-\imath H_0(t-t_0)/\hbar}\rangle_0}_{=\mathrm{Tr}\left(\frac{e^{-\beta H_0}}{Z}\, e^{\imath H_0(t-t_0)/\hbar} A\, e^{-\imath H_0(t-t_0)/\hbar}\right) = \mathrm{Tr}\left(\frac{e^{-\beta H_0}}{Z} A\right) = \langle A\rangle_0} \\
&+ \frac{1}{\imath\hbar}\int_{t_0}^{t} dt' \,\langle [e^{\imath H_0(t-t_0)/\hbar} A\, e^{-\imath H_0(t-t_0)/\hbar},\, \underbrace{H_I'(t')}_{=e^{\imath H_0(t-t')/\hbar} H'\, e^{-\imath H_0(t-t')/\hbar} = -B(t')\cdot F(t')}]\rangle_0
\end{aligned}$$

$$\Rightarrow \quad \langle A(t)\rangle = \langle A\rangle_0 - \frac{1}{\imath\hbar}\int_{t_0}^{t} dt' \,\langle [A(t), B(t')]\rangle_0\, F(t')$$

Initially $t_0 \to -\infty$ the system is in equilibrium and $F(t')$ is switched on at a later instant.

$$\Delta\langle A(t)\rangle = \langle A(t)\rangle - \langle A\rangle_0 = \int_{-\infty}^{\infty} dt' \,\chi_{AB}(t-t')\, F(t')$$

$$\text{with} \quad \chi_{AB}(t-t') = \frac{\imath}{\hbar}\Theta(t-t')\langle [A(t), B(t')]\rangle_0$$

with dynamical susceptibility or linear response function χ_{AB} and the step function

$$\Theta(x) = \begin{cases} 1 & x \geq 0 \\ 0 & x < 0 \end{cases},$$

which ensures causality.

Fourier transform of the dynamical susceptibility

$$\chi_{AB}(z) = \int_{-\infty}^{\infty} dt\, e^{\imath z t}\chi_{AB}(t) \qquad \text{with complex } z$$

Consider a very slowly switched on periodic perturbation ($\epsilon \to 0, \epsilon > 0$)

$$H' = -\left(BF_\omega e^{-\imath\omega t'} + B^\dagger F_\omega^\star\, e^{\imath\omega t}\right) e^{\epsilon t'}$$

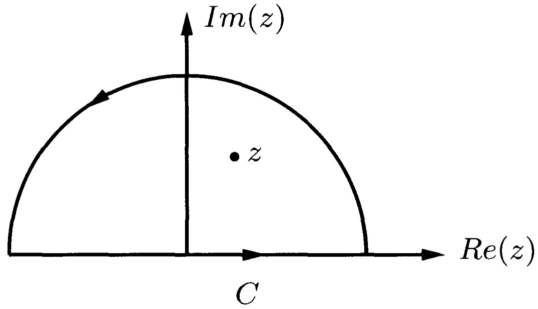
$$\begin{aligned}
\Rightarrow \Delta\langle A(t)\rangle &= \int_{-\infty}^{\infty} dt' \left(\chi_{AB}(t-t')\, F_\omega e^{-\imath\omega t'} + \chi_{AB^\dagger}(t-t')\, F_\omega^\star\, e^{\imath\omega t'}\right) \underbrace{e^{\epsilon t'}}_{\longrightarrow 1} \\
&= \chi_{AB}(\omega)\, F_\omega\, e^{-\imath\omega t} + \chi_{AB^\dagger}(-\omega)\, F_\omega^\star\, e^{-\imath\omega t}
\end{aligned}$$

The effect of the periodic perturbation on $\Delta\langle A(t)\rangle$ is proportional to the force.

Resonances in the susceptibility: strong reaction to forces at the corresponding frequency.

A.4 Dispersion Relations

Causality $\Rightarrow \quad \chi_{AB}(t) = 0$ for $t < 0$
$\Rightarrow \quad \chi_{AB}(z)$ is analytical in the upper half plane (due to $e^{-\text{Im}\, zt}$ in the Fourier transform)
$\Rightarrow \quad \chi_{AB}(z) = \frac{1}{2\pi\imath}\int\limits_c dz'\, \frac{\chi_{AB}(z')}{z'-z}$ (Cauchy's integral theorem)



← The semicircular part of the integration path does not contribute if $\chi_{AB}(z')$ is sufficiently small at infinity.

$$\Rightarrow \quad \chi_{AB}(z) = \frac{1}{2\pi\imath}\int\limits_{-\infty}^{\infty} dx'\, \frac{\chi_{AB}(x')}{x'-z}$$

$$\xrightarrow{\text{for real } z} \quad \chi_{AB}(x) = \lim_{\epsilon\to 0}\chi_{AB}(x+\imath\epsilon) = \lim_{\epsilon\to 0}\int \frac{dx'}{2\pi\imath}\,\frac{\chi_{AB}(x')}{x'-x-\imath\epsilon}$$

$$\lim_{\epsilon\to 0}\int\limits_{-\infty}^{+\infty}\frac{dx'}{2\pi\imath}\,\frac{f(x')}{x'-x-\imath\epsilon} = \lim_{\epsilon\to 0}\left(\int\limits_{-\infty}^{x-\epsilon}\frac{dx'}{2\pi\imath} + \int\limits_{x+\epsilon}^{+\infty}\frac{dx'}{2\pi\imath}\right)\frac{f(x')}{x'-x} + \frac{1}{2}\underbrace{\oint\frac{dz}{2\pi\imath}\,\frac{f(z)}{z-x}}_{=f(x)}$$

$$= P\int\frac{dx'}{2\pi\imath}\frac{f(x')}{x'-x} + \int\frac{dx'}{2}\, f(x')\,\delta(x'-x)\,,$$

with the Cauchy principal value defined as

$$P\int dx'\,\frac{f(x')}{x'-x} = \lim_{\epsilon\to 0}\left(\int\limits_{-\infty}^{x-\epsilon} dx' + \int\limits_{x+\epsilon}^{\infty} dx'\right)\frac{f(x')}{x'-x}$$

Or formal:

$$\boxed{\frac{1}{x'-x-\imath\epsilon} = P\left(\frac{1}{x'-x}\right) + \pi\imath\,\delta(x'-x)\,,}$$

i.e.

$$\chi_{AB}(x) = P\int\frac{dx'}{2\pi\imath}\,\frac{\chi_{AB}(x')}{x'-x} + \frac{1}{2}\chi_{AB}(x)$$

$$\Rightarrow \quad \chi_{AB}(x) = \frac{1}{\pi\imath}P\int dx'\,\frac{\chi_{AB}(x')}{x'-x}$$

i.e.

$$\begin{aligned}
\operatorname{Re}\chi_{AB}(x) &= \operatorname{Re}\left\{\frac{1}{\pi\imath}P\int dx'\,\frac{\imath\operatorname{Im}\chi_{AB}(x') + \operatorname{Re}\chi_{AB}(x')}{x'-x}\right\} \\
&= \frac{1}{\pi}\,P\int dx'\,\frac{\operatorname{Im}\chi_{AB}(x')}{x'-x} \\
\operatorname{Im}\chi_{AB}(x) &= -\frac{1}{\pi}\,P\int dx'\,\frac{\operatorname{Re}\chi_{AB}(x')}{x'-x}
\end{aligned}$$

A.5 Spectral Representation

Definition: Dissipative response $\chi''_{AB}(t) = \frac{1}{2\hbar}\langle[A(t),B(0)]\rangle$,
Fourier transform: $\chi''_{AB}(\omega) = \int\limits_{-\infty}^{+\infty} dt\, e^{\imath\omega t}\,\chi''_{AB}(t)$.
Due to $\Theta(t) = \lim_{\epsilon\to 0}\int\limits_{-\infty}^{+\infty}\frac{d\omega}{2\pi}\,e^{-\imath\omega t}\,\frac{\imath}{w+\imath\epsilon}$ we get

$$\begin{aligned}
\chi_{AB}(\omega) &= \int\limits_{-\infty}^{+\infty} dt\, e^{\imath\omega t}\Theta(t)2\imath\,\chi''_{AB}(t) \\
&= \frac{1}{\pi}\int\limits_{-\infty}^{+\infty} d\omega'\,\frac{\chi''_{AB}(w')}{\omega'-\omega-\imath\epsilon} \\
&= \underbrace{\frac{1}{\pi}P\int d\omega'\,\frac{\chi''_{AB}(\omega')}{\omega'-\omega}}_{=:\chi'_{AB}(\omega)} + \imath\chi''_{AB}(\omega) \\
&= \chi'_{AB}(\omega) + \imath\chi''_{AB}(\omega)
\end{aligned} \tag{A.8}$$

Decomposition into real and imaginary parts if $\chi''_{AB}(\omega)$ is real.

A.6 Fluctuation-Dissipation Theorem

Due to

$$\chi''_{AB}(t) = \frac{1}{2\hbar}\left\{\langle A(t)B(0)\rangle - \langle B(0)A(t)\rangle\right\}$$

it is

$$\chi''_{AB}(\omega) = \frac{1}{2\hbar}\{G^{>}_{AB}(\omega) - \underbrace{G^{<}_{AB}(\omega)}_{=G^{>}_{AB}(\omega)\,e^{-\beta\hbar\omega}}\}$$

thus

$$\boxed{\chi''_{AB}(\omega) = \frac{1}{2\hbar}\,G^{>}_{AB}(\omega)(1-e^{-\beta\hbar\omega})}$$

is the so-called **fluctuation-dissipation theorem** or with (A.8)

$$\chi_{AB}(\omega) = \frac{1}{2\pi\hbar} \int\limits_{-\infty}^{+\infty} d\omega' \, \frac{G^{>}_{AB}(\omega')(1 - e^{-\beta\hbar\omega'})}{\omega' - \omega - \imath\epsilon} \tag{A.9}$$

Classical limit: $\beta\hbar\omega \ll 1$ ($\leftarrow$ frequency and temperature region)

$$\Rightarrow \chi''_{AB}(\omega) = \frac{\beta\omega}{2} \, G^{>}_{AB}(\omega)$$

i.e.

$$\chi_{AB}(\omega = 0) = \beta \int \frac{d\omega'}{2\pi} \, G^{>}_{AB}(\omega') = \beta G^{>}_{AB}(t = 0) \,,$$

where $\chi_{AB}(\omega = 0)$ is the static susceptibility and $G^{>}_{AB}(t = 0)$ is the equal-time correlation function of A and B.
The name fluctuation-dissipation theorem is appropriate since $G_{AB}(\omega)$ is a measure of the correlation between fluctuations of A and B, whilst χ''_{AB} describes the dissipation.

That χ''_{AB} has to do with dissipation can be seen as follows: Consider a perturbation of the form $H' = \Theta(t)(A^\dagger F e^{-\imath\omega t} + AF^\star e^{\imath\omega t})$, where F is complex. The golden rule gives a transition rate per unit time from the state n into the state m:

$$\Gamma_{n\to m} = \frac{2\pi}{\hbar} \left\{ \delta(E_m - E_n - \hbar\omega) \, |\langle m|A^\dagger F|n\rangle|^2 \; + \; \delta(E_m - E_n + \hbar\omega) |\langle m|AF^\star|n\rangle|^2 \right\}$$

$\Rightarrow$ The power of the external force ($\hat{=}$ the energy absorbed per unit time)

$$\begin{aligned}
W &= \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \, \Gamma_{n\to m}(E_m - E_n) \\
&= \frac{2\pi}{Z} \left\{ \sum_{n,m} e^{-\beta E_n} \langle n|A|m\rangle \langle m|A^\dagger|n\rangle |F|^2 \, \delta(E_m - E_n - \hbar\omega) \cdot \overbrace{\frac{E_m - E_n}{\hbar}}^{=\omega} \right. \\
&\quad \left. + \sum_{n,m} e^{-\beta E_n} \langle n|A^\dagger|m\rangle \langle m|A|n\rangle |F|^2 \, \delta(E_m - E_n + \hbar\omega) \cdot \underbrace{\frac{E_m - E_n}{\hbar}}_{=-\omega} \right\} \\
&= \frac{\omega}{\hbar} \left\{ G^{>}_{AA^\dagger}(\omega) - G^{<}_{A^\dagger A}(\omega) \right\} |F|^2 \; = \; 2\omega \chi''_{AA^\dagger}(\omega) \cdot |F|^2
\end{aligned}$$

A.7 Example of Application: Harmonic crystal

Assumption: A Bravais lattice, i.e. a lattice with one atom per unit cell.

$$\text{Index} \quad \mathbf{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} \quad \text{and equilibrium position of an atom} \quad \mathbf{a_n} = \begin{pmatrix} n_x \cdot a_x \\ n_y \cdot a_y \\ n_z \cdot a_z \end{pmatrix}$$

with $n_{x,y,z} = 1, \ldots, N_{x,y,z}$ and the number of lattice points $N = N_x \cdot N_y \cdot N_z$.

Displacement from the equilibrium position $\quad \mathbf{u_n} = \mathbf{x_n} - \mathbf{a_n}$

Harmonic approximation of the Hamiltonian (Taylor expansion of the potential energy around the equilibrium position):

$$\hat{H} = \sum_{\mathbf{n}} \frac{\hat{p}_{\mathbf{n}}^2}{2M} + \sum_{\mathbf{n},\mathbf{n}'} \hat{\mathbf{u}}_{\mathbf{n}} \, \mathbf{D}_{\mathbf{n},\mathbf{n}'} \hat{\mathbf{u}}_{\mathbf{n}'} \quad \text{with} \quad \hat{p}_{\mathbf{n}} = -\imath\hbar \nabla_{\mathbf{u_n}}$$

Normal coordinates Q diagonalize the potential energy in the harmonic approximation.

$$\hat{\mathbf{u}}_{\mathbf{n}} = \frac{1}{\sqrt{NM}} \sum_{\mathbf{k},\lambda} e^{\imath \mathbf{k}\cdot\mathbf{a_n}} \, \boldsymbol{\epsilon}(\mathbf{k},\lambda) \, \hat{Q}_{\mathbf{k},\lambda} \,, \tag{A.10}$$

where $\boldsymbol{\epsilon}(\mathbf{k},\lambda)$ are the three polarization vectors ($\lambda = 1,2,3$) and $\mathbf{k}$ is the wave vector with components $k_i = n_i \frac{2\pi}{N_i a_i}$ due to periodic boundary conditions.
Thus

$$\hat{H} = -\sum_{\mathbf{k},\lambda} \frac{\hbar^2}{2M} \Delta_Q + \sum_{\mathbf{k},\lambda} \omega_{\mathbf{k},\lambda}^2 \, Q_{\mathbf{k},\lambda}^2$$

Define a creation and annihilation operators like for the harmonic oscillator:

$$\hat{Q}_{\mathbf{k},\lambda} = \sqrt{\frac{\hbar}{2\omega_{\mathbf{k},\lambda}}} \left(a_{\mathbf{k},\lambda} + a_{\mathbf{k},\lambda}^{\dagger} \right) \tag{A.11}$$

Thus

$$\hat{H} = \sum_{\mathbf{k},\lambda} \hbar\omega_{\mathbf{k},\lambda} \left(a_{\mathbf{k},\lambda}^{\dagger} a_{\mathbf{k},\lambda} + \frac{1}{2} \right)$$

Commutation relations: $\left[a_{\mathbf{k},\lambda},\, a_{\mathbf{k}',\lambda}^{\dagger}\right] = \delta_{\lambda\lambda'}\delta_{\mathbf{k}\mathbf{k}'}$ and $\left[a_{\mathbf{k},\lambda},\, a_{\mathbf{k}',\lambda'}\right] = \left[a_{\mathbf{k}',\lambda}^{\dagger},\, a_{\mathbf{k}',\lambda'}^{\dagger}\right] = 0$.
Dynamical susceptibility for the displacements:

$$\chi^{ij}(\mathbf{n}-\mathbf{n}',t) = \frac{\imath}{\hbar}\Theta(t)\langle[u_{\mathbf{n}}^i(t),\, u_{\mathbf{n}'}^j(0)]\rangle \tag{A.12}$$

$$\text{or} \quad \chi''^{ij}(\mathbf{n}-\mathbf{n}',t) = \frac{1}{2\hbar}\langle[u_{\mathbf{n}}^i(t),\, u_{\mathbf{n}'}^j(0)]\rangle \tag{A.13}$$

Thus

$$\chi^{ij}(\mathbf{n}-\mathbf{n}',t) = 2\imath\Theta(t)\, \chi''^{ij}(\mathbf{n}-\mathbf{n}',t)$$

Remark: $(\mathbf{n}-\mathbf{n}')$ instead of $(\mathbf{n},\mathbf{n}')$ due to translational invariance.

Phonon correlation function:

$$D^{ij}(\mathbf{n}-\mathbf{n}',t) = \langle u^i_{\mathbf{n}}(t)\, u^j_{\mathbf{n}'}(0)\rangle$$

Insert (A.11) into (A.10), and use this ($\hat{\mathbf{u}}$ expressed in terms of a, $a^\dagger$) in (A.13):

$$\chi''^{ij}(\mathbf{n}-\mathbf{n}',t) = \frac{1}{2\hbar}\,\frac{1}{NM}\sum_{\substack{\mathbf{k},\mathbf{k}'\\ \lambda,\lambda'}} e^{\imath\mathbf{k}\mathbf{a}_{\mathbf{n}}+\imath\mathbf{k}'\mathbf{a}_{\mathbf{n}'}}\,\epsilon^i(\mathbf{k},\lambda)\,\epsilon^j(\mathbf{k}'\lambda')$$
$$\times\frac{\hbar}{\sqrt{4\omega_{\mathbf{k},\lambda}\omega_{\mathbf{k}',\lambda'}}}\left\langle\left[\left(a_{\mathbf{k},\lambda}(t)+\mathbf{a}^\dagger_{-\mathbf{k},\lambda}(t)\right)\,,\,\left(a_{\mathbf{k}',\lambda'}(0)+\mathbf{a}^\dagger_{-\mathbf{k}',\lambda'}(0)\right)\right]\right\rangle$$

with $a_{\mathbf{k},\lambda}(t) = e^{-\imath\omega_{\mathbf{k},\lambda}t}\,a_{\mathbf{k},\lambda}(0)$

Auxiliary calculation: For $H=\hbar\omega a^\dagger a$ it is $a(t) = e^{+\imath\omega t a^\dagger a}a\,e^{-\imath\omega t a^\dagger a}$, thus

$$\langle n|a(t)|m\rangle = e^{+\imath\omega(n-m)t}\underbrace{\langle n|a|m\rangle}_{\propto\,\delta_{n,m-1}} = e^{-\imath\omega t}\langle n|a|m\rangle$$

Thus

$$\begin{aligned}
&\left[\left(a_{\mathbf{k},\lambda}(t)+a^\dagger_{-\mathbf{k},\lambda}(t)\right),\left(a_{\mathbf{k}',\lambda'}(0)+a^\dagger_{-\mathbf{k}',\lambda'}(0)\right)\right]\\
&=\left[a^\dagger_{-\mathbf{k},\lambda}(t),a_{\mathbf{k}',\lambda'}(0)\right]+\left[a_{\mathbf{k},\lambda}(t),a^\dagger_{-\mathbf{k}',\lambda'}(0)\right]\\
&=-\,e^{-\imath\omega_{\mathbf{k},\lambda}t}\delta_{-\mathbf{k},\mathbf{k}'}\,\delta_{\lambda,\lambda'}+e^{\imath\omega_{\mathbf{k},\lambda}t}\delta_{\mathbf{k},-\mathbf{k}'}\delta_{\lambda,\lambda'}
\end{aligned}$$

$$\Rightarrow \chi''^{ij}(\mathbf{n}-\mathbf{n}',t) = \frac{1}{4NM}\sum_{\mathbf{k},\lambda} e^{\imath\mathbf{k}(\mathbf{a}_{\mathbf{n}}-a_{\mathbf{n}'})}\,\epsilon^i(\mathbf{k},\lambda)\underbrace{\epsilon^{*j}(\mathbf{k},\lambda)}_{=\epsilon^j(-\mathbf{k},\lambda)}\frac{1}{\omega_{\mathbf{k},\lambda}}(e^{-\imath\omega_{\mathbf{k},\lambda}t}-e^{\imath\omega_{\mathbf{k},\lambda}t})$$

The polarization vectors for Bravais lattices are real, thus

$$\chi''^{ij}(\mathbf{n}-\mathbf{n}',t) = \frac{-\imath}{2NM}\sum_{\mathbf{k},\lambda} e^{\imath\mathbf{k}(\mathbf{a}_{\mathbf{n}}-\mathbf{a}_{\mathbf{n}'})}\frac{\epsilon^i(\mathbf{k},\lambda)\epsilon^j(\mathbf{k},\lambda)}{\omega_{\mathbf{k},\lambda}}\,\sin(\omega_{\mathbf{k},\lambda}t)$$

It is $\chi^{ij}(\mathbf{n}-\mathbf{n}',t) = 2\imath\,\Theta(t)\,\chi''^{ij}(\mathbf{n}-\mathbf{n}',t)$, thus

$$\chi^{ij}(\mathbf{n}-\mathbf{n}',t) = \frac{1}{NM}\sum_{\mathbf{k},\lambda} e^{\imath\mathbf{k}(\mathbf{a}_{\mathbf{n}}-\mathbf{a}_{\mathbf{n}'})}\frac{\epsilon^i(\mathbf{k},\lambda)\epsilon^j(\mathbf{k},\lambda)}{\omega_{\mathbf{k},\lambda}}\,\sin(\omega_{\mathbf{k},\lambda}t)\,\Theta(t)$$

$$\text{or}\quad \chi^{ij}(\mathbf{n}-\mathbf{n}',\omega) = \frac{1}{NM}\sum_{\mathbf{k},\lambda} e^{\imath\mathbf{k}(\mathbf{a}_{\mathbf{n}}-\mathbf{a}_{\mathbf{n}'})}\frac{\epsilon^i(\mathbf{k},\lambda)\epsilon^j(\mathbf{k},\lambda)}{\omega_{\mathbf{k},\lambda}}\underbrace{\int_0^\infty dt\,e^{\imath\omega t}\,\sin(\omega_{\mathbf{k},\lambda}t)}_{=\lim\limits_{\epsilon\to0}\frac{1}{2}\left\{\frac{1}{\omega+\omega_{\mathbf{k},\lambda}+\imath\epsilon}-\frac{1}{\omega-\omega_{\mathbf{k},\lambda}+\imath\epsilon}\right\}}$$

Auxiliary calculation:

$$\frac{1}{\imath}\int_0^\infty dt\,e^{\imath\tilde{\omega}t} = \lim_{\epsilon\to0}\frac{1}{\imath}\int_0^\infty dt\,e^{\imath\tilde{\omega}t}e^{-\epsilon t} = \lim_{\epsilon\to0}-\frac{1}{\imath}\,\frac{1}{\imath\tilde{\omega}-\epsilon} = \lim_{\epsilon\to0}\frac{1}{\tilde{\omega}+\imath\epsilon}$$

Spatial Fourier transform:

$$\begin{aligned}\chi^{ij}(\mathbf{q},\omega) &= \sum_{\mathbf{n}} e^{-\imath\mathbf{q}\mathbf{a_n}}\chi^{ij}(\mathbf{n},\omega)\\ &= \frac{1}{2NM}\sum_{\mathbf{k},\lambda}\underbrace{\sum_{\mathbf{n}} e^{-\imath\mathbf{a_n}(\mathbf{k}-\mathbf{q})}}_{=N\,\delta_{\mathbf{k},\mathbf{q}}}\frac{\epsilon^i(\mathbf{k},\lambda)\epsilon^j(\mathbf{k},\lambda)}{\omega_{\mathbf{k},\lambda}}\left\{\frac{1}{\omega+\omega_{\mathbf{k},\lambda}+\imath\epsilon}-\frac{1}{\omega-\omega_{\mathbf{k},\lambda}+\imath\epsilon}\right\}\\ &= \frac{1}{2M}\sum_{\lambda}\frac{\epsilon^i(\mathbf{q},\lambda)\epsilon^j(\mathbf{q},\lambda)}{\omega_{\mathbf{q},\lambda}}\left\{\frac{1}{\omega+\omega_{\mathbf{q},\lambda}+\imath\epsilon}-\frac{1}{\omega-\omega_{\mathbf{q},\lambda}+\imath\epsilon}\right\}\end{aligned}$$

For the decompositions

$$\chi^{ij}(\mathbf{n}-\mathbf{n}',\omega) = \chi'^{ij}(\mathbf{n}-\mathbf{n}',\omega) + \imath\,\chi''^{ij}(\mathbf{n}-\mathbf{n}',\omega)$$

this leads to

$$\chi'^{ij}(\mathbf{n}-\mathbf{n}',\omega) = \frac{1}{2NM}\sum_{\mathbf{k},\lambda} e^{\imath\mathbf{k}(\mathbf{a_n}-\mathbf{a_{n'}})}\frac{\epsilon^i(\mathbf{k},\lambda)\epsilon^j(\mathbf{k},\lambda)}{\omega_{\mathbf{k},\lambda}}\times\left\{P\left(\frac{1}{\omega+\omega_{\mathbf{k},\lambda}}\right)-P\left(\frac{1}{\omega-\omega_{\mathbf{k},\lambda}}\right)\right\}$$

$$\chi''^{ij}(\mathbf{n}-\mathbf{n}',\omega) = \frac{\pi}{2NM}\sum_{\mathbf{k},\lambda} e^{\imath\mathbf{k}(\mathbf{a_n}-\mathbf{a_{n'}})}\frac{\epsilon^i(\mathbf{k},\lambda)\epsilon^j(\mathbf{k},\lambda)}{\omega_{\mathbf{k},\lambda}}\times\left\{\delta(\omega-\omega_{\mathbf{k},\lambda})-\delta(\omega+\omega_{\mathbf{k},\lambda})\right\}$$

or

$$\chi'^{ij}(\mathbf{q},\omega) = \frac{1}{2M}\sum_{\lambda}\frac{\epsilon^i(\mathbf{q},\lambda)\ epsilon^j(\mathbf{q},\lambda)}{\omega_{\mathbf{q},\lambda}}\times\left\{P\left(\frac{1}{\omega+\omega_{\mathbf{q},\lambda}}\right)-P\left(\frac{1}{\omega-\omega_{\mathbf{q},\lambda}}\right)\right\}$$

$$\chi''^{ij}(\mathbf{q},\omega) = \frac{\pi}{2M}\sum_{\lambda}\frac{\epsilon^i(\mathbf{q},\lambda)\epsilon^j(\mathbf{q},\lambda)}{\omega_{\mathbf{q},\lambda}}\times\{\delta(\omega-\omega_{\mathbf{q},\lambda})-\delta(\omega+\omega_{\mathbf{q},\lambda})\}$$

The phonon correlation function can be either calculated directly, or determined with the help of the fluctuation-dissipation theorem from $\chi''^{ij}(\mathbf{n}-\mathbf{n}',\omega)$:

$$\begin{aligned}D^{ij}(\mathbf{n}-\mathbf{n}',\omega) &= 2\hbar\,\frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}-1}\,\chi''^{ij}(\mathbf{n}-\mathbf{n}',\omega)\\ &= 2\hbar\,(1+n(\omega))\chi''^{ij}(\mathbf{n}-\mathbf{n}',\omega)\\ &= \frac{\pi\hbar}{NM}\sum_{\mathbf{k},\lambda} e^{\imath\mathbf{k}(\mathbf{a_n}-\mathbf{a_{n'}})}\frac{\epsilon^i(\mathbf{k},\lambda)\epsilon^j(\mathbf{k},\lambda)}{\omega_{\mathbf{k},\lambda}}\\ &\quad\times\left\{(1+n_{\mathbf{k},\lambda})\delta(\omega-\omega_{\mathbf{k},\lambda})-n_{\mathbf{k},\lambda}\delta(\omega+\omega_{\mathbf{k},\lambda})\right\}\end{aligned}$$

or

$$\begin{aligned}D^{ij}(\mathbf{q},\omega) &= 2\hbar(1+n(\omega))\,\chi''^{ij}(\mathbf{q},\omega)\\ &= \frac{\pi\hbar}{M}\sum_{\lambda}\frac{\epsilon^i(\mathbf{q},\lambda)\epsilon^j(\mathbf{q},\lambda)}{\omega_{\mathbf{q},\lambda}}\left\{(1+n_{\mathbf{q},\lambda})\delta(\omega-\omega_{\mathbf{q},\lambda})-n_{\mathbf{q},\lambda}\delta(\omega+\omega_{\mathbf{q},\lambda})\right\}\end{aligned}$$

with $n_{q,\lambda} = \langle a^\dagger_{\mathbf{q},\lambda} a_{\mathbf{q},\lambda} \rangle = \frac{1}{e^{\beta\hbar\omega_{\mathbf{q},\lambda}}-1}$ the average thermal occupation number for phonons of wave vector $\mathbf{q}$ and polarization λ.

The phonon resonances in $D^{ij}(\mathbf{q},\omega)$ for a particular $\mathbf{q}$ are sharp δ-function-like peaks at the positions $\pm\omega_{\mathbf{q},\lambda}$.

The expansion of the density-density correlation function, which determines the inelastic neutron scattering cross-section, contains the phonon correlation function $D^{ij}(\mathbf{q},\omega)$.
$\rightsquigarrow$ The excitations of the many-particle system (in this case the phonons) express themselves as resonances in the scattering cross-section.

In reality, the phonons interact with one another and also with other excitations of the system, e.g, with the electrons in a metal → Damping of the phonons.
Replace ϵ by a finite damping constant → The phonon resonances then acquire a finite width.

Appendix B

Recap: Lorentz transformations

B.1 Infinitesimal Lorentz transformation

The subset $\mathcal{L}_+^\dagger$ where $\det(\Lambda) = +1$ (*proper*) and $\Lambda^0{}_0 \geq 1$ (*orthochronous*) is called **proper orthochronous Lorentz group** or simply **restricted Lorentz group**. It is a continuous group – a so called Lie group. The easiest way of analysing a continuous group is through infinitesimal transformations. Finite transformations are then obtained by repeated application of the infinitesimal transformation – an exponentiation.

We write

$$\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \Delta\omega^\mu{}_\nu$$

for the Lorentz transformation. Substitution in the constraint $g = \Lambda^T g \Lambda$ gives

$$g_{\rho\sigma} = (\delta^\mu{}_\rho + \Delta\omega^\mu{}_\rho) g_{\mu\nu} (\delta^\nu{}_\sigma + \Delta\omega^\nu{}_\sigma) = g_{\rho\sigma} + g_{\mu\sigma}\Delta\omega^\mu{}_\rho + g_{\rho\nu}\Delta\omega^\nu{}_\sigma + \mathcal{O}(\Delta\omega^2)\,.$$

There following statements must be satisfied:

$$\Delta\omega_{\sigma\rho} = -\Delta\omega_{\rho\sigma} \qquad \text{or} \qquad \begin{array}{l} \Delta\omega^0{}_i = +\Delta\omega^i{}_0 \\ \Delta\omega^i{}_j = -\Delta\omega^j{}_i \end{array}\,.$$

In other words, the infinitesimal 4×4-matrix $\Delta\omega_{\mu\nu}$ must be antisymmetrical. This leaves us with 6 free variables. The conditions $\det(\Lambda) = +1$ ans $\Lambda^0{}_0 \geq 1$ are guaranteed by the assumption that the transformation is an infinitesimal deviation from the identity matrix. Using the notation $\Delta\omega^0{}_i = -\Delta\eta_i$ and $\Delta\omega^i{}_j = \epsilon^i{}_j{}^k\Delta\theta_k = \epsilon_{ijk}\Delta\theta_k$, the matrix $\Delta\omega$ with its elements $\Delta\omega^\mu{}_\nu$ can be written as

$$\Delta\omega = \begin{pmatrix} 0 & -\Delta\eta^1 & -\Delta\eta^2 & -\Delta\eta^3 \\ -\Delta\eta^1 & 0 & \Delta\theta^3 & -\Delta\theta^2 \\ -\Delta\eta^2 & -\Delta\theta^3 & 0 & \Delta\theta^1 \\ -\Delta\eta^3 & \Delta\theta^2 & \Delta\theta^1 & 0 \end{pmatrix} = \imath\Delta\theta_i\mathcal{I}^i - \imath\Delta\eta_i\mathcal{K}^i\,.$$

The matrices $\mathcal{I}^i$ and $\mathcal{K}^i$ can be directly be read off from the equation, but will be later later explicitly represented after the meaning of this matrices is determined.
Example I: Rotations. An infinitesimal rotation about the x^3-axis ($\Delta\theta_3 = \theta/N$):

$$\Lambda = R_3\left(\frac{\theta}{N}\right) : \quad \begin{pmatrix} x'^0 \\ x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & \frac{\theta}{N} & 0 \\ 0 & -\frac{\theta}{N} & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix}, \quad \Rightarrow \Delta\omega = \imath\frac{\theta}{N}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\imath & 0 \\ 0 & \imath & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \imath\frac{\theta}{N}\mathcal{I}^3$$

For $\theta/N \ll 1$ we can approximate $(1 + \frac{\theta}{N}\mathcal{I}^3) \approx e^{\frac{\theta}{N}\mathcal{I}^3}$ and we have a finite rotation by the angle θ via

$$R_3(\theta) = \lim_{N\to\infty} R_3^N\left(\frac{\theta}{N}\right) = \lim_{N\to\infty}\left(\mathbb{1} + \imath\frac{\theta}{N}\mathcal{I}^3\right)^N = \lim_{N\to\infty}\left(e^{\imath\frac{\theta}{N}\mathcal{I}^3}\right)^N$$
$$= e^{\imath\theta\mathcal{I}^3} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos\theta & \sin\theta & 0 \\ 0 & -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

We can identify $\mathcal{I}^3$ as the generatrix of the rotation about the x^3-axis.

Rotation group

Rotations about the three axes x^1, x^2, x^3 are described by

$$R_i(\theta) = e^{\imath\theta\mathcal{D}^i}$$

where

$$\mathcal{D}^1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\imath \\ 0 & 0 & \imath & 0 \end{pmatrix}, \quad \mathcal{D}^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \imath \\ 0 & 0 & 0 & 0 \\ 0 & -\imath & 0 & 0 \end{pmatrix}, \quad \mathcal{D}^3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\imath & 0 \\ 0 & \imath & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The generator $\mathcal{D}^i$ satisfy the $\mathfrak{su}(2)$-algebra

$$\left[\mathcal{D}^i, \mathcal{D}^j\right] = \imath\epsilon^{ij}{}_k\mathcal{D}^k = \imath\epsilon_{ijk}\mathcal{D}^k .$$

Example II: Lorentz boosts. An infinitesimal boost along the x^1-axis:

$$\Lambda = L_1\left(\frac{\eta}{N}\right) : \quad \begin{pmatrix} x'^0 \\ x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} = \begin{pmatrix} 1 & -\frac{\eta}{N} & 0 & 0 \\ -\frac{\eta}{N} & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix}, \quad \Rightarrow \Delta\omega = \frac{\eta}{N}\begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = -\imath\frac{\eta}{N}\mathcal{K}^1$$

For $\eta/N \ll 1$ we can approximate $(1 - \imath\frac{\theta}{N}\mathcal{K}^1) \approx e^{-\imath\frac{\eta}{N}\mathcal{K}^1}$ and we have a finite rotation by the boost via

$$L_1(\eta) = \lim_{N\to\infty} L_1^N\left(\frac{\eta}{N}\right) = \lim_{N\to\infty}\left(\mathbb{1} - \imath\frac{\eta}{N}\mathcal{K}^1\right)^N = \lim_{N\to\infty}\left(e^{-\imath\frac{\theta}{N}\mathcal{K}^1}\right)^N$$
$$= e^{-\imath\eta\mathcal{K}^1} = \begin{pmatrix} \cosh\eta & -\sinh\eta & 0 & 0 \\ -\sinh\eta & \cosh\eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Boosts

Boosts along the three axes x^1, x^2, x^3 are described by

$$L_i(\eta) = e^{-\imath\eta\mathcal{I}^i}$$

where

$$\mathcal{I}^1 = \begin{pmatrix} 0 & -\imath & 0 & 0 \\ -\imath & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{I}^2 = \begin{pmatrix} 0 & 0 & -\imath & 0 \\ 0 & 0 & 0 & 0 \\ -\imath & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \mathcal{I}^3 = \begin{pmatrix} 0 & 0 & 0 & -\imath \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -\imath & 0 & 0 & 0 \end{pmatrix}.$$

The generators $\mathcal{I}^i$ do not form a closed algebra and the Lorentz boosts also do not form a subset of the Lorentz group. Instead we have

$$\left[\mathcal{I}^i, \mathcal{I}^j\right] = -\imath\epsilon^{ij}{}_k\mathcal{D}^k = -\imath\epsilon_{ijk}\mathcal{D}^k .$$

Lorentz algebra

A general infinitesimal Lorentz transformation in the restricted Lorentz group $\mathcal{L}_+^\uparrow$

$$\lambda^\mu{}_\nu = \delta^\mu{}_\nu + \Delta\omega^\mu{}_\nu$$

can be expressed via the generators of rotations and boosts

$$\Delta\omega = \imath\Delta\theta_i\mathcal{D}^i - \imath\Delta\eta_i\mathcal{I}^i .$$

The generators form an algebra with

$$\left[\mathcal{D}^i, \mathcal{D}^j\right] = \imath\epsilon_{ijk}\mathcal{D}^k , \quad \left[\mathcal{I}^i, \mathcal{I}^j\right] = -\imath\epsilon_{ijk}\mathcal{D}^k , \quad \left[\mathcal{D}^i, \mathcal{I}^j\right] = \imath\epsilon_{ijk}\mathcal{I}^k .$$

One gets a finite transformations by exponentiation of the infinitesimal transformations

$$R_i(\theta) = e^{\imath\theta\mathcal{D}^i} , \qquad L_i(\eta) = e^{-\imath\eta\mathcal{I}^i} .$$

B.2 Matrix representation of a Lorentz boost

We want to look at a boost in x^1 direction and define

$$\beta := \frac{v}{c} = \tanh \xi$$

$$\begin{aligned}
\Rightarrow \quad \gamma &:= \frac{1}{\sqrt{1-(v/c)^2}} \\
&= \frac{1}{\sqrt{1-\tanh^2 \xi}} \\
&= \frac{1}{\sqrt{1-\frac{\sinh^2 \xi}{\cosh^2 \xi}}} \\
&= \frac{1}{\frac{1}{\cosh \xi} \underbrace{\sqrt{\cosh^2 \xi - \sinh^2 \xi}}_{=1}} \\
&= \cosh \xi
\end{aligned}$$

Then we have

$$\begin{aligned}
\beta\gamma &= \frac{v/c}{\sqrt{1-(v/c)^2}} \\
&= \frac{\tanh \xi}{\sqrt{1-(v/c)^2}} \\
&= \cosh \xi \cdot \tanh \xi \\
&= \sinh \xi \, .
\end{aligned}$$

With this, we can write the transformed $x^0 = ct$ and x^1 component as

$$\begin{aligned}
x'^1 &= \frac{x^1 - vt}{\sqrt{1-(v/c)^2}} \\
&= \frac{1}{\sqrt{1-(v/c)^2}}\, x^1 - ct\, \frac{v/c}{\sqrt{1-(v/c)^2}} \\
&= \cosh \xi \cdot x^1 - \sinh \xi \cdot x^0
\end{aligned}$$

$$\begin{aligned}
x'^0 = ct' &= \frac{ct - (v/c)x^1}{\sqrt{1-(v/c)^2}} \\
&= \cosh \xi \cdot x^0 - \sinh \xi \cdot x^1 \, ,
\end{aligned}$$

while x^2 and x^3 remain unchanged. We can therefore write the transformation as a matrix equation:

$$\begin{pmatrix} x'^0 \\ x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} = \left(\begin{array}{cc|cc} \cosh \xi & -\sinh \xi & 0 & 0 \\ -\sinh \xi & \cosh \xi & 0 & 0 \\ \hline 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right) \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix} \, .$$

Appendix C

Alternative derivation of the Dirac equation

C.1 Derivation of the Dirac equation through the transformation behaviour of spinors

Rotation in $\mathbb{R}^3$: $\mathbf{r}' = \mathcal{R}\mathbf{r}$ with $\mathcal{R}\mathcal{T}\mathcal{R} = 1$, i.e. $\mathcal{R} \in \mathrm{O}(3)$

Example:
Rotation about the x, y, z axis:

$$\mathcal{R}_z(\theta) = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ -\sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\mathcal{R}_x(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & \sin\phi \\ 0 & -\sin\phi & \cos\phi \end{pmatrix}$$

$$\mathcal{R}_y(\psi) = \begin{pmatrix} \cos\psi & 0 & -\sin\psi \\ 0 & 1 & 0 \\ \sin\psi & 0 & \cos\psi \end{pmatrix}$$

O(3) is a **non-abelian group**, i.e. its elements do not commute in general.
O(3) is a **Lie group**, i.e. a continuous group with a non-finite number of elements.

A general rotation has three parameters, e.g. Euler angles.
$\Rightarrow$ There exist three (hermitian) **generators**:

$$J_z = \frac{1}{\imath}\frac{d\mathcal{R}_z(\theta)}{d\theta}\bigg|_{\theta=0} = \begin{pmatrix} 0 & -\imath & 0 \\ \imath & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$J_x = \frac{1}{\imath}\frac{d\mathcal{R}_x(\phi)}{d\phi}\bigg|_{\phi=0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$J_y = \frac{1}{\imath}\frac{d\mathcal{R}_y(\psi)}{d\psi}\bigg|_{\psi=0} = \begin{pmatrix} 0 & 0 & \imath \\ 0 & 0 & 0 \\ -\imath & 0 & 0 \end{pmatrix}$$

Infinitesimal rotation: e.g. $\mathcal{R}_z(\delta\theta) \approx 1 + \imath J_z \delta\theta$, $\mathcal{R}_x(\delta\phi) \approx 1 + \imath J_x \delta\phi$
E.g. the commutator is:

$$\begin{aligned}&\mathcal{R}_z(\delta\theta)\mathcal{R}_x(\delta\phi)\mathcal{R}_z^{-1}(\delta\theta)\mathcal{R}_x^{-1}(\delta\phi)\\=&1-\left(\delta\theta^2+\delta\phi^2\right)-2\underbrace{[J_z,\,J_x]}_{\imath J_y}\delta\theta\,\delta\phi+\mathcal{O}(\delta^3)\end{aligned}$$

$\Rightarrow$ **J** is the angular momentum operator with the commutation relation $\boxed{[J_x,\,J_y]=\imath J_z}$ and cyclic permutations.

Rotation by an finite angle:
e.g. $\theta = N\cdot\delta\theta$ $(N\to\infty)$, $\delta\theta=\theta/N$

$$\begin{aligned}\Rightarrow\quad \mathcal{R}_z(\theta)&=\Big[\mathcal{R}_z(\delta\theta)\Big]^N\\&=\Big(1+\imath J_z\delta\theta\Big)^N\\&=\left(1+\imath J_z\frac{\theta}{N}\right)^N\xrightarrow[N\to\infty]{}\exp(\imath J_z\theta)\end{aligned}$$

In general: rotation about an axis $\mathbf{n}$ by an angle θ:

$$\boxed{\mathcal{R}_{\mathbf{n}}(\theta)=\exp\left(\imath\mathbf{J}\cdot\boldsymbol{\theta}\right)=\exp\left(\imath(\mathbf{J}\cdot\mathbf{n})\,\theta\right)}$$

Consider now SU(2): 2×2 unitary matrices with determinants 1, $\mathcal{U}\mathcal{U}^\dagger=1$, $\det\mathcal{U}=1$. Every element in SU(2) can be written as

$$\boxed{\mathcal{U}=\exp\left(\imath\frac{\boldsymbol{\sigma}\cdot\boldsymbol{\theta}}{2}\right),\qquad \boldsymbol{\theta}=(\theta_x,\,\theta_y,\,\theta_z)=|\theta|\cdot\mathbf{n}}\qquad(*)$$

with

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad\sigma_y=\begin{pmatrix}0&-\imath\\\imath&0\end{pmatrix},\quad\sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

the Pauli matrices. $\mathbf{J}=\frac{1}{2}\boldsymbol{\theta}$ is the angular momentum operator ($\hbar=1$).
One has the commutation relations

$$\boxed{\left[\frac{\sigma_x}{2},\,\frac{\sigma_y}{2}\right]=\imath\frac{\sigma_z}{2}\quad\text{and cyclic permutations}\,.}$$

In other words: SU(2) is a 2-dimensional representation of the rotation group and acts on the space of the double- (or Pauli-)spinors $\begin{pmatrix}\xi_1\\\xi_2\end{pmatrix}$.

SU(2) and O(3) have a similar structure, however two elements each of SU(2) correspond to one element of O(3) due to the factor of 1/2 in the exponent of $(*)$.

C.1.1 SL$(2,\mathbb{C})$ and the Lorentz group

$\mathrm{SL}(2,\mathbb{C}) = \{\mathcal{U} \mid \mathcal{U}: \text{ complex } 2\times 2\text{-matrix with } \det\mathcal{U} = 1\}$
In analogy to the correspondence between SU(2) and the rotation group, there is a correspondence between SL$(2,\mathbb{C})$ and the Lorentz group.

Pure Lorentz boosts: e.g. movement along the x axis with velocity v:

$$x' = \frac{x+vt}{\sqrt{1-\frac{v^2}{c^2}}}\,, \quad y' = y\,, \quad z' = z\,, \quad t' = \frac{t+\frac{v}{c^2}x}{\sqrt{1-\frac{v^2}{c^2}}}$$

Definition:

$$\gamma = \frac{1}{\sqrt{1-\frac{v^2}{c^2}}}\,, \quad \beta = \frac{v}{c}\,, \quad x^0 = ct\,, \quad x^1 = x \quad \text{etc.}$$

$$\Rightarrow x'^0 = \gamma(x^0+\beta x^1) \quad x'^1 = \gamma(\beta x^0 + x^1)\,, \quad x'^2 = x^2\,, \quad x'^3 = x^3$$

Because of $\gamma^2 - (\gamma\beta)^2 = 1$, we can set

$$\boxed{\gamma =: \cosh\phi\,, \quad \gamma\beta =: \sinh\phi\,, \quad \frac{v}{c} =: \tanh\phi\,.}$$

This leads to the matrix representation

$$\Rightarrow \begin{pmatrix} x'^0 \\ x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} = \underbrace{\begin{pmatrix} \cosh\phi & \sinh\phi & 0 & 0 \\ \sinh\phi & \cosh\phi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_{=:\,\mathcal{B}\,,\ \textbf{Boost matrix}} \begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix}$$

Generator of this boost transformation is

$$K_x = \frac{1}{\imath}\frac{\partial\mathcal{B}}{\partial\phi}\Big|_{\phi=0} = -\imath \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

and analogous for the other spatial directions

$$K_y = -\imath \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\,, \quad K_z = -\imath \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}\,.$$

In this 4×4-matrix notation the generators of the rotations are given by:

$$J_x = -\imath \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}\,, \quad J_y = -\imath \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}\,, \quad J_z = -\imath \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\,.$$

General Lorentz transformation: consisting of boosts in 3 directions and rotations about 3 axis, i.e. 6 generators (see above).

Commutation relations:

$$\left.\begin{array}{l}[K_x,\, K_y] = -\imath J_z \\ [J_x,\, J_y] = \imath J_z \\ [J_x,\, K_y] = \imath K_z\end{array}\right\} \text{ and cyclic permutations}$$
$$[J_x, K_x] = 0 \ \text{ etc.}$$

n.b.: Pure Lorentz transformations *do not* form a group, because **K** does not represent a closed algebra under the commutation relations. E.g. for 2 infinitesimal boosts, the term

$$e^{\imath K_x \delta\phi}\, e^{\imath K_y \delta\psi}\, e^{-\imath K_x \delta\phi}\, e^{-\imath K_y \delta\psi} = 1 - [K_x,\, K_y]\delta\phi\,\delta\psi + K_x^2(\delta\phi)^2 K_y^2(\delta\psi)^2 + \dots$$

contains a rotation about the z axis because of $[K_x,\, K_y] = -\imath J_z$ ($\rightsquigarrow$ Thomas precession).

C.1.2 Transformation behaviour of Pauli matrizen under Lorentz transformations

Remark:
$\mathbf{K} = \pm\imath\frac{\boldsymbol{\sigma}}{2}$ satisfies the above commutation relation $\rightsquigarrow$ two types of spinors related to + resp. −.

Definition:
The generators

$$\left.\begin{array}{l}\mathbf{A} := \frac{1}{2}\left(\mathbf{J} + \imath\mathbf{K}\right) \\ \mathbf{B} := \frac{1}{2}\left(\mathbf{J} - \imath\mathbf{K}\right)\end{array}\right\} \quad \Longrightarrow \quad \begin{array}{rcll}[A_x,\, A_y] &=& \imath A_z & \text{cycl.} \\ [B_x,\, B_y] &=& \imath B_z & \text{cycl.} \\ [A_i,\, B_j] &=& 0 & (i, j = x, y, z)\end{array}$$

generate both a group SU(2) respectively and both groups commute, i.e. the Lorentz group is in essence equivalent SU(2) ⊗ SU(2) and states that transform in a well-defined way are denoted with two angular momenta: $(j,\, j')$, j corresponds to A, j' corresponds to B.

In particular:

$$\begin{array}{llll}(j,\, 0) & \longrightarrow & \mathbf{J}^{(j)} = \ \ \imath\mathbf{K}^{(j)} & (\mathbf{B} = 0) \\ (0,\, j) & \longrightarrow & \mathbf{J}^{(j)} = -\imath\mathbf{K}^{(j)} & (\mathbf{A} = 0)\end{array}$$

Definition: 2 types of spinors:

- Type I:
  $(\frac{1}{2},\, 0)$: $\mathbf{J}^{(1/2)} = \boldsymbol{\sigma}/2$, $\quad \mathbf{K}^{(1/2)} = -\imath\boldsymbol{\sigma}/2$, $\quad$ spinor ξ.
  Let be $\boldsymbol{\theta}$ and $\boldsymbol{\phi}$ the parameters of a rotation and a pure Lorentz transformation respectively. Then ξ transforms like

$$\xi \quad\longrightarrow\quad \exp\left(\imath\frac{\boldsymbol{\sigma}}{2}\cdot\boldsymbol{\theta} + \frac{\boldsymbol{\sigma}}{2}\cdot\boldsymbol{\phi}\right)\xi = \underbrace{\exp\left(\imath\frac{\boldsymbol{\sigma}}{2}\cdot(\boldsymbol{\theta} - \imath\boldsymbol{\phi})\right)}_{=:\mathcal{U}}\xi$$

- Type II:
  $(0,\ \frac{1}{2})$: $\mathbf{J}^{(1/2)} = \boldsymbol{\sigma}/2$, $\quad \mathbf{K}^{(1/2)} = \imath\boldsymbol{\sigma}/2$, $\quad$ spinor η.

$$\eta \quad \longrightarrow \quad \underbrace{\exp\left(\imath\frac{\boldsymbol{\sigma}}{2}\cdot(\boldsymbol{\theta}+\imath\boldsymbol{\phi})\right)}_{=:\mathcal{N}}\eta$$

n.b.: These are non-equivalent representations of the Lorentz group, i.e. there exists **no** matrix $\mathcal{S}$ in such a way that $\mathcal{N} = \mathcal{S}\mathcal{U}\mathcal{S}^{-1}$. Instead there are connected via $\mathcal{N} = \zeta\mathcal{U}^*\zeta^{-1}$ where $\zeta = -\imath\sigma_2$. Furthermore it is $\det\mathcal{U} = \det\mathcal{N} = 1$.
$\rightsquigarrow$ $\mathcal{U}$ and $\mathcal{N}$ form group $\mathrm{SL}(2,\mathbb{C})$. 6 parameters $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$, $ad - bc = 1$
Therefore there are two *different* types of 2-component spinors, which transform differently under Lorentz transformations, ξ and η. These correspond to the representations $(1/2,\ 0)$ and $(0,\ 1/2)$ of the Lorentz group.
Essentially the **Dirac equation** is a relation between these spinors.

Parity operator: $\mathbf{r} \to \mathbf{r}'$

- $\Rightarrow$ velocity in the Lorentz boost: $\mathbf{v} \to -\mathbf{v}$
- $\Rightarrow$ generator $\mathbf{K} \to -\mathbf{K}$ ($\widehat{=}$ vector), but $\mathbf{J} \to +\mathbf{J}$ (angular momentum is an axial or pseudo vector)
- $\Rightarrow$ representations $(j,\ 0)$ and $(0,\ j)$ are exchanged under parity: $(j,\ 0) \to (0,\ j)$ and therefore $\xi \to \eta$

If we consider the parity, we see it is no longer sufficient to view ξ and η separately, but the **4-spinor**

$$\psi = \begin{pmatrix} \xi \\ \eta \end{pmatrix}$$

Under a Lorentz transformation:

$$\begin{aligned}\begin{pmatrix} \xi \\ \eta \end{pmatrix} \longrightarrow & \begin{pmatrix} \exp\left(\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta}-\imath\boldsymbol{\phi})\right) & 0 \\ 0 & \exp\left(\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta}+\imath\boldsymbol{\phi})\right) \end{pmatrix}\begin{pmatrix} \xi \\ \eta \end{pmatrix} \\ = & \begin{pmatrix} D(\Lambda) & 0 \\ 0 & \bar{D}(\Lambda) \end{pmatrix}\begin{pmatrix} \xi \\ \eta \end{pmatrix},\end{aligned}$$

where $\bar{D}(\Lambda) = \zeta D^*(\Lambda)\zeta^{-1}$ and Λ the Lorentz transformation: $x'^{\mu} = \Lambda^{\mu}{}_{\nu}\, x^{\nu}$.

Under parity transformation:

$$\begin{pmatrix} \xi \\ \eta \end{pmatrix} \Longrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} \xi \\ \eta \end{pmatrix}$$

The 4-spinor ψ is a *irreducible* representation of the Lorentz group *extended* by parity (is *not* unitary b.c. $\exp(\boldsymbol{\theta}\cdot\boldsymbol{\phi}) \Leftrightarrow$ L group is not compact).

Consider now Lorentz boosts especially ($\theta = 0$) and define $\xi = \phi_\mathrm{R}$ and $\eta = \phi_\mathrm{L}$ (R: right, L: left)

$$\phi_\mathrm{R} \quad \Rightarrow \quad e^{\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\phi}}\,\phi_\mathrm{R} = \left\{\cosh\left(\frac{\phi}{2}\right) + \boldsymbol{\sigma}\cdot\underbrace{\mathbf{n}}_{\text{direction of the Lorentz boost}}\sinh\left(\frac{\phi}{2}\right)\right\}\phi_\mathrm{R}$$

Let $\phi_\mathrm{R}(0)$ be the spinor for a particle at rest, $\phi_\mathrm{R}(\mathbf{p})$ the spinor for a particle with momentum $\mathbf{p}$ respectively.

Because of $\cos(\phi/2) = [(r+1)/2]^{1/2}$, $\sinh(\phi/2) = [(r-1)/2]^{1/2}$ $r = \frac{1}{\sqrt{1-v^2}}$, (where we set $c = 1$), follows

$$\phi_\mathrm{R}(\mathbf{p}) = \left\{\left(\frac{r+1}{2}\right)^{1/2} + \boldsymbol{\sigma}\cdot\mathbf{p}\left(\frac{r-1}{2}\right)^{1/2}\right\}\phi_\mathrm{R}(0)\,.$$

Because for a particle with (total) energy E, mass m and momentum $\mathbf{p}$ holds $E = \gamma m$ ($c = 1$), it follows

$$\phi_\mathrm{R}(\mathbf{p}) = \frac{E + m + \boldsymbol{\sigma}\cdot\mathbf{p}}{[2m\,(E+m)]^{1/2}}\,\phi_\mathrm{R}(0)\,,$$

or analogous

$$\phi_\mathrm{L}(\mathbf{p}) = \frac{E + m - \boldsymbol{\sigma}\cdot\mathbf{p}}{[2m\,(E+m)]^{1/2}}\,\phi_\mathrm{L}(0) \quad \Rightarrow \quad \phi_\mathrm{L}(0) = \frac{E + m + \boldsymbol{\sigma}\cdot\mathbf{p}}{[2m\,(E+m)]^{1/2}}\,\phi_\mathrm{L}(\mathbf{p})$$

The spin of a resting particle cannot be defined as left- or right-handed $\rightsquigarrow$ $\phi_\mathrm{R}(0) = \phi_\mathrm{L}(0)$.

$$\begin{aligned}
\Rightarrow \quad \phi_\mathrm{R}(\mathbf{p}) &= \frac{E + m + \boldsymbol{\sigma}\cdot\mathbf{p}}{[2m\,(E+m)]^{1/2}}\cdot\frac{E + m + \boldsymbol{\sigma}\cdot\mathbf{p}}{[2m\,(E+m)]^{1/2}}\,\phi_\mathrm{R}(\mathbf{p}) \\
&= \frac{(E+m)^2 + 2\boldsymbol{\sigma}\cdot\mathbf{p}(E+m) + p^2}{2m(E+m)}\,\phi_\mathrm{L}(\mathbf{p}) \\
&= \frac{E + \boldsymbol{\sigma}\cdot\mathbf{p}}{m}\,\phi_\mathrm{L}(\mathbf{p})\,,
\end{aligned}$$

respectively

$$\phi_\mathrm{L}(\mathbf{p}) = \frac{E - \boldsymbol{\sigma}\cdot\mathbf{p}}{m}\,\phi_\mathrm{L}(\mathbf{p})$$

We find in matrix form:

$$\boxed{\begin{pmatrix} -m & p_0 + \boldsymbol{\sigma}\cdot\mathbf{p} \\ p_0 - \boldsymbol{\sigma}\cdot\mathbf{p} & -m \end{pmatrix}\begin{pmatrix}\phi_\mathrm{R}(\mathbf{p}) \\ \phi_\mathrm{L}(\mathbf{p})\end{pmatrix}} \tag{C.1}$$

Definition: The 4-spinor

$$\psi(p) := \begin{pmatrix} \phi_{\mathrm{R}}(\mathbf{p}) \\ \phi_{\mathrm{L}}(\mathbf{p}) \end{pmatrix}$$

and the 4×4-matrices

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & -\sigma^i \\ \sigma^i & 0 \end{pmatrix}$$

let us write (C.1) write as

$$\left(\gamma^0 p_0 + \gamma^i p_i - m\right) \psi(p) = 0\,,$$

respectively

$$\boxed{(\gamma^\mu p_\mu - m)\,\psi(p) = 0}$$

what corresponds to the **Dirac equation**.

n.b.: ψ and γ^μ are given here in the so called **chiral** representation (since ϕ_{R} and ϕ_{L} are eigenstates of the chirality operator, what we will see later). The **standard** representation – that we already get to know – results form a similarity transformation:

$$\boxed{\psi_{\mathrm{SR}} = \mathcal{S}\psi_{\mathrm{CR}}\,, \quad \gamma^\mu = \mathcal{S}\gamma^\mu_{\mathrm{CR}}\mathcal{S}^{-1}\,, \quad \text{where } \mathcal{S} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \mathcal{S}^{-1}}$$

$$\psi_{\mathrm{SR}} = \frac{1}{\sqrt{2}}\begin{pmatrix} \phi_{\mathrm{R}} + \phi_{\mathrm{L}} \\ \phi_{\mathrm{R}} - \phi_{\mathrm{L}} \end{pmatrix}$$

$$\gamma^0_{\mathrm{SR}} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\gamma^i_{\mathrm{SR}} = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}$$

For a *particle at rest* this surely yields the more adept representation:

$$\begin{aligned} \psi_{\mathrm{SR}} &= u(0)e^{-\imath mt} && \text{positive energy} \\ \psi_{\mathrm{SR}} &= v(0)e^{+\imath mt} && \text{negative energy}\,, \end{aligned}$$

with the already known 4-spinors:

$$u^1(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad u^2(0) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad v^1(0) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad v^2(0) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

Lorentz boost in moving co-system ($\boldsymbol{\theta} = 0$) in chiral representation:

$$\begin{pmatrix} \phi_{\mathrm{R}} \\ \phi_{\mathrm{L}} \end{pmatrix} \quad \rightarrow \quad \begin{pmatrix} \phi'_{\mathrm{R}} \\ \phi'_{\mathrm{L}} \end{pmatrix} = \underbrace{\begin{pmatrix} e^{\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\phi}} & 0 \\ 0 & e^{-\frac{1}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\phi}} \end{pmatrix}}_{u_{\mathrm{CR}}} \begin{pmatrix} \phi_{\mathrm{R}} \\ \phi_{\mathrm{L}} \end{pmatrix}$$

$\Rightarrow$ Boos matrix in standard representation:

$$u_{\mathrm{SR}} = \mathcal{S} u_{\mathrm{CR}} \mathcal{S}^{-1} = \begin{pmatrix} \cosh\frac{\phi}{2} & \boldsymbol{\sigma}\cdot\mathbf{n}\,\sinh\frac{\phi}{2} \\ \boldsymbol{\sigma}\cdot\mathbf{n}\,\sinh\frac{\phi}{2} & \cosh\frac{\phi}{2} \end{pmatrix}$$

and through

$$\cos\frac{\phi}{2} = \left(\frac{E+m}{2m}\right)^{1/2}, \quad \sin\frac{\phi}{2} = \left(\frac{E-m}{2m}\right)^{1/2}, \quad \tanh\frac{\phi}{2} = \frac{p}{E+m},$$

where $p = \sqrt{E^2 - m^2}$, follows

$$u_{\mathrm{SR}}(p) = \begin{pmatrix} 1 & 0 & \frac{p_z}{E+m} & \frac{p_x - \imath p_y}{E+m} \\ 0 & 1 & \frac{p_x + \imath p_y}{E+m} & \frac{-p_z}{E+m} \\ \frac{p_z}{E+m} & \frac{p_x - \imath p_y}{E+m} & 1 & 0 \\ \frac{p_x + \imath p_y}{E+m} & \frac{-p_z}{E+m} & 0 & 1 \end{pmatrix}.$$

The corresponding spinors *psi* (which are identical with the ones we derived from the explicit solution of the Dirac equation) are given by

$$\begin{aligned} \psi^\alpha(x) &= u^\alpha(p) e^{-\imath px}, \qquad & u^\alpha(p) &= u_{\mathrm{SR}}(p)\, u^\alpha(0) \\ \psi^\alpha(x) &= v^\alpha(p) e^{+\imath px}, \qquad & v^\alpha(p) &= u_{\mathrm{SR}}(p)\, v^\alpha(0) \end{aligned}$$

where $\alpha = 1, 2$, or explicitly written out

$$\boxed{u^1 = N \begin{pmatrix} 1 \\ 0 \\ \frac{p_z}{E+m} \\ \frac{p_x + \imath p_y}{E+m} \end{pmatrix}, \quad u^2 = N \begin{pmatrix} 0 \\ 1 \\ \frac{p_x - \imath p_y}{E+m} \\ \frac{-p_z}{E+m} \end{pmatrix}, \quad v^1 = N \begin{pmatrix} \frac{p_z}{E+m} \\ \frac{p_x + \imath p_y}{E+m} \\ 1 \\ 0 \end{pmatrix}, \quad v^2 = N \begin{pmatrix} \frac{p_x - \imath p_y}{E+m} \\ \frac{-p_z}{E+m} \\ 0 \\ 1 \end{pmatrix},}$$

where the normalization is given by $N = \sqrt{\frac{E+m}{2m}}$, what gives $\bar{u}^\alpha u^\alpha = 1$.

It is

$$\begin{aligned} \bar{u}^\alpha(p)\, u^{\alpha'}(p) &= \delta_{\alpha\alpha'} \\ \bar{v}^\alpha(p)\, v^{\alpha'}(p) &= -\delta_{\alpha\alpha'} \\ \bar{u}^\alpha(p)\, v^{\alpha'}(p) &= 0 \\ u^{\alpha\dagger}(p)\, u^{\alpha'}(p) = v^{\alpha\dagger}(p)\, v^{\alpha'}(p) &= \frac{E}{m}\,\delta_{\alpha\alpha'} \end{aligned}$$

Furthermore u and v satisfy (insertion in the Dirac equation)

$$\begin{aligned}(\gamma^\mu p_\mu - m)\, u(p) &= (\not{p} - m)\, u(p) = 0 \\ (\gamma^\mu p_\mu + m)\, v(p) &= (\not{p} + m)\, v(p) = 0\,,\end{aligned}$$

and the adjoint spinors satisfy

$$\begin{aligned}\bar{u}(p)\,(\gamma^\mu p_\mu - m) &= \bar{u}(p)\,(\not{p} - m) = 0 \\ \bar{v}(p)\,(\gamma^\mu p_\mu + m) &= \bar{v}(p)\,(\not{p} + m) = 0\,.\end{aligned}$$

The operator

$$\boxed{P_+ := \sum_\alpha u^\alpha(p)\bar{u}^\alpha(p)}$$

is a projection operator since

$$\begin{aligned}P_+^2 &= \sum_{\alpha,\beta} u^\alpha(p)\,\underbrace{\bar{u}^\alpha(p)u^\beta(p)}_{=\delta^{\alpha\beta}}\,\bar{u}^\beta(p) \\ &= \sum_\alpha u^\alpha(p)\bar{u}^\alpha(p) = P_+\end{aligned}$$

and projects on states with positive energy. One can show that the operator P_+ can be expressed as

$$P_+ = \frac{\not{p} + m}{2m}\,.$$

Analogous one defines

$$\boxed{P_- := -\sum_\alpha v^\alpha(p)\bar{v}^\alpha(p) = \frac{-\not{p} + m}{2m}}$$

Obviously one has $P_+ + P_- = 1$.

C.1.3 Lorentz covariance of the Dirac equation

When performing a Lorentz transformation from one reference frame I to another reference frame I', the coordinates transform like

$$x' = \Lambda x\,, \qquad \text{i.e. } x = \Lambda^{-1} x$$

and the Dirac spinor according to

$$\psi'(x') = \mathcal{S}(\Lambda)\psi(\Lambda^{-1}x')\,,$$

where the transformation matrix, $S(\Lambda)$, is blockdiagonal in chiral representation:

$$\mathcal{S}(\Lambda) = \begin{pmatrix} D(\Lambda) & 0 \\ 0 & \bar{D}(\Lambda) \end{pmatrix} .$$

The Dirac equation should be *form-invariant* under this Lorentz transformation

$$\boxed{\Big(\imath\gamma^\mu\partial_\mu - m\Big)\,\psi(x) = 0 \quad (\text{in } I) \quad \Longleftrightarrow \quad \Big(\imath\gamma^\mu\partial'_\mu - m\Big)\,\psi'(x') = 0 \quad (\text{in } I')}$$

For the derivation applies

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \frac{\partial x'^\nu}{\partial x^\mu}\frac{\partial}{\partial x'^\nu} = \Lambda^\nu{}_\mu \frac{\partial}{\partial x'^\nu} = \Lambda^\nu{}_\mu \partial'_\nu$$

and with $\mathcal{S}^{-1}\psi'(x') = \psi(x)$ follows for the Dirac equation in the reference frame I:

$$\Big(\imath\gamma^\mu\Lambda^\nu{}_\mu\partial'_\nu - m\Big)\,\mathcal{S}^{-1}(\Lambda)\psi'(x') = 0\,.$$

Multiplying above equation from the left with $\mathcal{S}(\Lambda)$ gives

$$\Big(\imath\mathcal{S}(\Lambda)\gamma^\mu\mathcal{S}^{-1}(\Lambda)\Lambda^\nu{}_\mu\partial'_\nu - mBig)\psi' = 0\,.$$

If $\boxed{\mathcal{S}(\Lambda)\gamma^\mu\mathcal{S}^{-1}(\Lambda) = (\Lambda^{-1})^\mu{}_\tau\gamma^\tau}$, then $\mathcal{S}(\Lambda)\gamma^\mu\mathcal{S}^{-1}(\Lambda)\Lambda^\nu{}_\mu = (\Lambda^{-1})^\mu{}_\tau\Lambda^\nu{}_\mu\gamma^\tau = \gamma^\nu$ and we arrive at the equation of the reference frame I'.

It remains to show that for all Lorentz transformations Λ

$$\boxed{\mathcal{S}^{-1}(\Lambda)\gamma^\mu\mathcal{S}(\Lambda) = \Lambda^\mu{}_\nu\gamma^\nu}$$

$\Big($Note that $\mathcal{S}^{-1}(\Lambda) = \mathcal{S}(\Lambda^{-1})\Big)$

Reminder:

$$\mathcal{S}(\Lambda) = \begin{pmatrix} \exp\Big(\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta} - \imath\boldsymbol{\phi})\Big) & 0 \\ 0 & \exp\Big(\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta} + \imath\boldsymbol{\phi})\Big) \end{pmatrix}$$

Due to the fact that every Lorentz transformation can be composed of 3 Lorentz boosts along the x-, y- and z-axes and 3 rotations about the same 3 axes, we will look at these cases separately.

Lorentz boosts, i.e. $\boldsymbol{\theta} = 0$; w.l.o.g. $\boldsymbol{\phi} = (\phi, 0, 0)$ (boost along the x axis)

$$\Rightarrow \mathcal{S}(\Lambda) = \begin{pmatrix} e^{+\frac{1}{2}\phi\sigma^x} & 0 \\ 0 & e^{-\frac{1}{2}\phi\sigma^x} \end{pmatrix} \quad \text{and} \quad \Lambda = \begin{pmatrix} \cosh\phi & \sinh\phi & 0 & 0 \\ \sinh\phi & \cosh\phi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

Now we have

$$\begin{aligned}
\mathcal{S}^{-1}\gamma^0\mathcal{S} = \mathcal{S}^{-1}\begin{pmatrix}0 & \mathbb{1}\\ \mathbb{1} & 0\end{pmatrix}\mathcal{S} &= \begin{pmatrix}e^{-\frac{1}{2}\phi\sigma^x} & 0\\ 0 & e^{+\frac{1}{2}\phi\sigma^x}\end{pmatrix}\begin{pmatrix}0 & \mathbb{1}\\ \mathbb{1} & 0\end{pmatrix}\begin{pmatrix}e^{+\frac{1}{2}\phi\sigma^x} & 0\\ 0 & e^{-\frac{1}{2}\phi\sigma^x}\end{pmatrix}\\
&= \begin{pmatrix}0 & e^{-\phi\sigma^x}\\ e^{\phi\sigma^x} & 0\end{pmatrix} = \begin{pmatrix}0 & \cosh\,\phi - \sigma^x \sinh\,\phi\\ \cosh\,\phi + \sigma^x\sinh\,\phi & 0\end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
\mathcal{S}^{-1}\gamma^1\mathcal{S} = \mathcal{S}^{-1}\begin{pmatrix}0 & -\sigma^x\\ \sigma^x & 0\end{pmatrix}\mathcal{S} &= \begin{pmatrix}0 & -\sigma^x e^{\phi\sigma^x}\\ \sigma^x e^{\phi\sigma^x} & 0\end{pmatrix}\\
&= \begin{pmatrix}0 & -\sigma^x\Big(\cosh\,\phi - \sigma^x\sinh\,\phi\Big)\\ \sigma^x\Big(\cosh\,\phi + \sigma^x\sinh\,\phi\Big) & 0\end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
\mathcal{S}^{-1}\gamma^{2,3}\mathcal{S} = \mathcal{S}^{-1}\begin{pmatrix}0 & -\sigma^{y,z}\\ \sigma^{y,z} & 0\end{pmatrix}\mathcal{S} &= \begin{pmatrix}0 & -e^{-\frac{1}{2}\phi\sigma^x}\sigma^{y,z}e^{-\frac{1}{2}\phi\sigma^x}\\ e^{\frac{1}{2}\phi\sigma^x}\sigma^{y,z}e^{\frac{1}{2}\phi\sigma^x} & 0\end{pmatrix}\\
&= \begin{pmatrix}0 & -\sigma^{y,z}\\ \sigma^{y,z} & 0\end{pmatrix} = \gamma^{2,3}
\end{aligned}$$

Furthermore we find:

$$\begin{aligned}
\Lambda^0{}_\nu\gamma^\nu &= \cosh\,\phi\gamma^0 + \sinh\,\phi\gamma^1 = \begin{pmatrix}0 & \cosh\,\phi - \sigma^x\sinh\,\phi\\ \cosh\,\phi + \sigma^x\sinh\,\phi & 0\end{pmatrix}\,,\\
\Lambda^1{}_\nu\gamma^\nu &= \sinh\,\phi\gamma^0 + \cosh\,\phi\gamma^1 = \begin{pmatrix}0 & \sinh\,\phi - \sigma^x\; cosh\,\phi\\ \sinh\,\phi + \sigma^x\cosh\,\phi & 0\end{pmatrix}\,,\\
\Lambda^{2,2}{}_\nu\gamma^\nu &= \gamma^{2,3}\,.
\end{aligned}$$

By comparing the left and right side one finds the given identity.

Rotations, i.e. $\boldsymbol{\phi} = 0$, w.l.o.g. $\boldsymbol{\theta} = (\theta, 0, 0)$ (rotation about the x axis). Analogous to previous case one finds

$$\mathcal{S}(\Lambda) = \begin{pmatrix}e^{\frac{i}{2}\theta\sigma^x} & 0\\ 0 & e^{\frac{i}{2}\theta\sigma^x}\end{pmatrix}$$

$$\Lambda = \begin{pmatrix}1 & 0 & 0 & 0\\ 0 & 1 & 0 & 0\\ 0 & 0 & \cos\,\theta & \sin\,\theta\\ 0 & 0 & -\sin\,\theta & \cos\,\theta\end{pmatrix}$$

C.1.4 Transformation behaviour of bilinear forms

We will again use the chiral representation

$$\psi = \begin{pmatrix}\phi_{\mathrm{R}}\\ \phi_{\mathrm{L}}\end{pmatrix}\,,$$

which transforms under Lorentz transformations like

$$\phi_R \longrightarrow \exp\left[\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta}-\imath\boldsymbol{\phi})\right]\phi_R\,; \qquad \phi_L \longrightarrow \exp\left[\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta}+\imath\boldsymbol{\phi})\right]\phi_L$$

$$\rightsquigarrow \quad \phi_R^\dagger \longrightarrow \phi_R^\dagger \exp\left[-\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta}+\imath\boldsymbol{\phi})\right]; \qquad \phi_L^\dagger \longrightarrow \phi_L^\dagger \exp\left[-\frac{\imath}{2}\boldsymbol{\sigma}\cdot(\boldsymbol{\theta}-\imath\boldsymbol{\phi})\right].$$

It is immediately clear that $\psi^\dagger\psi = \phi_R^\dagger\phi_R + \phi_L^\dagger\phi_L$ is *not* invariant. However the **adjoint** spinor has the components

$$\bar{\psi} = \psi^\dagger\gamma^0 = \begin{pmatrix}\phi_R^\dagger & \phi_L^\dagger\end{pmatrix}\begin{pmatrix}0 & \mathbb{1}\\ \mathbb{1} & 0\end{pmatrix} = \begin{pmatrix}\phi_L^\dagger & \phi_R^\dagger\end{pmatrix}$$

and therefore we have that

$$\boxed{\bar{\psi}\psi = \phi_L^\dagger\phi_R + \phi_R^\dagger\phi_L}$$

is invariant under Lorentz transformations (i.e. is "**scalar**").

Furthermore is under parity transformations $\phi_R \leftrightarrow \phi_L$, so that $\bar{\psi}\psi \to \bar{\psi}\psi$, which means that $\bar{\psi}\psi$ is a true scalar, i.e. it does not change it sign under parity transformations.

We now define the 4×4-matrix

$$\boxed{\gamma^5 = \imath\gamma^0\gamma^1\gamma^2\gamma^3 \underset{\text{in chiral repres.}}{=} \begin{pmatrix}\mathbb{1} & 0\\ 0 & -\mathbb{1}\end{pmatrix}.}$$

Then the expression is

$$\bar{\psi}\gamma^5\psi = \begin{pmatrix}\phi_R^\dagger & \phi_L^\dagger\end{pmatrix}\begin{pmatrix}\mathbb{1} & 0\\ 0 & -\mathbb{1}\end{pmatrix}\begin{pmatrix}\phi_R\\ \phi_L\end{pmatrix} = \phi_L^\dagger\phi_R - \phi_R^\dagger\phi_L$$

invariant under Lorentz transformations, but changes its sign under parity transformations, i.e. $\boxed{\bar{\psi}\gamma^5\psi \text{ is a } \textbf{pseudo scalar}}$.

We will now consider the quantity $\boxed{\bar{\psi}\gamma^\mu\psi}$ and show that it behaves like 4-vector under Lorentz transformations

$$\bar{\psi}\gamma^0\psi = \phi_R^\dagger\phi_R + \phi_L^\dagger\phi_L$$

$$\bar{\psi}\gamma^i\psi = \begin{pmatrix}\phi_R^\dagger & \phi_L^\dagger\end{pmatrix}\begin{pmatrix}0 & -\sigma\\ \sigma & 0\end{pmatrix}\begin{pmatrix}\phi_R\\ \phi_L\end{pmatrix} = -\phi_L^\dagger\sigma^i\phi_L + \phi_R^\dagger\sigma^i\phi_R\,.$$

Under spatial rotations ($\boldsymbol{\theta} \neq 0$, $\boldsymbol{\phi} = 0$) we find

$$\bar{\psi}\gamma^0\psi \longrightarrow \bar{\psi}\gamma^0\psi \qquad (*)$$

and for infinitesimal $\boldsymbol{\theta}$

$$\begin{aligned}
\bar{\psi}\boldsymbol{\gamma}\psi \quad \longrightarrow \quad & -\phi_{\mathrm{L}}^{\dagger} e^{-\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}} \boldsymbol{\sigma} e^{\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}} + \phi_{\mathrm{R}}^{\dagger} e^{-\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}} \boldsymbol{\sigma} e^{\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}} \\
=& -\phi_{\mathrm{L}}^{\dagger}\left(1-\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}\right)\boldsymbol{\sigma}\left(1+\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}\right)\phi_{\mathrm{L}} + \phi_{\mathrm{R}}^{\dagger}\left(1-\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}\right)\boldsymbol{\sigma}\left(1+\frac{\imath}{2}\boldsymbol{\sigma}\cdot\boldsymbol{\theta}\right)\phi_{\mathrm{R}} \\
=& -\phi_{\mathrm{L}}^{\dagger}\left(\boldsymbol{\sigma}-\boldsymbol{\theta}\times\boldsymbol{\sigma}\right)\phi_{\mathrm{L}} + \phi_{\mathrm{R}}^{\dagger}\left(\boldsymbol{\sigma}-\boldsymbol{\theta}\times\boldsymbol{\sigma}\right)\phi_{\mathrm{R}} \\
=& \;\; \bar{\psi}\gamma\psi - \boldsymbol{\theta}\times\left(\bar{\psi}\gamma\psi\right) \qquad\qquad (*)
\end{aligned}$$

The above equation $(*)$ describes the behaviour of a vector under rotations. Since the time-component is invariant under rotations due to $(**)$, the expression $\bar{\psi}\gamma^{\mu}\psi$ actually behaves like a 4-vector under rotations.

In a similar fashion one can show that $\bar{\psi}\gamma^{\mu}\psi$ behaves also like a 4-vector under *Lorentz boosts*. Under *parity transformations* one has $\bar{\psi}\gamma^{0}\psi \to \bar{\psi}\gamma^{0}\psi$, but $\bar{\psi}\boldsymbol{\gamma}\psi \to -\bar{\psi}\boldsymbol{\gamma}\psi$, which means we have a **polar** vector, i.e. $\bar{\psi}'(x')\gamma^{\mu}\psi'(x') = \Lambda^{\mu}{}_{\nu}\bar{\psi}(x)\gamma^{\nu}\psi(x)$.

Analogous, $\bar{\psi}\gamma^{\mu}\gamma^{5}\psi$ behaves like an **axial** vector, i.e. like a vector under Lorentz transformations, but under parity transformations one finds $\bar{\psi}\boldsymbol{\gamma}\gamma^{5}\psi \to \bar{\psi}\boldsymbol{\gamma}\gamma^{5}\psi$, i.e. $\bar{\psi}'(x')\gamma^{\mu}\gamma^{5}\psi'(x') \to \Lambda^{\mu}{}_{\nu}\bar{\psi}(x)\gamma^{\nu}\gamma^{5}\psi(x)\cdot\det(\Lambda)$.

We summarize:

- $\bar{\psi}\psi$ — scalar
- $\bar{\psi}\gamma^{5}\psi$ — pseudo scalar
- $\bar{\psi}\gamma^{\mu}\psi$ — polar vector
- $\bar{\psi}\gamma^{\mu}\gamma^{5}\psi$ — axial vector
- $\bar{\psi}(\gamma^{\mu}\gamma^{\nu}-\gamma^{\nu}\gamma^{\mu})\psi$ — antisym. tensor