Advanced Quantum Mechanics

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Contents

Introduction

This script has evolved from lectures in Advanced Quantum Mechanics at the University of Cologne given in the first year of a master's course in physics. It should replace neither one of the excellent books in the field nor the visit of the lecture itself. I would strongly recommend to read a book on advanced quantum mechanics (e.g., books from Sakurai, Schwabl, or Messiah) parallel to this lecture. Scattering theory on the level needed for this lecture is sometimes also covered in more elementary textbooks on quantum mechanics.
The script assumes that you are familiar with standard quantum mechanics as taught worldwide in bachelor courses in physics. This includes topics like the foundations of quantum mechanics, measurement principles, the Dirac notation (bra and ket), atomic physics and perturbation theory.
I would like to thank Richard Altenkirch who typed in a first version of these notes based on my blackboard presentation. The single most important source for the script is probably the book and lecture notes of my colleague Alexander Altland which I used especially in the chapter on second quantization. Thanks also for the input of many students in the summer semester of 2020, which helped to eliminate at least some of the typos.

Note that this is a preliminary version of the script. There has been no proof-reading and there will be many mistakes.

1 Second Quantization

In this chapter you will learn the language of second quantization. This is "the" language of quantum field theory in which we can formulate and describe (almost) all know phenomena in the world around us: the properties of matter, of light and of all known elementary particles. An important exception is quantum gravity: it is presently not clear how the ultimate quantum theory of, e.g., a black holes looks like. While in ordinary quantum mechanics one considers the properties of just a few quantum particles, we will develop the methods to describe many, sometimes an infinite number of particles. Most importantly, we will also be able to formulate a theory of how particles are created and destroyed. This will allow us to describe, e.g., how photons are created and absorbed.

1.1 Concepts of Quantum Mechanics

This section is a brief reminder on the basic structures underlying quantum mechanics. It assumes that you have heard (and understood) all this before.
Probably the single most important concept of quantum mechanics (and quantum field theory) is that the laws of nature are formulated in terms of **probability amplitudes** Ψ written as complex numbers. These are not directly observable but instead $|\Psi|^2$ gives the probability.

$$\Psi \in \mathbb{C}, \quad |\psi|^2 = \text{probability}$$

With this mathematical tool, one can describe the dual nature of quantum particles like the electron: like waves electrons show interference but when measured they can be viewed as a point-like particle. **Superposition**, i.e. the addition of probability amplitudes naturally leads to **interference**.

$$|\underbrace{\psi_1 + \psi_2}_{\text{linear theory}}|^2 = |\psi_1|^2 + |\psi_2|^2 + 2|\psi_1||\psi_2| \cdot \cos(\varphi_1 - \varphi_2) \quad \text{with:} \quad \psi_i = |\psi| e^{i\varphi_i}$$

The natural mathematical structure describing probability amplitudes, their addition and calculating the probabilities by taking the modulus square is the **Hilbert space**.[1] Therefore we describe a quantum mechanical **state** by a vector in a Hilbert space.

state = vector in Hilbert-space, $|\psi\rangle \in \mathcal{H}$

[1] Do you recall the definition of a Hilbert space and its scalar product? If not look it up!

Two simple examples are

i) QBit: $|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle = \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \in \mathbb{C}$

ii) wavefunction: $\psi : \mathbb{R}^3 \to \mathbb{C}$,

scalar product: $\langle\psi|\ \Phi\rangle = \int \psi^*(\vec{r})\,\Phi(\vec{r})\ \mathrm{d}^3 r$

After having decided how to describe states, the next step is to find out how properties of a states are measured. For this we have to identify which mathematical structure describes **observables**.

observable = linear, hermitian *operators* with $A = (A^*)^T = A^\dagger$

Some examples are

i) $\vec{S} = \frac{\hbar}{2}\vec{\sigma}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},\ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

for: $\mathcal{H} = \mathbb{C}^2$

ii) $\vec{p} = -i\,\hbar\vec{\nabla}$

But how can we obtain the result of a measurement? The answer is that in a (idealized) **measurement**

In an idealized measurements the *eigenvalues* $\alpha_n \in \mathbb{R}$ of the observables, $A\,|\psi_{n,i}\rangle = \alpha_n\,|\psi_{n,i}\rangle \quad i = 1, \ldots, m$ can be measured. Thereby, the eigenvalue α_n is measured with the probability

$$p_n = \sum_{i=1,\ldots,m} |\,\langle\psi_{ni}|\ \psi\rangle\,|^2 \qquad \text{, for } \langle\psi|\ \psi\rangle = 1\ \ \langle\psi_{n,i}|\ \psi_{n,j}\rangle = \delta_{ij}$$

By repeating these measurements one obtains the **expectation value**

$$\begin{aligned} \langle A\rangle &= \sum \alpha_n p_n = \sum \langle\psi|\ \psi_{ni}\rangle\,\langle\psi_{ni}|\,A\,|\psi_{ni}\rangle\,\langle\psi_{ni}|\ \psi\rangle \\ &= \sum \langle\psi|\ \psi_{mj}\rangle\,\langle\psi_{mj}|\,A\,|\psi_{ni}\rangle\,\langle\psi_{ni}|\ \psi\rangle = \langle\psi|\,A\,|\psi\rangle \end{aligned}$$

For example, consider

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{eigenvalue: } \pm\frac{\hbar}{2} \qquad \text{eigenvector: } \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

for $|\psi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ one measures $-\frac{\hbar}{2}$ with probability $\left|\frac{1}{\sqrt{2}}\,(1,-1)\,\binom{1}{0}\right|^2 = 50\%$

Above, we have described a highly idealized quantum mechanical measurement. Here one should emphasize that in practice most measurements done in experimental labs (e.g., measuring the resistance of a piece of metal) cannot be described in such terms. One can, nevertheless, use the above described concepts as a starting point to develop a theory of measurement. In many cases it turns out that macroscopic measurements can be described by certain expectation values (more precisely by correlation functions). This is a topic which is not captured in this lecture (in Cologne this topic is covered in the quantum field theory course).

An interesting question is how the state of a system is described *after* an idealized quantum measurement. Effectively, this can be described by the **collapse of the wave function**

after measurment of eigenvalue α_n: $\left|\tilde{\psi}\right\rangle = c\sum_i |\psi_{n,i}\rangle \langle\psi_{n,i}| \, \psi\rangle$,

c: normalisation

Note that the collapse of the wave function is a non-linear process, very different from all other laws of quantum mechanics where all evolution is always linear. One can actually avoid to use the collapse of the wave function when one is willing to include the observer (i.e. the experimental apparatus) in the quantum mechanical description. This approach is usually called "many-world interpretation" of quantum mechanics (a quite misleading term).

Above, we have found out how states and measurements are described. The missing element is the **time-evolution** of states which is governed by the

Schrödinger-equation: $i\hbar\partial_t |\psi(t)\rangle = H |\psi(t)\rangle$

H is the **Hamiltonian** which is hermitian, $H = H^\dagger$

A well known example is the single particle Hamiltonian

$$H = \frac{p^2}{2\,m} + V(\vec{r})$$

1.2 Identical particles

Our next goal will be to develop the quantum mechanics of many particles starting from the quantum mechanical description of a single particle. The key element of the following discussion will be to think about a deep question: Can one in principle distinguish one electron from another electron? And, if not, how is this reflected in their quantum mechanical description?

We start with a single particle whose state are elements of the Hilbert space $\mathbb{H}_1$. For the following, it will be useful to define a **basis** of $\mathbb{H}_1$. We therefore introduce

1-particle Hilbert-space $\mathbb{H}_1$ with basis $|\alpha_i\rangle$ or $\psi_i(r)$

An arbitrary wave function of the single particle is written a s a linear superposition of basis vectors, $|\Psi\rangle = \sum_i c_i |\alpha_i\rangle$ or $\Psi(r) = \sum c_i \psi_i(r)$.

These concepts are easily generalized to n quantum particles if they are *distinguishable* (e.g, one electron, one proton and one neutron). Then the wavefunction $\psi(r_1, r_2, \ldots, r_n)$ describes the quantum mechanical amplitude that particle k is at position r_k. Expressed in terms of the one-particle eigenfunctions this can be written as

$$\begin{aligned} \psi(r_1, r_2, \ldots, r_n) &= \sum c_{j_1,j_2,\ldots,j_n} \Psi_{j_1}(r_1)\Psi_{j_2}(r_2)\ldots\Psi_{j_n}(r_n) \\ |\psi\rangle &= \sum c_{j_1,j_2,\ldots,j_n} \underbrace{|\alpha_{j_1}\rangle\,|\alpha_{j_2}\rangle\ldots|\alpha_{j_n}\rangle}_{\text{particle k in state}|\alpha_{j_k}\rangle} \end{aligned}$$

The Hilbert space $\mathbb{H}_n^d$ of n *distinguishable* particles is therefore given by the product of n one-particle Hilbert spaces $\mathbb{H}_1$

n-distinguishable particles: $\mathbb{H}_n^d = \mathbb{H}_1 \otimes \mathbb{H}_1 \otimes \ldots \otimes \mathbb{H}_1$

In recent years it has been more and more realized that thinking about quantum mechanics and quantum field theory from the perspective of quantum information theory has proven to be extremely useful. By asking, for example, the question what information can be encoded in quantum states and how precisely a quantum state differs from a classical state, one can learn a lot about quantum physics and about the question of how to solve quantum mechanical problems. We will now encounter an early example of how useful this type of approach is by considering the description of indistinguishable particles.
As one electrons - as a matter of principle - cannot be distinguished from another electron, we have to include this property into our quantum mechanical description. Consider two indistinguishable particles. For those we have to postulate that $\psi(r_1, r_2)$ and $\psi(r_2, r_1)$ *have to describe the same state.* To formulate this property formally, we introduce the permutation operator, P_{ij} which exchanges particle i and particle j.

$$P_{ij}\Psi(r_1, ..., r_i, ...r_j, ...) = \Psi(r_1, ..., r_j, ...r_i, ...)$$

For identical particles we postulate

$$P_{ij}\psi = \psi \cdot \underbrace{e^{i\varphi}}_{\substack{\text{not} \\ \text{observable}}}$$

as multiplying a wave function by a global phase provides the same quantum state.
When we assume furthermore that $P_{ij}P_{ij} = \mathbb{1}$, we obtain

$$P_{ij}^2\psi = \underbrace{e^{i2\varphi}}_{=1}\psi \quad \rightarrow e^{i\varphi} = \pm 1$$

.
Nature has realized both of these option! One obtains

two types of particles:
"bosons" $e^{i\varphi} = 1 \Rightarrow \quad \psi(r_1, r_2) = \psi(r_2, r_1)$ symmetric
"fermions" $e^{i\varphi} = -1 \Rightarrow \quad \psi(r_1, r_2) = -\psi(r_2, r_1)$ antisymmetric

For the descriptions of two bosons (fermions) only symmetric (antisymmetric) wave functions are allowed. Electrons, protons, neutrons are all fermions, while photons, pions or the newly discovered Higgs particle are bosons.

note:

- in 2-dim also $e^{i\varphi} \neq \pm 1$ is possible (so-called *anyons*) or more exotic representations of permutation group
- causality & Lorentz invariance in 3-dimensions results in the spin-statistics theorem: bosons have integer $(0, 1, 2, \ldots)$, fermions half integer spin $(1/2, 3/2, 5/2, \ldots)$. We will not prove this statement. Note that it is not relevant for non-Lorentz-invariant matter, e.g. excitations in a solid.

For a definition of the Hilbert space we consider S_N, the set of all permutations P of n particles with:

$P = P_{i_1,j_1} P_{i_2,j_2} \ldots P_{i_m,j_m}$ and $(-1)^P = (-1)^m = \begin{cases} -1 & \text{odd number of permutations} \\ 1 & \text{even number} \qquad " \end{cases}$

Starting from the Hilbert space $\mathbb{H}_n^d$ of n distinguishable particles, we can introduce the Hilbert space of n bosons or n fermions by allowing only the symmetric or antisymmetric states.

symmetric n-particles Hilbert-space for n **bosons**:
$\mathbb{H}_n^S = \left\{ |\psi\rangle \in \mathbb{H}_n^d \mid P|\psi\rangle = |\psi\rangle \quad \forall P \in S_n \right\}$

antisymmetric Hilbert-space for n **fermions**:
$\mathbb{H}_n^A = \left\{ |\psi\rangle \in \mathbb{H}_n^d \mid P|\psi\rangle = (-1)^P |\psi\rangle \quad \forall P \in S_n \right\}$

A direct consequence is the **Pauli-principle**: 2 Fermions cannot occupy same state as such a state is not part of the Hilbert space:
$|\psi\rangle \in \mathbb{H}^A \qquad P_{12}|\alpha\rangle|\alpha\rangle = |\alpha\rangle|\alpha\rangle \neq -|\alpha\rangle|\alpha\rangle \notin \mathbb{H}^A$
One way to write down a completely antisymmetric wave function of N electrons occupying N single particle states, $\alpha_1, \ldots, \alpha_N$, is the so-called **Slater determinant**.

$$det \begin{vmatrix} \psi_{\alpha_1}(r_1) & \psi_{\alpha_1}(r_2) & \ldots & \psi_{\alpha_1}(r_N) \\ \psi_{\alpha_2}(r_1) & \psi_{\alpha_2}(r_2) & \ldots & \psi_{\alpha_2}(r_N) \\ \vdots & \ddots & \ddots & \vdots \\ \psi_{\alpha_N}(r_1) & \ldots & \ldots & \psi_{\alpha_N}(r_N) \end{vmatrix} \in \mathbb{H}_N^A$$

Here one uses that the determinant by definition produces something completely antisymmetric. Starting from a given single-particle basis $\Psi_{\alpha_i}(r)$ one can use the slater determinants to build a basis of the N particle fermionic Hilbert space $\mathbb{H}_N^A$.

For $N = 2$ one obtains

$$\psi_{\alpha_1}(r_1)\psi_{\alpha_2}(r_2) - \psi_{\alpha_2}(r_1)\psi_{\alpha_1}(r_2).$$

For a gold atom with $N = 79$ electrons, one would have to write

$$79! \approx 10^{117}$$

terms, clearly not a good idea! We will therefore **not** use Slater determinants in the following but will be looking for something more physical and more easy to handle.

1.3 Creation and Annihilation operators

1.3.1 Fock space

We have learned that describing N identical particle by a wave function $\psi(r_1, \ldots, r_N)$ is clearly not a good idea. What to do instead?

- We want to use $\mathbb{H}^{A/S}$ directly (never using $\psi(r_1, \ldots, r_N)$)
- The main idea is that we will **just count** how frequently a given quantum state is occupied. Counting is the only meaningful thing to do for indistinguishable particle.

This simple idea is most easily understood by doing simple examples.
Consider the single-particle Hilbert space $\mathbb{H}_1$ with the basis $\{|\alpha_1\rangle, |\alpha_2\rangle, |\alpha_3\rangle\}$ and corresponding wave functions $\psi_{\alpha_i}(r) = \langle r| \alpha_i\rangle$. To describe the state with 2 bosons in the first state, none in the second state, and 2 in the third state, we can use the following simple notation:

$$|2, 0, 2\rangle$$

. This is much shorter than writing the totally symmetric wave function

$$\begin{aligned}\frac{1}{\sqrt{6}}[&\Psi_{\alpha_1}(r_1)\Psi_{\alpha_1}(r_2)\Psi_{\alpha_3}(r_3)\Psi_{\alpha_3}(r_4) + \Psi_{\alpha_1}(r_1)\Psi_{\alpha_1}(r_3)\Psi_{\alpha_3}(r_2)\Psi_{\alpha_3}(r_4)\\ &+ \Psi_{\alpha_1}(r_1)\Psi_{\alpha_1}(r_4)\Psi_{\alpha_3}(r_2)\Psi_{\alpha_3}(r_3) + \Psi_{\alpha_1}(r_2)\Psi_{\alpha_1}(r_3)\Psi_{\alpha_3}(r_1)\Psi_{\alpha_3}(r_4)\\ &+ \Psi_{\alpha_1}(r_2)\Psi_{\alpha_1}(r_4)\Psi_{\alpha_3}(r_1)\Psi_{\alpha_3}(r_3) + \Psi_{\alpha_1}(r_3)\Psi_{\alpha_1}(r_4)\Psi_{\alpha_3}(r_1)\Psi_{\alpha_3}(r_2)]\end{aligned}$$

Similarly, for one fermion in the first, and one in the third state we write

$$\begin{aligned}|1, 0, 1\rangle &\hat{=} \frac{1}{\sqrt{2}}\left(|\alpha_1\rangle\,|\alpha_3\rangle - |\alpha_3\rangle\,|\alpha_1\rangle\right)\\ &\hat{=} \frac{1}{\sqrt{2}}\left(\psi_{\alpha_1}(r_1)\psi_{\alpha_3}(r_2) - \psi_{\alpha_1}(r_2)\psi_{\alpha_3}(r_1)\right)\end{aligned}$$

To formalize this, we first combine the Hilbert spaces of 0, 1, 2, ... particles to one large Hilbert space, the so-called Fock space

$$\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \dots$$
$$\text{with} \quad \mathcal{F}_n = \begin{cases} \mathbb{H}_n^S & \text{for Bosons} \\ \mathbb{H}_n^A & \text{for Fermions} \end{cases}$$

with: $\mathcal{F}_0$ = 1-dim Hilbert-space with basis $|0\rangle = |0, 0, \dots, 0\rangle$
$\hat{=}$ no particle present = vacuum state

To define a basis in this Hilbert space, we start from a **given single-particle basis**. By counting how often each state is occupied, we obtain

Basis in *Fock-space*: $|n_1, n_2, n_3, \dots\rangle \in \mathbb{F}$
defined for given single-particle basis $\{|\alpha_1\rangle, |\alpha_2\rangle, \dots\}$ of the *single-particle* Hilbert space $\mathbb{H}_1$
with $n_i \in \mathbb{N}_0$ for bosons or $n_i \in \{0, 1\}$ for fermions

Then an arbitrary wave function in $\mathcal{F}$ takes the form

$$|\psi\rangle = \sum_{n_i} c_{n_1,n_2,\dots} |n_1, n_1, \dots\rangle$$

This result is a major achievement. We have not only found a very economic way to write N-particle wave functions but also found a way to describe superposition of states with different particle number which was not possible in the old first-quantized quantum mechanics. This will be important to describe things like photons, superconductivity or antiparticles as we will see.

1.3.2 Creation & Annihilation

We have found out that simple counting is the best way to describe indistinguishable particles. What is left is that we have to learn how to add and subtract using operators. There is one problem in your first quantum mechanics course, where you had precisely learned how to do this. Remember the solution of the harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

To solve this problem algebraically, one can use a simple trick. One defines "raising" and "lowering" operators

$$a^\dagger = \sqrt{\frac{m\omega}{2}} \left(x - \frac{i}{m\omega} p \right), a = \sqrt{\frac{m\omega}{2}} \left(x + \frac{i}{m\omega} p \right),$$
$$\hat{N} = a^\dagger a, \text{ eigenvalue of } \hat{N} = 0, 1, 2, \dots \text{ (counting)}$$

Then $H = \hbar\omega\left(\hat{N} + \frac{1}{2}\right)$ where the operator $\hat{N} = a^\dagger a$ has eigenvalues $0, 1, 2, \ldots$ and is therefore ideally suited for counting. Based on the eigenstates of $\hat{N}$, one obtains in this case an algebra of counting

$$\begin{aligned}
&\hat{N}\,|n\rangle = n\,|n\rangle \\
&a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle && \text{adding 1} \\
&a\,|n\rangle = \sqrt{n}\,|n-1\rangle && \text{substraction 1}
\end{aligned}$$

In the case of the harmonic oscillator this was just a convenient trick to solve the problem. Now we want to use this math (not the physics) to count indistinguishable particles.
We therefore *define* operators, which describe adding and subtracting one particle, i.e., we define creation and annihiliation operators. We thereby have to know, how these operators act on the basis $|n_1, n_2, \ldots\rangle$ of the Fock space (defined by counting particles in a given single particle basis).

Definition: creation & annihilation operators

bosons: $a_i^\dagger\,|n_1, \ldots, n_i, \ldots\rangle \equiv \sqrt{n_i+1}\,|n_1, \ldots, n_i+1, \ldots\rangle$

fermions: $a_i^\dagger\,|n_1, \ldots, 1, \ldots\rangle = 0$

$a_i^\dagger\,|n_1, \ldots, 0, \ldots\rangle = (-1)^{\sum_{j<i} n_j}\,|n_1, \ldots, 1, \ldots\rangle$

annihilation operator: $a_i = \left(a_1^\dagger\right)^\dagger \qquad \left(\langle\varphi|\,a_i\,|\psi\rangle = \langle\psi|\,a_i^\dagger\,|\varphi\rangle^*\right)$

bosons: $a_i\,|n_1, \ldots, n_i, \ldots\rangle \equiv \sqrt{n_i}\,|n_1, \ldots, n_i-1, \ldots\rangle$

fermions: $a_i\,|n_1, \ldots, 0, \ldots\rangle = 0$

$a_i\,|n_1, \ldots, 1, \ldots\rangle = (-1)^{\sum_{j<i} n_j}\,|n_1, \ldots, 0, \ldots\rangle$

For bosons, we just copied the definition from the harmonic oscillator. For fermions, the fact that $a^\dagger\,|1\rangle = 0$ is enforced by the constraint that only $n = \{0, 1\}$ are allowed elements of the Fock space. Less obvious is the factor $(-1)^{\sum_{j<i} n_j}$. As we will see below, it encodes the Pauli principle and is needed to obtain simple rules to do calculations with the fermionic creation and annihilation operators.
As we have learned to raise the number of particles by one, we can now build the basis of the Hilbert space just starting from the vacuum, the state without any particles.

for bosons & fermions:

$$\begin{aligned}
&\text{vacuum: } |0\rangle = |0, 0, 0, \ldots\rangle \quad \text{with; } a_i\,|0\rangle = 0\ \forall a_i \\
&|n_1, n_2, \ldots\rangle = \prod_i \frac{1}{\sqrt{n!}}\left(a_i^\dagger\right)^{n_i}|0\rangle
\end{aligned} \tag{1.1}$$

For fermions the order or operator matters - here we use the convention that one starts from the right with $i = 0$.
Later, all calculations will be based on the creation and annihilation operators. It is therefore important to work out the rules for these calculation, i.e., the **algebra of $\mathbf{a_i^\dagger, a_i}$** which directly follows form the definitions given above.

$$
\begin{aligned}
\textbf{bosons:}\quad i \neq j \qquad & a_i^\dagger a_j^\dagger = a_j^\dagger a_i^\dagger \mathrel{\hat{=}} \text{ sym. wave function} \\
& a_i^\dagger a_j = a_j a_i^\dagger \\
i = j \qquad & \left(a_i a_i^\dagger - a_i^\dagger a_i\right) |n_1, \ldots, n_i, \ldots\rangle = \\
& = \left(\underbrace{\left(\sqrt{n_i + 1}\right)^2 - \left(\sqrt{n_i}\right)^2}_{=1} \right) |n_1, \ldots, n_i, \ldots\rangle
\end{aligned}
$$

These rules can be written in a compact way using the commutator:

commutator: $\quad [A, B] = AB - BA$

We obtain

bosonic commutation relations:

$$
\begin{aligned}
[a_i, a_j^\dagger] &= \delta_{ij} \\
[a_i^\dagger, a_j^\dagger] &= [a_i, a_j] = 0
\end{aligned}
\tag{1.2}
$$

For fermions we find instead

$$
\begin{aligned}
\textbf{fermions:}\quad i \neq j \qquad & a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger \quad \text{due to } (-1)^{\sum_{j<i} n_i} \mathrel{\hat{=}} \text{antisym wave function} \\
& a_i^\dagger a_j^\dagger |0\rangle = -a_j^\dagger a_i^\dagger |0\rangle \\
i = j \qquad & a_i^\dagger a_i |\ldots, n_i, \ldots\rangle = n_i |\ldots, n_i, \ldots\rangle \\
& a_i a_i^\dagger |\ldots, n_i, \ldots\rangle = (1 - n_i) |\ldots, n_i, \ldots\rangle
\end{aligned}
$$

Defining

anticommutator: $\quad \{A, B\} = AB + BA$

we can write in a compact way

fermionic commutation relations:

$$
\begin{aligned}
\{a_i, a_j^\dagger\} &= \delta_{ij} \\
\{a_i^\dagger, a_j^\dagger\} &= \{a_i, a_j\} = 0
\end{aligned}
\tag{1.3}
$$

Some important consequences are:

$\hat{n}_i = a_i^\dagger a_i$ count particles (for both bosons & fermions)

as $\hat{n}_i \,|\ldots, n_i, \ldots\rangle = n_i \,|\ldots, n_i, \ldots\rangle$. As a consequence, one obtains $\hat{n}_i a_i^\dagger \,|\ldots, n_i, \ldots\rangle = a_i^\dagger \,(n_i + 1) \,|\ldots, n_i, \ldots\rangle$ as $a_i^\dagger$ raises the particle number by 1. These results can be written in the form (counting algebra)

$$\left.\begin{aligned} [\hat{n}_i, a_i^\dagger] &= a_i^\dagger \\ [\hat{n}_i, a_i] &= -a_i \end{aligned}\right\} \text{bosons \& fermions} \tag{1.4}$$

This formula expresses in a compact way all properties needed for counting. Please check that starting from this equation, one can derive that $a_i^\dagger$ raises $\hat{n}_i$ by an integer.
Let us check Eq. (1.4) for fermions: $[a_i^\dagger a_i \ , \ a_i^\dagger] = a_i^\dagger a_i a_i^\dagger - a_i^\dagger a_i^\dagger a_i$. To simplify such an expression, one usually performs a procedure called **normal ordering**. Here one moves creation operators to the left and destruction operators to the right using the commutation relations. $a_i^\dagger a_i a_i^\dagger - a_i^\dagger a_i^\dagger a_i \underbrace{=}_{\substack{\{a_i a_i^\dagger\}=1 \\ a_i a_i^\dagger + a_i^\dagger a_i = 1}} a_i^\dagger - \underbrace{a_i^\dagger a_i^\dagger}_{=0} a_i - \underbrace{a_i^\dagger a_i^\dagger}_{=0} a_i = a_i^\dagger$.

Here we used that $\{a_i^\dagger, a_j^\dagger\} = 0 \underset{i=j}{\Longrightarrow} a_i^\dagger a_i^\dagger + a_i^\dagger a_i^\dagger = 0 \Longrightarrow \left(a_i^\dagger\right)^2 = 0$, reflecting again the Pauli principle.

Concluding remarks: The logic of the previous chapter was that we started from the definition of Fock space, then defined creation & annihilation operators and obtained finally their commutation relations and the rules for counting expressed in Eq. (1.4). An alternative (and, perhaps, deeper) approach is the reverse order: One can start by asking the question, how one can realize "counting" (and therefore Eq. (1.4)) on the operator level. Two realizations are the bosonic and fermionic commutation relations, (1.2) and (1.3). Postulating the existence of a vacuum state, one can then build up the Hilbert space as in Eq. (1.1).

1.4 Operators in Fock-space

In this chapter we will learn the essence of second quantization: we express all types of operators (including the Hamiltonian) in creation and annihiliation operators. We will furthermore see what quantum fields are.

1.4.1 Basis change

We have defined the basis of the Fock space and therefore also the creation operator $a_\lambda^\dagger$ relative to a *given* single particle basis $|\lambda\rangle$, $|\lambda\rangle = a_\lambda^\dagger |0\rangle$ and λ denotes a set of quantum numbers (you can think of $\lambda = 1, 2, \ldots$ just enumerating the basis vectors). For the following, it will be important to learn how to change this basis. We denote the vectors of

the new basis by $|\tilde{\lambda}\rangle$ and express them in terms of the old basis vectors $|\lambda\rangle$ using

$$|\tilde{\lambda}\rangle = \underbrace{\sum_{\lambda} |\lambda\rangle \langle\lambda|}_{=\mathbb{1}} \tilde{\lambda}\rangle = \sum_{\lambda} U_{\tilde{\lambda}\lambda} |\lambda\rangle$$

where $U_{\tilde{\lambda}\lambda} = \langle\lambda| \tilde{\lambda}\rangle$ is a unitary matrix.
For the changed basis, we want to define a new creation operator $\tilde{a}^\dagger_{\tilde{\lambda}}$ such that $|\tilde{\lambda}\rangle = \tilde{a}^\dagger_{\tilde{\lambda}} |0\rangle = \sum_{\lambda} U_{\tilde{\lambda}\lambda} a^\dagger_\lambda |0\rangle$. Therefore the old and new operators have to be related in the following way

$$\tilde{a}^\dagger_{\tilde{\lambda}} = \sum_{\lambda} U_{\tilde{\lambda}\lambda} a^\dagger_\lambda = \sum_{\lambda} \langle\lambda| \tilde{\lambda}\rangle a^\dagger_\lambda$$
$$\tilde{a}_{\tilde{\lambda}} = \left(\tilde{a}^\dagger_{\tilde{\lambda}}\right)^\dagger = \sum_{\lambda} \langle\tilde{\lambda}| \lambda\rangle a_\lambda$$

We should check that the new operators fulfill the same commutation relations as the old one. For fermions, e.g., we find

$$\left\{\tilde{a}^\dagger_{\tilde{\lambda}_1},\, \tilde{a}_{\tilde{\lambda}_2}\right\} = \sum_{\lambda\lambda'} \langle\lambda \left|\tilde{\lambda}_1\right\rangle \left\langle\tilde{\lambda}_2\right| \lambda'\rangle \underbrace{\left\{a^\dagger_\lambda,\, a_{\lambda'}\right\}}_{=\delta_{\lambda\lambda'}} = \sum_{\lambda} \left\langle\tilde{\lambda}_2\right| \lambda\rangle \langle\lambda \left|\tilde{\lambda}_1\right\rangle = \langle\tilde{\lambda}_2|\tilde{\lambda}_1\rangle = \delta_{\tilde{\lambda}'\tilde{\lambda}}$$

1.4.2 Field operator in real- & momentum-space

After having learnt how to change a basis, we will discuss two special basis sets which play an important role when formulating quantum field theory: the real-space and the momentum-space basis.
The single-particle state $|\vec{x}\rangle$ describes a particle with wave function $\Psi(\vec{r}) = \delta^3(\vec{r} - \vec{x})$ localized at point $\vec{x}$. The overlap to another wave function is given by

$$\langle\vec{x}| \varphi\rangle = \int \delta(\vec{r} - \vec{x})\, \varphi(\vec{r})\, \mathrm{d}^3 r = \phi(\vec{x})$$

and therefore one also obtains

$$\langle\vec{x}| \vec{x'}\rangle = \int \delta(\vec{r} - \vec{x})\ \delta\left(\vec{r} - \vec{x}'\right) \mathrm{d}^3 r = \delta\left(\vec{x} - \vec{x}'\right).$$

We use this to define the **field operator** $\Psi^\dagger(\vec{x})$, which creates a particle located at point $\vec{x}$. We can, e.g., use the formulas from the previous chapter to obtain

$$\Psi^\dagger(\vec{x}) = \sum_{\lambda} \langle\lambda\, |\vec{x}\rangle a^\dagger_\lambda, \qquad a^\dagger_\lambda = \int \langle\vec{x}|\, \lambda\rangle\, \Psi^\dagger(\vec{x}) \mathrm{d}^3\vec{x} \tag{1.5}$$

Repeating the last calculation of the previous section, we obtain directly the commutation relations

$$\text{fermions:} \quad \left\{\Psi(\vec{x}),\ \Psi^\dagger(\vec{x}')\right\} = \langle\vec{x}|\vec{x}'\rangle = \delta^3(\vec{x}-\vec{x}')$$
$$\text{bosons:} \quad \left[\Psi(\vec{x}),\ \Psi^\dagger(\vec{x}')\right] = \langle\vec{x}|\vec{x}'\rangle = \delta^3(\vec{x}-\vec{x}')$$

Note that $\Psi(\vec{x})$ is an *operator* but **not** a wave function and also $\vec{x}$ is just a label **not** an operator. $\Psi(\vec{x})$ is example of a **quantum field**, i.e., a real-space operator destroying (or creationg) a particle. Later we will see that also other fields, like the electric or magnetic field. $\vec{E}(\vec{r})$, $\vec{B}(\vec{r})$, should be viewed as quantum fields.

Let us practice this a new notation. How can we obtain a single particle with wave function $\varphi(\vec{r})$ using the field operator $\Psi^\dagger(\vec{x})$? The following formula gives the answer:

$$|\varphi\rangle = \int \mathrm{d}^3x\, \varphi(\vec{x})\, \Psi^\dagger(\vec{x})\ |0\rangle$$

This should be read from right to left: We start with the vacuum state, then we create a linear superpostion of particles located at point $\vec{x}$ weighted with the wave function $\varphi(\vec{x})$. The result is the desired state.

To check this, let us calculate $\varphi(\vec{x}_0) = \langle\vec{x}_0|\varphi\rangle$ using that $|x_0\rangle = \Psi^\dagger(x_0)\,|0\rangle$. We therefore obtain

$$\langle x_0|\ \varphi\rangle = \langle 0|\ \Psi(x_0) \int \mathrm{d}^3x\, \varphi(x)\, \Psi^\dagger(x)\ |0\rangle$$

To proceed, we use a standard trick: *normal ordering*, i.e., we move all annihilation operators to the right. For this we need the anticommutation relation $\Psi(x_0)\Psi^\dagger(x) + \Psi^\dagger(x)\Psi(x_0) = \delta^3(\vec{x}-\vec{x}_0)$ and then $\Psi(x_0)\,|0\rangle = 0$ to eliminate the second term.

$$\langle x_0|\ \varphi\rangle = \langle 0| \int \mathrm{d}^3x\, \delta^3(\vec{x}-\vec{x}_0)\, \varphi(\vec{x})\,|0\rangle - \underbrace{0}_{\Psi(x_0)|0\rangle=0} = \varphi(x_0)\,\langle 0|\ 0\rangle = \varphi(x_0)$$

Momentum space: Besides field operators in position space, also operators which generate a particle in a momentum eigenstate are very useful. Momentum eigenstates are just plane waves, $e^{i\vec{k}\vec{x}}$. To normalize those, we consider a 3-dimensional box of length L with periodic boundary conditions. In this case only discreet momenta, $\vec{k} = (k_x, k_y, k_z)$, are allowed with

$$k_i = \frac{2\pi}{L}\, n_i = \Delta K n_i \qquad i = x, y, z, \quad n_i \in \mathbb{Z}$$

We normalize the single-particle eigenstates with

$$\left\langle \vec{k}_n \middle|\ \vec{k}_m \right\rangle = \delta_{\vec{K}_n, \vec{K}_m}$$

and therefore have

$$\langle\vec{x}|\,\vec{k}_n\rangle = \frac{1}{\sqrt{V}} e^{i\vec{k}_n\vec{x}}$$

where $V = L^3$ is the volume of the box.
Using the previously obtained relation (1.5), we can define the creation operator in momentum space using the position-space field operators

$$c_{\vec{k}}^\dagger = \int \frac{e^{i\vec{k}\vec{x}}}{\sqrt{V}} \Psi^\dagger(\vec{x}) \mathrm{d}^3x \qquad \Psi^\dagger(x) = \sum_{\vec{k}} \frac{e^{-i\vec{k}\vec{x}}}{\sqrt{V}} c_{\vec{k}}^\dagger \tag{1.6}$$

Here, $c_{\vec{k}}^\dagger$ creates a particle with momentum $\hbar\vec{k}$.
As we have normalized the eigenstates to 1, we obtain the usual commutation relations

$$\begin{aligned} \text{fermions:} \quad & \left\{c_K,\ c_{K'}^\dagger\right\} = \delta_{KK'} \\ \text{bosons:} \quad & \left[c_K,\ c_{K'}^\dagger\right] = \delta_{KK'} \end{aligned} \tag{1.7}$$

In the following, we will often use the limit of an infinite box $L, V \to \infty$. In this case it is useful to derive a few simple relations of sums and integrals. In one dimension, the sum over all discreet momenta $k_n = n\Delta k$ can be written as $\sum_{k_n} \cdots = \frac{1}{\Delta k} \sum_{k_n} \Delta k \ldots$ which for $L \to \infty$ gives the integral $L \int \frac{dk}{2\pi} \ldots$ as $\Delta k = 2\pi/L$. Correspondingly, we have in $d = 3$

$$\sum_{\vec{k}} \cdots = V \int \frac{\mathrm{d}^3\,\vec{k}}{(2\pi)^3} \cdots$$

The total number of particles, for example, can be written for $V \to \infty$ as

$$N = \sum_{\vec{K}} c_{\vec{K}}^\dagger c_{\vec{K}} = V \int \frac{\mathrm{d}^3\,K}{(2\pi)^3} c_{\vec{K}}^\dagger c_{\vec{K}} = \int \Psi^\dagger(\vec{x}) \Psi(\vec{x}) \mathrm{d}^3x$$

and we can write Eq. (1.6) as

$$\Psi^\dagger(\vec{x}) = \sqrt{V} \int \frac{d^3\vec{k}}{(2\pi)^3} e^{-i\vec{k}\vec{x}} c_{\vec{k}}^\dagger$$

In a number of books different conventions for the normalization of momentum states are used. To translate various conventions it is useful to rewrite the commutation relations (1.7) in the continuum. Using $\frac{1}{V} \int e^{i(\vec{k}-\vec{k}')\vec{x}} d^3x = \delta_{\vec{k}\vec{k}'}$, we can write for $V \to \infty$

$$\left\{c_{\vec{k}},\ c_{\vec{k}'}^\dagger\right\} = \delta_{\vec{k},\vec{k}'} = \frac{1}{V} \underbrace{\int e^{i(\vec{k}-\vec{k}')\vec{x}}\, d^3x}_{(2\pi)^3\delta^3(\vec{k}-\vec{k}')} = \frac{(2\pi)^3}{V} \delta^3(\vec{k}-\vec{k}')$$

1.4.3 Single-particle operators

Our next main goal will be to translate an arbitrary operator from the languange for first quantization to second quantization. We will do this by writing the operator in terms of creation and annihilation operators. Consider, for example, the Hamiltion operator describing N electrons in an external potential $V_a(r)$ which interact with the potential $V(r_i - r_j) = \frac{e^2}{|r_i - r_j|}$.

$$H = \underbrace{\sum_{i=1}^{N} \frac{p_i^2}{2m} + V_a(r_i)}_{\text{single-particle operator}} + \underbrace{\frac{1}{2} \sum_{r_i \neq r_j} V(\vec{r_i} - \vec{r_j})}_{\text{interaction}}$$

The first two terms are a so-called single-particle operator, defined below (the last term, the interaction will be treated in the next section).
A single-particle operator, by definition, acts on each particle i separately and one can simply sum over i to obtain the operator A^N acting in the N-particle hilbert space.

$$A^{(N)} = \sum_{i=1}^{N} A_i$$

Formally, the operator A in Fock space is obtained as a sum of all these operators acting in the N particle subspace.

$$A = A^{(0)} \oplus A^{(1)} \oplus A^{(2)} \oplus \dots$$

The trick to translate this operator to the language of second quantization is simple: we write both the operator A and the creation and annihilation operators in the eigenbasis $\{|\lambda_i\rangle\}$ of $A^{(1)} = \sum_{\lambda} \lambda_i |\lambda_i\rangle \langle\lambda_i|$ such that $|\lambda_i\rangle = a^\dagger_{\lambda_i} |0\rangle$. In this basis it is very simple to calculate the effect of A: just multiply the eigenvalue by the number of particles which are in the corresponding eigenstate.

$$A |n_{\lambda_1}, n_{\lambda_2}, \dots\rangle = \sum \lambda_i n_{\lambda_i} |n_{\lambda_1}, n_{\lambda_2}, \dots\rangle = \sum_{\lambda_i} \lambda_i a^\dagger_{\lambda_i} a_{\lambda_i} |n_{\lambda_1}, n_{\lambda_2}, \dots\rangle$$

From this we can read off directly

$$A = \sum_i \underbrace{\langle\lambda_i| A^{(1)} |\lambda_j\rangle}_{=\lambda_i \delta_{ij}} a^\dagger_{\lambda_i} a_{\lambda_i}$$

The only remaining step is to find the corresponding formula for another single-particle basis $|\alpha_i\rangle$. For this we use the formulas derived previously

$$a^\dagger_{\lambda_i} = \sum_K \langle\alpha_K|\, \lambda_i\rangle\, a^\dagger_{\alpha_K} \quad a_{\lambda_i} = \sum_{K^\dagger} \langle\lambda_i|\, \alpha_{K'}\rangle\, a_{\alpha_{K'}}$$

Using $\sum \langle\alpha_K|\,\lambda_i\rangle\,\langle\lambda_i|\,A^{(1)}\,|\lambda_j\rangle\,\langle\lambda_j|\,\alpha_{K'}\rangle = \langle\alpha_K|\,A^{(1)}\,|\alpha_{K'}\rangle$ we obtain

$$A = \sum_{KK'} \langle\alpha_K|\,A^{(1)}\,|\alpha_{K'}\rangle\, a^\dagger_{\alpha_K} a_{\alpha_{K'}} \tag{1.8}$$

Above, the operator in Fock space has been obtained directly from the single-particle matrix elements $\langle\alpha_K|\,A^{(1)}\,|\alpha_{K'}\rangle$.
It is important to learn to read such an equation to get an intuitive understanding. What is a operator $A^{(1)}$ acting on a single particle doing? According to the formula $A^{(1)} = \sum_{KK'} |\alpha_K\rangle\,\langle\alpha_K|\,A^{(1)}\,|\alpha_{K'}\rangle\,\langle\alpha_{K'}|$ the operator transforms an initial state $|\alpha_{K'}\rangle$ into $|\alpha_K\rangle$ with the amplitude $\langle\alpha_K|\,A^{(1)}\,|\alpha_{K'}\rangle$. This is precisely how one should also read the second-quantized version, Eq. (1.8): the operator removes one particles in $|\alpha_{K'}\rangle$ by $a_{\alpha_{K'}}$ and add it back in the state $|\alpha_K\rangle$ by $a^\dagger_{\alpha_K}$. This happens with the amplitude $\langle\alpha_K|\,A^{(1)}\,|\alpha_{K'}\rangle$.
A few examples are given below.

1. **momentum**: $P = \sum_{i=1}^{N} -i\hbar\frac{\partial}{\partial\vec{r}_i}$,
   momentum basis: $\left\langle\vec{K}\right| -i\hbar\vec{\nabla}\left|\vec{K}\right\rangle = \delta_{K,\,K'}\hbar\vec{K}$

   $\Rightarrow \quad \vec{P} = \sum_{\vec{K}} \hbar\vec{K} c^\dagger_{\vec{K}} c_{\vec{K}}$

   real-space basis (here: one dimensional):

   $$\langle x_0|\,P\,|x_0'\rangle = \langle x_0|\,-i\hbar\frac{d}{dx}\,|x_0'\rangle = \int \delta(\vec{r}-\vec{x}_0)(-i\hbar\frac{\partial}{\partial r}\delta(\vec{r}-\vec{x}_0')\mathrm{d}^3r = -i\hbar\delta'(x-x_0')$$
   $$\Rightarrow \quad P = \int \mathrm{d}x_0\mathrm{d}x_0'(-i\hbar)\delta'(x-x_0')\Psi^\dagger(x_0)\Psi(x_0') = \int \mathrm{d}x\Psi^\dagger(x)\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi(x)$$

2. **kinetic energy**: $\quad T^{(N)} = \sum_{i=1}^{N} -\frac{\hbar^2}{2m}\vec{\nabla}_i^2$
   use same arguements as above

   $$T = \int \mathrm{d}^3x\,\Psi^\dagger(x)\left(-\frac{\hbar^2}{2m}\right)\vec{\nabla}^2\Psi(x) == \int \mathrm{d}^3x\,\frac{\hbar^2}{2m}(\vec{\nabla}\Psi^\dagger(x))\vec{\nabla}\Psi(x)$$
   $$= \sum_K \frac{\hbar^2\vec{K}^2}{2m} c^\dagger_K c_K$$

3. **Potential-energy**: $U^{(N)} = \sum_{i=1}^{N} U(r_i)$

   $$U = \int \mathrm{d}^3x\,U(\vec{x})\Psi^\dagger(x)\Psi(x)$$

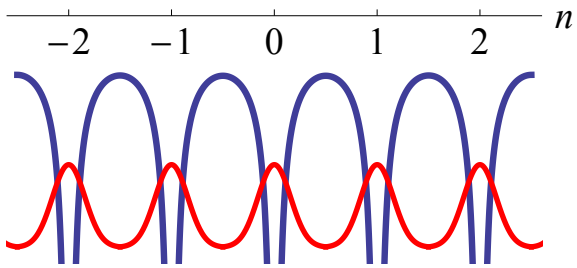


Figure 1.1: Blue: Periodic potential arising from a periodic arrangement of, e.g., hydrogen ions. When the atoms are far apart, electrons tunnel from one groundstate of each atom to the next with a small tunneling rate $-t$.

4. **Hopping on a lattice**: Consider a regular lattice of, e.g., hydrogen atoms arranged on a line in such a way that there is little overlap between their groundstate wave function, see Fig. 1.1. We denote by $c_i^\dagger$ the operator creating an electron in the groundstate wave function of atom i (we ignore spin, discussed below in Sec. 1.4.5). The electrons can tunnel from groundstate of one atoms to the neighboring atome with the rate $-t$ (a calculation gives $t > 0$). This simple picture can litteraly be translated to a Hamiltonian using that $c_{i+1}^\dagger c_i$ describes the process where one electron moves from site i where it is annihilated to site $i+1$, where it is created. Including also the reverse process, the Hamiltonian is therefore given by

$$H = -t \sum_i c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i$$

Note that H is hermitian. You can diagonalize H by a Fourier transformation of the operators, i.e., by introducing a new field $f_k^\dagger = \frac{1}{\sqrt{N}} \sum_j c_j^\dagger e^{ikj}$ where N is the number of lattice sites (homework problem).

In conclusion, we have found a simple way to write operators using the language of second quantization. In contrast to the first-quantized version, there is no need to introduce N coordinates $\vec{r}_i$, $i = 1, .., N$ to describe N particles. Just quantum fields with simple commutation relations are sufficient.

1.4.4 Two particle operators

As a next step, we want to translate more complicated operators describing two-particle interaction processes into the language of second quantization. These are operators of the type

$$V = \frac{1}{2} \sum_{i \neq j} V(r_i, r_j)$$

where the **Coulomb interaction** $V(r_1, r_2) = \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$ is probably the most important example.

We will not give a detailed derivation in this section: one can follow the procedures described in more detail in the previous paragraph to obtain all results.

For a two-particle operator, we need its matrix elements in the same basis in which the creation and annihilation operators are defined.

$$\langle\lambda_1|\langle\lambda_2|V^{(2)}\left|\lambda_2'\right\rangle\left|\lambda_1'\right\rangle = \int \Psi^*_{\lambda_1}(r_1)\Psi^*_{\lambda_2}(r_2)V(r_1, r_2)\Psi_{\lambda_2'}(r_2)\Psi_{\lambda_1'}(r_1)\,\mathrm{d}^3r_1\,\mathrm{d}^3r_2$$

The operator in second quantization reads

for bosons *and* fermions:

$$V = \frac{1}{2}\sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'}\langle\lambda_1|\langle\lambda_2|V^{(2)}\left|\lambda_2'\right\rangle\left|\lambda_1'\right\rangle\; a^\dagger_{\lambda_1}a^\dagger_{\lambda_2}a_{\lambda_2'}a_{\lambda_1'} \tag{1.9}$$

The interpretation is the same which we used in the previous section: V describes that two particles in states λ_1', λ_2' are transferred to the states λ_1, λ_2 (by annihilating the first two and creating the second two).

Note that the order of operators in important in Eq. (1.9) is important as for fermions we have $a_{\lambda_2'}a_{\lambda_1'} = -a_{\lambda_1'}a_{\lambda_2'}$.

An important example is an interaction which depends only of the position of two particles $V^{\mathrm{int}} = \frac{1}{2}\sum_{i\neq j} V^{\mathrm{int}}(r_i - r_j)$.

$$\begin{aligned} V^{\mathrm{int}} &= \frac{1}{2}\int \mathrm{d}^3x\,\mathrm{d}^3x'\; V^{\mathrm{int}}(x-x')\Psi^\dagger(x)\Psi^\dagger(x')\Psi(x')\Psi(x) \\ &= \frac{1}{2}\int \mathrm{d}^3x\,\mathrm{d}^3x'\; \underbrace{\Psi^\dagger(x')\Psi(x')}_{\text{density at } x'}\; V^{\mathrm{int}}(x'-x)\; \underbrace{\Psi^\dagger(x)\Psi(x)}_{\text{density at } x} \end{aligned} \tag{1.10}$$

The resulting formula takes the form expected from classical physics when one realizes that $\Psi^\dagger(x)\Psi(x)$ is the density of particles at point x.

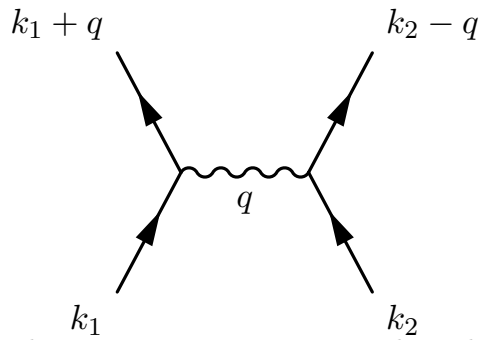
One also often uses the interaction written in **momentum space**. Starting from the matrix element

$$\begin{aligned} \left\langle \vec{K}_1\vec{K}_2\middle|V^{\mathrm{int}}(1-2)\middle|\vec{K}_1\vec{K}_2\right\rangle &= \frac{1}{V^2}\int \mathrm{d}^3r_1\,\mathrm{d}^3r_2\; e^{i(\vec{K}_1'-\vec{K}_1)r_1}\; e^{i(\vec{K}_2'-\vec{K}_2)r_2}V^{\mathrm{int}}(r_1-r_2) \\ &= \frac{1}{V^2}\int \mathrm{d}^3r\,\mathrm{d}^3R\;\; e^{i(K_1'+K_2'-(K_1+K_2))R}\;\; e^{i\frac{1}{2}(K_1'-K_1-(K_2'+K_2))r}\; V^{\mathrm{int}}(r) \\ &= \frac{1}{V}\delta_{\vec{K}_1+\vec{K}_2,\,\vec{K}_1'+\vec{K}_2'}\; V^{\mathrm{int}}(K_1-K_1') \end{aligned}$$

with $V^{\mathrm{int}}(K) = \int V(x)e^{-ikx}$, we obtain

$$V^{\text{int}} = \frac{1}{2V} \sum_{k_1,k_2,k_1',k_2'} V^{\text{int}}(k_1 - k_1') c_{k_1}^\dagger c_{k_2}^\dagger c_{k_2'} c_{k_1'} \delta_{\vec{k}_1+\vec{k}_2,\, \vec{k}_1'+\vec{k}_2'} =$$
$$= \frac{1}{2V} \sum_{k_1,\, k_2,\, q} V^{\text{int}}(q) c_{k_1+q}^\dagger c_{k_2-q}^\dagger c_{k_2} c_{k_1}$$

A useful way to visualize this expression is shown here:



which shows visually, that there are two incoming particle with momenta k_1 and k_2 (described by annihilation operators) and outgoing ones with momenta $k_1 + q$ and $k_2 - q$ (creation operators). At each vertex, where three lines join, the momentum is conserved. We will not use such diagrams in the lecture a lot, but they are an important building block for any calculation using perturbation theory, a topic covered in Quantum Field Theory lectures (but not in this course).

1.4.5 Hamiltonian with spin

It is straightforward to include more quantum numbers in the language of second quantization: one justs adds one more index to the field operators. The most important example is the spin of an electron. We denote the extra label σ sometimes by $\sigma = \pm\frac{1}{2}$ but more often by $\sigma = \uparrow \,/\, \downarrow$. The new field operators are, for example, written as $\Psi_\uparrow^\dagger(x)$ or $c_{\downarrow,k}^\dagger$. Their anti-commutation relation simply read

$$\{\Psi_\sigma(r),\ \Psi_{\sigma'}^\dagger(r')\} = \delta^3(r - r')\, \delta_{\sigma\sigma'}$$

To describe a spin in first-quantized language, the spinor notation is used, for example, $\vec{\varphi}(\vec{r}) = \begin{pmatrix} \varphi_\uparrow(r) \\ \varphi_\downarrow(r) \end{pmatrix}$. It describes a single electron which has the probability amplitude $\varphi_\sigma(r)$ to be at position r with spin σ. The same wave function of a single electron is written in second quantization as

$$|\varphi\rangle = \int \varphi_\uparrow(r)\, \Psi_\uparrow^\dagger(r) + \varphi_\downarrow(r)\, \Psi_\downarrow^\dagger(r)\ |0\rangle\ \mathrm{d}^3 r$$

In first-quantized languange, the Hamiltonian describing N particles in the presence of a magnetic field has the form

$$H = \sum_i \frac{\left(\vec{p}_i - \frac{e}{c}\vec{A}(r_i)\right)^2}{2m} + U(r_i) + \frac{1}{2}\sum_{i\neq j} V(r_i - r_j) - \sum_i g\mu_B \vec{B}(r_i)\vec{S}_i$$

In second-quantized form this translates to

$$\begin{aligned} H = &\sum_{\sigma=\uparrow/\downarrow} \int \mathrm{d}^3x\ \Psi^\dagger_\sigma(x)\ \frac{\left(-i\hbar\vec{\nabla} - \frac{e}{c}\vec{A}(x)\right)^2}{2m}\ \Psi_\sigma(x) + U(x)\,\Psi^\dagger_\sigma(x)\,\Psi_\sigma(x) \\ &+ \frac{1}{2}\sum_{\sigma,\,\sigma'} \int \mathrm{d}^3x\,\mathrm{d}^3x'\ V(x-x')\,\Psi^\dagger_\sigma(x)\Psi^\dagger_{\sigma'}(x')\,\Psi_{\sigma'}(x')\Psi_\sigma(x) \\ &- g\,\mu_B \int \mathrm{d}^3x\,\vec{B}(\vec{x}) \sum_{\alpha,\,\beta} \Psi^\dagger_\alpha(x)\,\frac{\vec{\sigma}_{\alpha,\,\beta}}{2}\,\Psi_\beta(x) \end{aligned} \tag{1.11}$$

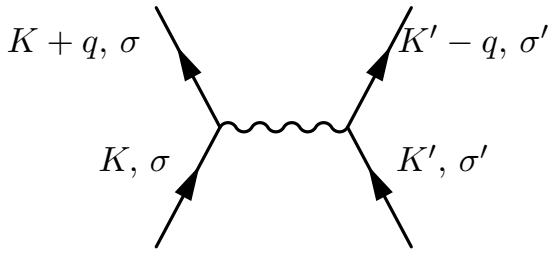
where we have just replaced the densities by $\sum_\sigma \Psi^\dagger_\sigma(x)\Psi_\sigma(x)$ while the spin density at site x is written as

$$\sum_{\alpha,\,\beta} \Psi^\dagger_\alpha(x)\,\frac{\vec{\sigma}_{\alpha,\,\beta}}{2}\,\Psi_\beta(x)$$

Please check that this is just the second-quantized version of the first-quantized operator $\sum_i \vec{S}_i\delta^3(x - r_i)$.
For vanishing vector potential $\vec{A}$, magnetic field $\vec{B}$ and single-particle potential U one obtains in momentum space:

$$H = \sum_{\sigma=\uparrow/\downarrow}\ \sum_K\ \epsilon(K)\,c^\dagger_{K,\sigma}c_{K,\sigma} + \frac{1}{2}\sum_{\sigma\sigma',KK',q} V(\vec{q})\ c^\dagger_{K+q,\sigma}c^\dagger_{K'-q,\sigma'}c_{K',\sigma'}c_{K,\sigma}$$

with the kinectic energy $\epsilon(K) = \frac{(\hbar K)^2}{2m}$.
The correspondig Feynman diagram



has the property that at the vertex the incoming spin is equal to the outgoing spin as the Coulomb interaction does not change the spin.
The language of second quantization is used whenever one describes more than one or two quantum particles. An important example are **electrons in a solid**. As you probably

know from your solid state lecture, their properties are described by electronic bands. The bandstructure $\epsilon_{n,k}$ describes how the energy of a given band n depends on (quasi-) momentum k defined in the first Brillouin zone. We will not explain these concepts in this lecture (assuming you have heard this before) but this paragraph describes how easily this can be translated to the language of second quantization. The band label n just enters as an extra index. Ignoring interactions, the Hamiltonian of a solid with several bands can simply be written as

$$H = \sum_{n,k,\sigma} \epsilon_{n,k}\, c^\dagger_{n,k,\sigma} c_{n,k,\sigma}$$

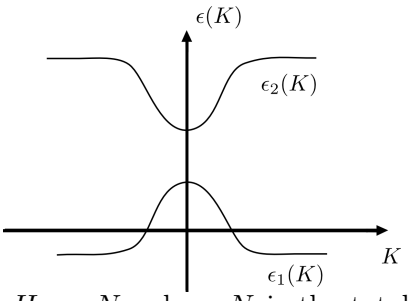
where $c^\dagger_{n,k,\sigma}$ creates an electron in band n with momentum k and spin σ.
The ground state of such a system is characterized by the fact that all states up to a maximal energy – the Fermi energy or, equivalently, the chemical potential μ – are occupied. This ground state is called Fermi sea and we denote it by $|FS\rangle$ and it is given by

$$|FS\rangle = \prod_{n,k,\sigma \text{ with } \epsilon_{n,k,\sigma}<\mu} c^\dagger_{n,k,\sigma}\,|0\rangle$$

This ground state has the property that

$$\left\langle FS\,|c^\dagger_{n,k,\sigma}\, c_{n,k,\sigma}\,|FS\right\rangle = \begin{cases} 1 & \text{for} \quad \epsilon_K - \mu < 0 \\ 0 & \qquad\quad \epsilon_K - \mu > 0 \end{cases}$$

As a simple, but instructive example let us consider a semiconductor with two bands where the upper band is completely empty and the lower one occupied with $\epsilon_{1,k} < \mu$ and $\epsilon_{2,k} > \mu$. The ground state is given by $|GS\rangle = \prod_{K,\sigma} c^\dagger_{1\,K,\sigma}\,|0\rangle$.



For the following it is useful to discuss the combination $H - \mu N$, where N is the total number of particles, as this combination enters, e.g., the Boltzmann weight $e^{-(H-\mu N)/(k_B T)}$ of each state. For the two bands, we obtain

$$H - \mu N = \sum_{k,\sigma} (\epsilon_{1,k} - \mu)\, c^\dagger_{1,k,\sigma} c_{1,k,\sigma} + (\epsilon_{2,k} - \mu)\, c^\dagger_{2,k,\sigma} c_{2,k,\sigma}$$

For many applications it is useful to think about this system in a different way. We want to view the ground state $|GS\rangle$ defined above as a **new vacuum**, i.e., as a state without particles. This is achieved by rewriting the occupied band in terms of **hole operators**.

We define

$$\begin{aligned} h^\dagger_{K,\uparrow} &= c_{1,-K,\downarrow} & h^\dagger_{K,\downarrow} &= -c_{1,-K,\uparrow} \\ h_{K,\uparrow} &= c^\dagger_{1,-K,\downarrow} & h_{K,\downarrow} &= -c^\dagger_{1,-K,\uparrow} \end{aligned} \tag{1.12}$$

From this definition, we find that the new operators fulfill the standard commutation relations of fermions

$$\left\{ h^\dagger_{K,\sigma},\ h_{K',\sigma'} \right\} = \delta_{K,K'}\,\delta_{\sigma,\sigma'}$$

What have we gained? All states in band 1 are occupied and therefore $c^\dagger_{1,k,\sigma}\,|GS\rangle = 0$. In the hole variables this implies that $h_{K,\sigma}\,|GS\rangle = 0$. As furthermore $c_{2,K,\sigma}\,|GS\rangle = 0$ (the second band is empty), we can now identify $|GS\rangle$ with the vacuum state of the new variables

$$|GS\rangle = |0\rangle$$

Using that $c^\dagger_{1\,K,\sigma}\,c_{1\,K,\sigma} = h_{-K,-\sigma}h^\dagger_{-K,-\sigma} = 1 - h^\dagger_{-K,-\sigma}h_{-K,-\sigma}$ and $\epsilon_{1,k} = \epsilon_{1,-k}$, the Hamiltonian is written in the new variables

$$H - \mu N = \sum_{K,\sigma} (\mu - \epsilon_{1,K})\ h^\dagger_{K,\sigma}h_{K,\sigma} + \sum_{K,\sigma} (\epsilon_{2,K} - \mu)\, c^\dagger_{2,K,\sigma}\,c_{2,K,\sigma} + \text{const.}$$

Note that now both $\mu - \epsilon_{1,k}$ and $\epsilon_{2,k} - \mu$ are positive: it costs a finite energy to add an extra particle. As you know from your solid state lecture, using holes is an efficient way to describe the properties of semiconductors. Their band structure is inverted and they have opposite charge compared to electrons (as $c^\dagger_{1\,K,\sigma}\,c_{1\,K,\sigma} = 1 - h^\dagger_{-K,-\sigma}h_{-K,-\sigma}$).

1.4.6 Dynamics of fields

As the reader is probably aware from his or her Quantum Mechanics course, there are two different ways how one can view the time evolution of a quantum-mechanical system. Following Schrödinger, one considers the time evolution of the wave function described by the **Schrödinger equation**

$$i\hbar\partial_t\,|\Psi(t)\rangle = H\ |\Psi(t)\rangle$$

which can also be rewritten using the unitary time-evolution operator U_t with

$$|\Psi(t)\rangle = U_t\ |\Psi(0)\rangle\,, \qquad i\hbar\partial_t\,U_t = H\,U_t$$

An equivalent, alternative point of view is, however, to attribute the time evolution *not* to the wave function but instead to the operator by using that $\langle A\rangle = \langle\Psi(t)|\,A\,|\Psi(t)\rangle = \langle\Psi(0)|\,U_t^\dagger\,A\,U_t\,|\Psi(0)\rangle$.
One can therefore introduce time-dependent "Heisenberg" operators

$$A^{\mathrm{H}}(t) = U_t^\dagger\,A\,U_t$$

following the **Heisenberg equation of motion**

$$i\hbar\partial_t A^{\mathrm{H}}(t) = \left[A^{\mathrm{H}}(t),\, H\right]$$

where this equation is only valid if A was time-independent in the Schrödinger version discussed above. The reader is encouraged to check this equation using the definition of A^H and the property of U_t given above.

We want to use these definitions to calculate the time-evolution of the Heisenberg operator $\Psi^H(r,t)$ describing the destruction of a particle at point r (not to be confused with the wave function). For simplicity, we will omit the index H in $\Psi^H(r,t)$ and write instead just $\Psi(r,t)$. We will calculate the time evolution using for the Hamiltonian

$$\begin{aligned} H = &\int -\frac{\hbar^2}{2m}\,\Psi^\dagger(r,t)\nabla^2\Psi(r,t) + U(r)\Psi^\dagger(r,t)\Psi(r,t) \\ &+ \frac{1}{2}\int U(r-r')\Psi^\dagger(r,t)\Psi^\dagger(r',t)\Psi(r',t)\Psi(r,t) \end{aligned}$$

We will consider the first term in $[\Psi, H]$ in a theory of fermions using that the (anti-) commutation relation of the Heisenberg operators is the same as that of the Schrödinger operators (check this!). As usually, we simplify the equations by normal ordering (moving creation operators to the left using the anticommutation relation $\Psi(r)\Psi^\dagger(x) = -\Psi^\dagger(x)\Psi(r) + \delta(x-r)$ (omitting the time-index)

$$\begin{aligned} &\left[\Psi(r),\, \int \Psi^\dagger(\vec{x})\,\left(-\frac{\hbar^2\nabla^2}{2m}\right)\,\Psi(\vec{x})\right] = \\ &\int dx\,\Psi(r)\Psi^\dagger(x)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\Psi(x) - \Psi^\dagger(x)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\Psi(x)\Psi(r) = \\ &\int dx\,(-1)\Psi^\dagger(x)\Psi(r)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\Psi(x) + \delta(r-x)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\Psi(x) \\ &- \Psi^\dagger(x)\left(-\frac{\hbar^2\nabla^2}{2m}\right)\Psi(x)\Psi(r) \underbrace{=}_{\substack{\text{with } \Psi(x)\Psi(r) \\ = -\Psi(r)\Psi(x)}} -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\,\Psi(r) \end{aligned}$$

Repeating similar calculations for the other terms, one obtains both for fermions and bosons the Heisenberg equation of motions

$$\begin{aligned} &i\hbar\partial_t\Psi(r,t) = [\Psi(r,t),\, H] \\ &= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2}\,\Psi(r,t) + U(r)\Psi(r) + \int \mathrm{d}^3\vec{x}\,\Psi^\dagger(x)\Psi(x)V(x-r)\Psi(r) \end{aligned}$$

Without interaction these equations *look like* the Schrödinger equation. The interpretation is, however, completly different: these are Heisenberg equations of motion for field operators.

Due to the non-linearities and the finite size of the Hilbert space, it is in general impossible to solve these equations analytically or numerically. In the course Quantum Field Theory I

methods for solving such problems using perturbation theory are discussed. This problem is, however, not covered in this lecture notes.

1.5 Bose-Einstein Condensation (BEC) and superfluidity

As an application of the power of field theoretical techniques we will study the Bose-Einstein condensation (BEC) of bosons in the presence of interactions. This will provide a very different point of view on this problem compared to the non-interacting case which was probably studied by most readers in a statistical physics course. In this chapter one of the most important concepts of physics is introduced: the concept of spontaneous symmetry breaking which not only determines the properties of all solids but is for example, an important building block of the standard model of particle physics (it is an important element of the Higgs mechanism).
Superfluidity and superconductivity, allowing for transport of mass or charge without any friction, are arguably some of the most fascinating subjects in physics - as can already be seen from the large number of Nobel prizes in this field (Kamerlingh Onnes 1913, Landau 1962, Bardeen, Cooper, Schrieffer 1972, Josephson 1973, Bednorz, Müller 1987, Lee, Osheroff, Richardson 1996, Cornell, Ketterle, Wiemann 2001, Abrikosov, Ginzburg, Legett 2003).

1.5.1 Spontaneous symmetry breaking

But let us start by recalling basic facs of the BEC of *non-interacting* bosons. Here the key observation is, that below the transition temperature, $T < T_c$, the ground state wave function (i.e., the $k = 0$ state) is macroscopically occupied

$$\frac{\left\langle n_{\vec{K}=0} \right\rangle}{V} = \frac{\left\langle c^\dagger_{\vec{K}=0}\, c_{\vec{K}=0} \right\rangle}{V} = n_s > 0 \;\text{ for } V \to \infty \tag{1.13}$$

where n_s is the superfluid density and we used the following definition of the expectation value

$$\langle A \rangle = \frac{1}{Z} \mathrm{tr}\, e^{-\frac{H-\mu N}{k_b T}} A \equiv \frac{1}{Z} \sum_i \langle \Psi_i |\, e^{-\frac{H-\mu N}{k_b T}} A \,| \Psi_i \rangle$$

where the trace "tr" is defined by summing over a basis of the Fock space with basis vectors $|\Psi_i\rangle$ and $Z = \mathrm{tr}\, e^{-\frac{H-\mu N}{k_b T}}$ is the partition sum (I assume that the reader is familiar with these concepts, if not, I would recommend reading a statistical physics textbook).
We will use Eq. (1.13) to calculate

$$\left\langle \Psi^\dagger(x)\Psi(y) \right\rangle = \frac{1}{V} \sum_{K,\,K'} \left\langle c^\dagger_{\vec{K}}\, c_{\vec{K'}} \right\rangle e^{i\vec{K}\vec{x}}\, e^{-i\vec{K'}\vec{y}}$$

for large distances $x - y$. This is greatly simplified by observing that $\left\langle c^\dagger_{\vec{K}}\, c_{\vec{K'}} \right\rangle = 0$

for $K \neq K'$. This is a consequence of momentum conservation: each eigenstate $|\Psi_n\rangle$ of the Hamiltonian H can be chosen as an eigenstate of the total momentum operator P. As $c^\dagger_{\vec{K}} c_{\vec{K'}}$ changes the momentum by $\vec{K} - \vec{K'}$, the overlap of $c^\dagger_{\vec{K}} c_{\vec{K'}} |\Psi_n\rangle$ with $|\Psi_n\rangle$ has to vanish (they have different momentum). Therefore also the expectation value (a sum over such overlaps) must be zero for $K \neq K'$. For $K = K'$ the occupations of the non-interacting systems are given by the well-known result (not derived here) $\left\langle c^\dagger_K c_K \right\rangle = \left(e^{\beta(\epsilon(K)-\mu)} - 1\right)^{-1}$. We will not use this formula but instead use that for $x - y \to \infty$ only the $k = 0$ states contribute to obtain

$$\lim_{|x-y|\to\infty} \left\langle \Psi^\dagger(x)\Psi(y) \right\rangle = \frac{1}{V} \sum_K \left\langle c^\dagger_K c_K \right\rangle e^{i\vec{K}(\vec{x}-\vec{y})} = \frac{1}{V} \left\langle c^\dagger_{K=0} c_{K=0} \right\rangle = n_s > 0 \tag{1.14}$$

for a BEC. This is an important observation: a BEC is characterized by correlations which do not decay in the limit of an infinitely large distance. This is surprising as usally all correlations decay at finite temperature due to thermal fluctuations.
To reconcile the infinite-range correlations of Eq. (1.14) with the fact that all physics is local, we introduce a radically new interpretation (justified in more detail below). We argue that the origin of the infinite-range correlation is, that our field operators obtain a finite expectation value

$$\lim_{|x-y|\to\infty} \left\langle \Psi^\dagger(x)\, \Psi(y) \right\rangle = \lim_{|x-y|\to\infty} \left\langle \Psi^\dagger(x) \right\rangle \left\langle \Psi(y) \right\rangle = n_s$$

We can say, that the system behaves "as if"

$$\left\langle \Psi^\dagger(x) \right\rangle = \sqrt{n_s} e^{i\varphi_0}, \qquad \langle \Psi(x) \rangle = \sqrt{n_s} e^{-i\varphi_0} \tag{1.15}$$

where φ_0 is an undetermined phase.
To appreciate how strange Eq. (1.15) is, we will show that Eq. (1.15) apparently contradicts the conservation of particle number. We will even give two different "proofs" of $\langle \Psi \rangle = 0$. As the total number of particles $\hat{N}$ is conserved, $\left[\hat{N},\, H\right] = 0$, we can choose all eigenstates of H as eigenstates of $\hat{N}$. We conculde

$$\hat{N} |n\rangle = n |n\rangle\,, \quad \langle n| \underbrace{\left(\Psi^\dagger |n\rangle\right)}_{n+1\text{particles}} = 0 \quad \Rightarrow \left\langle \Psi^\dagger \right\rangle = 0$$

Even more instructive is the following equivalent argument: we know that all observables are invariant under the change of the **phase** of all single-particle wave function which corresponds to the symmetry transformation

$$|\phi\rangle \to e^{i\varphi\hat{N}} |\phi\rangle\,.$$

Such a symmetry (multiplication by a phase) is called a **U(1) symmetry**. If we assume that the groundstate obeys this symmetry, then we find that

$$\langle\phi|\,\Psi^\dagger\,|\phi\rangle = \langle\phi|\,e^{-i\varphi\hat{N}}\Psi^\dagger\,e^{i\varphi\hat{N}}\,|\phi\rangle = \langle\phi|\,e^{-i\varphi}\,\Psi^\dagger\,|\phi\rangle = e^{-i\varphi}\,\langle\phi|\,\Psi^\dagger\,|\phi\rangle \tag{1.16}$$

using that $\Psi^\dagger$ increases the total number of particles by 1 making $\hat{N}$ to the left of $\Psi^\dagger$ larger by one compared to $\hat{N}$ to the right of $\Psi^\dagger$. As φ is arbitrary, we can use the equation $\left\langle\Psi^\dagger\right\rangle = e^{-i\varphi}\left\langle\Psi^\dagger\right\rangle$ to "prove" again that $\left\langle\Psi^\dagger\right\rangle = 0$.

While these proofs are formally fully correct in a finite system, they can, however, be "circumvented" in an infinitely large system. To reconcile the finite expectation value in Eq. (1.15) with the result Eq. (1.16) there is only one option: we have to assume that the BEC state *does not* have the symmetry that it is invariant under multiplication by $e^{i\varphi\hat{N}}$!

This phenomenon is called "spontaneous symmetry breaking". You have probably seen this before, for example, in your statistical physics course when discussing the phase transition in the Ising model. "Spontaneous symmetry breaking" describes that the state of the system does not have to have the symmetries of the underlying Hamiltonian. A good example is a magnet: while the Hamiltonian is symmetric under a reversal of the magnetization, $M \to -M$, the ferromagnetic groundstate selects "spontaneously" one direction of M.

For a BEC a similar effect takes place: the system "spontaneously" selects one phase φ_0. Thereby the $U(1)$ symmetry is "spontaneously broken" and is therefore not a symmetry of the thermal state below the transition temperature.

The previous discussion was far from rigorous. It started from the ad-hoc assumption (1.15) that the annihilation and creation operators obtain a finite expectation value. We will now shows that we can indeed perform a certain limiting procedure where one obtains rigorously a finite expectation value. We start by modfying the Hamiltonian is such a way that the $U(1)$ symmetry is explicitely broken by the parameter α

$$H = \sum\left(\epsilon_K - \mu\right)c_K^\dagger c_K + \alpha\,c_{K=0}^\dagger + \alpha^*\,c_{K=0} \tag{1.17}$$

As it is often done, we write here H for $H - \mu\hat{N}$ as this is convenient to describe grand canonical ensembles with $\hat{N} = \sum_K c_K^\dagger c_K$. You can check that for this Hamiltionian the particle number is not conserved, $[H, \hat{N}] = \alpha\,c_{K=0}^\dagger - \alpha^*\,c_{K=0}$. We will now study the limit $\alpha \to 0$ together with the infinite-volume limit $V \to \infty$.

The α-term in (1.17) can be easily be absorbed by defining new operators $\tilde{c}$ with

$$c_K = \tilde{c}_K + \frac{\alpha}{\mu}\delta_{\vec{K},\,0} \quad , c_K^\dagger = \tilde{c}_K^\dagger + \frac{\alpha^*}{\mu}\delta_{K,\,0} \quad , \left[\tilde{c}_K,\,\tilde{c}_{K'}^\dagger\right] = \left[c_K,\,c_{K'}^\dagger\right] = \delta_{K,\,K'} \tag{1.18}$$

In these new variables H takes the form

$$H = \sum\left(\epsilon_K - \mu\right)\tilde{c}_K^\dagger\tilde{c}_K + \frac{|\alpha|^2}{\mu^2}$$

The value of the chemical potential μ is determined from the density of particles

$$n = \frac{\langle N\rangle}{V} = \frac{1}{V}\sum_K \left\langle c_K^\dagger\, c_K\right\rangle = \frac{1}{V}\sum_K \left\langle \tilde{c}_K^\dagger\, \tilde{c}_K\right\rangle + \underbrace{\frac{\alpha}{\mu}\left\langle \tilde{c}_0^\dagger\right\rangle + \frac{\alpha^*}{\mu}\left\langle \tilde{c}_0\right\rangle}_{=0\,;\,\text{as}\left[\sum_K \tilde{c}_K^\dagger \tilde{c}_K, H\right]} + \frac{|\alpha|^2}{\mu^2} \tag{1.19}$$

The number of particles in the mode with momentum k is given by the Bose distribution $\left\langle \tilde{c}_K^\dagger \tilde{c}_K\right\rangle = \left(e^{(\epsilon(K)-\mu)/k_BT}-1\right)^{-1}$. As μ is very close to zero in the BEC phase, the occupation of the $k=0$ mode is given by

$$\left\langle \tilde{c}_{K=0}^\dagger \tilde{c}_{K=0}\right\rangle = \left(e^{-\mu/k_BT}-1\right)^{-1} \approx \frac{k_BT}{-\mu} \propto V$$

We therefore conclude that the occupation of the ground state per volume n_S is given by

$$n_S = \frac{\left\langle c_{k=0}^\dagger c_{k=0}\right\rangle}{V} = \frac{1}{V}\underbrace{\left(\frac{k_BT}{-\mu}\right.}_{K=0\text{ mode}} + \left.\frac{|\alpha|^2}{\mu^2}\right) \tag{1.20}$$

As μ vanishes in the thermodynamic limit, we can ignore it for all finite momenta and we obtain from Eq. (1.19) that the total density is given by

$$n = n_s + \int \frac{d^3k}{(2\pi)^3}\,\frac{1}{e^{\epsilon_k/k_BT}-1}$$

From this equation, one can determine n_s for given n and T.
For Eq. (1.20) consider the limit $\left|\frac{k_BT}{-\mu}\right| \ll \frac{|\alpha|^2}{\mu^2}$ such that $n_s = \frac{|\alpha|^2}{\mu^2 V}$ and therefore

$$\mu = -\sqrt{\frac{|\alpha|^2}{V n_s}}$$

(as $\mu < 0$). Plugging this result in the equality $\left|\frac{k_BT}{-\mu}\right| \ll \frac{|\alpha|^2}{\mu^2}$ from which we started and solving for α we obtain the condition $|\alpha| \gg \frac{k_BT}{\sqrt{V n_s}}$ which is alway fulfilled when we consider the limit $V\to\infty$ at any finite α. In this limit we will calculate $\left\langle \Psi^\dagger\right\rangle = \frac{1}{\sqrt{V}}\sum_K \left\langle c_K^\dagger\right\rangle$ using Eq. (1.18) and $\left\langle \tilde{c}_k^\dagger\right\rangle = 0$. We obtain

$$\lim_{\alpha\to 0}\lim_{V\to\infty}\left\langle \Psi^\dagger\right\rangle = \lim_{\alpha\to 0}\lim_{V\to\infty}\frac{\alpha^*}{\sqrt{V}\mu} = \lim_{\alpha\to 0}\sqrt{n_s}\frac{\alpha^*}{|\alpha|} = \sqrt{n_s}e^{-i\varphi_0}$$

where ϕ_0 is the phase of α. We have therefore shown that $\Psi^\dagger$ has precisely the type of expectation value which we previously had only conjectured, see Eq. (1.15), under the condition that one first takes the thermodynamic limit, $V\to\infty$, and only afterwards the limit $\alpha\to 0$. In contrast, in the opposite limit one finds

$$\lim_{V\to\infty}\lim_{\alpha\to 0}\left\langle \Psi^\dagger \right\rangle = \lim_{V\to\infty}\lim_{\alpha\to 0}\frac{\alpha^*}{\sqrt{V}\mu} = 0$$

In conclusion, we have found a natural way to describe the infinite-range BEC correlations by giving the field operator a finite expectation value. The infinite-range correlations are thereby described just by a local expectation value. As in the case of other spontaneously broken symmetries, this can formally be justified by introducing a symmetry breaking term in the Hamiltonian, and then considering first the infinite volume limit and then the limit of a vanishing symmetry breaking term. Above we discussed the familiar case without interaction: the real advantage of this approach is, however, that it allows for a simple description of the interacting case.

1.5.2 Bogoliubov quasi particles

Interactions drastically modify Bose Einstein condensates and ultimately lead to the phenomenon of superfluidity: a superfluid can flow without any friction. If you therefore cool down a rotating liquid until it becomes superfluid, its rotation will go on practically forever without any friction.

We consider a Hamiltonian which describes well a diluted gas of bosonic atoms (as in the Nobel-prize winning experiments of Cronelll, Ketterle and Wiemann, Nobelprize 2001). As the distance of the atoms is much larger than their radius, the interaction potential of two atoms, $V(r-r') \approx U\delta^3(\vec{r}-\vec{r}')$, is practically local.[2] The Hamiltonian therefore has in real space the form

$$H = \int \frac{\hbar^2}{2m}\vec{\nabla}\Psi^\dagger(x)\nabla\Psi(x) - \mu\Psi^\dagger(x)\Psi(x) + \frac{U}{2}\Psi^\dagger(x)\Psi^\dagger(x)\Psi(x)\Psi(x)\,dx$$

In the following it is convenient to use the Hamiltionian in a momentum-space representation

$$H = \sum_K (\epsilon_K - \mu)c_K^\dagger c_K + \frac{U}{2V}\sum_{K_1,\,K_2} c_{K_1+q}^\dagger c_{K_2-q}^\dagger c_{K_2}c_{K_1}$$

with $\epsilon_K = \hbar^2K^2/2m$ as usually. To describe the finite expectation value $\langle\Psi^\dagger\rangle = \sqrt{n_s}$ as in Eq. (1.15)[3], we again shift the fields by $\sqrt{n_s}$ (assuming $n_s \geq 0$) which is for us at the moment an unknown constant, to be determined from the condition that the expectation value vanishes for the shifted fields, $\left\langle\tilde{\Psi}\right\rangle = 0$ with

$$\Psi^\dagger = \sqrt{n_s} + \tilde{\Psi}^\dagger, \qquad c_K^\dagger = \sqrt{n_sV}\delta_{K,0} + \tilde{c}_K^\dagger$$

[2] We ignore here some issues related to the description of the two-particle scattering by a delta function. In reality U one has to parametrize U by the scattering length, a concept which we will introduce later in the chapter 4 on scattering theory.

[3] The arbitrariy phase ϕ_0 has been set to 0

As the next step, we Taylor-expand H in $\tilde{c}_K$ which turns out to be a good approximation for low temperatures (and not too large U), when there are few excitations. We find up to quadratic order

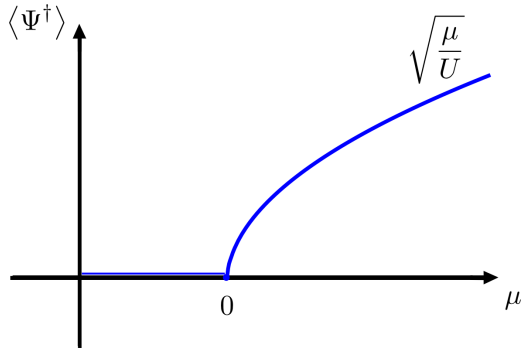
$$H = V\left(-\mu n_s + \frac{U}{2}n_s^2\right) + \sqrt{V}\left(-\mu\sqrt{n_s} + U n_s^{3/2}\right)\left(\tilde{c}^\dagger_{K=0} + \tilde{c}_{K=0}\right) + \tag{1.21}$$

$$+ \sum_K (\epsilon_K - \mu)\,\tilde{c}^\dagger_K \tilde{c}_K + \frac{n_s U}{2}\sum_K \left(\tilde{c}_K\tilde{c}_{-K} + \tilde{c}^\dagger_K\tilde{c}^\dagger_{-K} + 4\tilde{c}^\dagger_K\tilde{c}_K\right) + \mathcal{O}\left(\tilde{c}^3\right) \tag{1.22}$$

We have still to determine n_s. This can be done in two equivalent ways. One is to minimize the energy, i.e. the first term in H, $-\mu n_s + \frac{U}{2}n_s^2$ taking into account that we defined $n_s \geq 0$. The second one is to eliminate the prefactor $-\mu\sqrt{n_s} + U n_s^{3/2}$ of the term *linear* in $\tilde{c}$ and $\tilde{c}^\dagger$ which ensures that $\left\langle\tilde{\Psi}\right\rangle = 0$. Why are these two conditions equivalent? At the minimum the first derivative vanishes and therefore the first term in the Taylor expansion.

$$\text{minimize } -\mu n_s + \frac{U}{2}n_s^2 \text{ for } n_s \geq 0 \quad \Rightarrow \quad \begin{cases} n_s = 0 & \text{for } \mu < 0 \\ n_s = \frac{\mu}{U} & \text{for } \mu > 0 \end{cases}$$

We therefore obtain for $\left\langle\psi^\dagger\right\rangle = \sqrt{n_s}$ the result shown in the figure.



$\Rightarrow$ BEC for $\mu > 0$
spontaneous symmetry breaking

As all linear terms cancel, the Hamiltonian take the approximate form

$$H \approx \text{const.} + \sum_{K>0}\left[\left(\epsilon_K + U n_s\right)\left(\tilde{c}^\dagger_K\tilde{c}_K + \tilde{c}^\dagger_{-K}\tilde{c}_{-K}\right) + U n_s\left(\tilde{c}^\dagger_K\tilde{c}^\dagger_{-K} + \tilde{c}_K\tilde{c}_{-K}\right)\right]$$

Our next goal is to bring this quadratic Hamiltonian into a simple form $\sum_k E_k b^\dagger_k b_k$ with suitably chosen bosonic operators $b^\dagger_K$ and b_K. Here we employ the so-called **Bogoliubov transformation** starting from

$$\tilde{c}^\dagger_K = u_K b^\dagger_K + v_K b_{-K}\,; \quad \tilde{c}_K = u_K b_K + v_K b^\dagger_{-K}$$
$$\text{with:} \quad u_{-K} = u_K\,,\; v_{-K} = v_K\,, \quad \in \mathbb{R}$$

We will choose the unknow prefactors u_K and v_K to reach two goals: (i) $b^\dagger_K$ and b_K have to fulfill bosonic commutation relations and (ii) the Hamiltonian should take the simple

form $\sum_k E_k b_k^\dagger b_k$.
Starting from the first condition

$$\left[b_K,\, b_{K'}^\dagger\right] = \delta_{K,\,K'}\ , \quad [b_K,\, b_{K'}] = \left[b_K^\dagger,\, b_{K'}^\dagger\right] = 0$$

we calculate the known commutation relations

$$\begin{aligned}
\delta_{K,K'} = \left[\tilde{c}_{K'}, \tilde{c}_K^\dagger\right] &= \left[\ u_{K'} b_{K'} + v_{K'} b_{-K'}^\dagger, u_K b_K^\dagger + v_K b_{-K}\right] \\
&= u_{K'} u_K \left[b_{K'}, b_K^\dagger\right] + v_{K'} u_K \left[b_{-K'}^\dagger, b_K^\dagger\right] \\
&+ v_{K'} v_K \left[b_{-K'}^\dagger, b_{-K}\right] + u_{K'} v_K \left[b_{K'}, b_{-K}\right] \\
&= u_K^2 \delta_{K,\,K'} - v_K^2 \delta_{K,\,K'} \equiv \delta_{K,\,K'}
\end{aligned}$$

$$\Rightarrow \quad u_K^2 - v_K^2 = 1$$

Using that $\cosh^2 x - \sinh^2 x = 1$ we can therefore use the following parametrization

$$u_K = \cosh(\varphi_K) \quad , \quad v_K = \sinh(\varphi_K)$$

or, equivalently,

$$u_K = \frac{1}{\sqrt{1-\alpha_K^2}} \quad , \quad v_K = \frac{\alpha_K}{\sqrt{1-\alpha_K^2}} \quad \text{with:}\ \ \alpha_K = \tanh(\varphi_K)$$

The inverse transformation is given by

$$b_k^\dagger = u_K \tilde{c}_K^\dagger - v_K \tilde{c}_{-K}$$

(i.e., by reversing the 'angle', $\varphi_k \to -\varphi_k$). We will now express H in terms of the new operators. First we calculate the two combination of operators which enter in H

$$\begin{aligned}
\tilde{c}_K^\dagger \tilde{c}_K + \tilde{c}_{-K}^\dagger \tilde{c}_{-K} &= \left(u_K^2 + v_K^2\right) \left(b_K^\dagger b_K + b_{-K}^\dagger b_{-K}\right) + 2 u_K v_K \left(b_K^\dagger b_{-K}^\dagger + b_K b_{-K}\right) \\
\tilde{c}_K^\dagger \tilde{c}_{-K}^\dagger + \tilde{c}_K \tilde{c}_{-K} &= 2 u_K v_K \left(b_K^\dagger b_K + b_{-K}^\dagger b_{-K}\right) + \left(u_K^2 + v_K^2\right) \left(b_K^\dagger b_{-K}^\dagger + b_K b_{-K}\right)
\end{aligned}$$

Using this result, we obtain for H

$$\begin{aligned}
\rightarrow \quad H = \text{const.} &+ \sum_{K>0} \left[(\epsilon_K + U n_s) \left(u_K^2 + v_K^2\right) + U n_s 2 u_K v_K\right] \left(b_K^\dagger b_K + b_{-K}^\dagger b_{-K}\right) \\
&+ \sum_{K>0} \left[(\epsilon_K + U n_s)\, 2 u_K v_K + U n_s \left(u_K^2 + v_K^2\right)\right] \left(b_K^\dagger b_{-K}^\dagger + b_K b_{-K}\right)
\end{aligned}$$

The terms in the first line have the desired form but we want to get rid of the terms in the

second line by the right choice of α_k. This leads to the condition

$$\frac{1}{1-\alpha_K^2}\left[\left(\epsilon_K + Un_s\right)2\alpha_K + Un_s\left(1+\alpha_K^2\right)\right] = 0$$

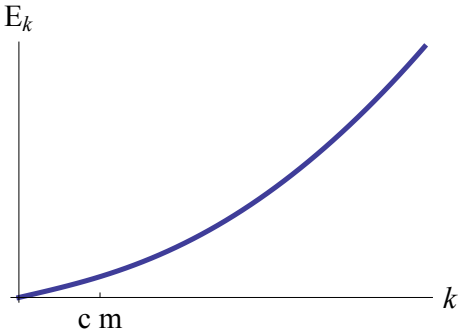
$$\Rightarrow \quad \alpha_K = -\left(\frac{\epsilon_K}{Un_s}+1\right) + \sqrt{\left(\frac{\epsilon_K}{Un_s}+1\right)^2 - 1}$$

Using this result we find

$$H = \text{const.} + \sum_K E_K b_K^\dagger b_K$$

$$\text{with:} \quad E_K = \sqrt{\epsilon_K\left(\epsilon_K + 2Un_s\right)} \cong \begin{cases} \hbar\,|k|\,c & \text{for} \quad \epsilon_K \ll 2Un_s \\ \epsilon_K = \frac{(\hbar k)^2}{2m} & \text{for} \quad \epsilon_K \gg 2Un_S \end{cases}$$

$$\text{with:} \quad c = \sqrt{\frac{Un_s}{m}}$$



Energy of the excitations in a BEC as a function of momentum.

For $\hbar\,|k| \ll cm$ the dispersion (i.e. the energy-momentum relation) is linear

$$E_K \approx c\,\hbar\,|K| \qquad \text{for } K \to 0 \tag{1.23}$$

while for large momenta the old quadratic dispersion still describes the excitations. This is an important result. A more careful analysis shows that the new excitations are weakly interacting. While our formula is quantitatively correct only for small U, qualitatively the results holds even for strongly interacting bosons: only the value of the speed c is modified. We have found that the excitations of the BEC are described by a new type of particles, the Bogoliubov quasi particles created by $b_k^\dagger$ and characterized by a linear dispersion. They describe the collective behavior of the original bosons (with quadratic dispersion) but have otherwise little to do with them. That interacting systems can lead to new types of quasi particles with new properties and, sometimes, new quantum numbers is a deep result at

the center of modern physics. Also the so-called elementary particles (electrons, quarks, photons,...) are probably "only" quasi particles of some other, not yet identified theory (one candidate is string theory).

The Bogoliubov quasi particles are an example of a so-called "Goldstone mode". The most important property of a Goldstone mode is that its energy vanishes in the limit of zero momentum $\lim_{K\to 0} E_K = 0$, a consequence of the so-called "Goldstone theorem" which states that such a mode exists in all systems with local interactions where a continuous symmetry (a symmetry described by a continuous real variable – the phase in our example) is spontaneously broken. While we will not give a formal derivation of the Goldstone theorem, the main argument is simple and takes in our case the following form: The phase ϕ_0 of $\langle\Psi\rangle$ describing the groundstate (see, e.g., Eq. (1.15)) is arbitrary. Changing this phase uniformly does therefore not cost any energy. The $k = 0$ Goldstone mode is precisely this mode.

Let us check this claim. An infinitesimal change $\delta\varphi$ of the phase of the wave function is described by

$$\Psi \to \Psi e^{i\,\delta\varphi} \approx \Psi\,(1 + i\,\delta\varphi) = \Psi + \delta\Psi \qquad \text{with } \delta\Psi = i\Psi\,\delta\varphi \tag{1.24}$$

In the limit $K \to 0$ we have $\alpha_{K\to 0} = -1 + \mathcal{O}\,(|K|)$ and therefore the change of the $k = 0$ mode is $\lim_{K\to 0} \tilde{c}_K^\dagger \propto \left(b_0^\dagger - b_0\right)$. It is therefore purely imaginary fully consistent with (1.24) as we have chosen $\langle\Psi\rangle$ to be real.

Another important example for a spontaneously broken symmetry is a solid: due to the periodic arrangement of atoms translation invariance is broken. The corresponding Goldstone modes are the phonons which also have an energy linear in momentum. Similarly, in a ferromagnet the spin-rotation symmetry is spontaneously broken (ignoring spin-orbit interactions and dipolar interactions here). In this case, the corresponding Goldstone mode, the spin waves, have a quadratic dispersion, $E_k \propto k^2$.

1.5.3 Superfluidity

The linear energy-momentum relation, Eq. (3.1) has a profound consequence: it leads to superfluidity. Superfluids can flow without any friction.

To make this surprising fact, first observed in superfluid ^{4}He, plausible we consider a thought experiment, where we investigated whether a particle moving through the superfluid will have any friction: A test particle with mass M moves with velocity $v = \frac{|\vec{p}|}{M}$ through a superfluid. We will investigate whether a process exist which can slow down the test particle by exciting a quasi-particle in the condensate with momentum q and energy $E_q = c\,|\vec{q}|$. After the collision the test particle has momentum $\vec{p} - \vec{q}$ and therefore energy conservation implies $\frac{p^2}{2m} = \frac{(\vec{p}-\vec{q})^2}{2M} + c\,|\vec{q}|$ and therefore we obtain

$$c\,|\vec{q}| = \frac{p^2}{2M} - \frac{(\vec{p}-\vec{q})^2}{2M} = \frac{2\vec{p}\,\vec{q} - q^2}{2M} < \frac{\vec{p}\,\vec{q}}{M} = \frac{|p|\,|q|\,\cos(\varphi)}{M} \leq v\,|q| \tag{1.25}$$

As this equation has no solution for $v < c$ it implies that a test particle with $v < c$ can not be slowed down by absorbing emitting a quasiparticle when moving through the superfluid. One can show (using that E_k is a convex function) that the same argument remains true for many-particle scattering. We conclude that the test particle experiences no friction as long as its velocity is smaller than a critical velocity v_c.[4]

Instead of considering the flow of a test particle, we can, equivalently, go to a frame of reference where the test particle is at rest while the superfluid moves. We therefore conclude that the superfluid itself will flow without friction as long as it is slower than v_c. If one therefore cools down a rotating liquid below the transition to a superfluid, it will continue to rotate without friction practically forever.

Note that superfluidity resulted from the repulsive interaction of the bosons as c is proportional to $\sqrt{U}$.

In conclusion, the example of superfluidity has shown how powerful the language of second quantization is to describe complex phenomena involving an arbitrarily large number of particles. We were able to identify a new set of quasi particles and obtained that superfluidity becomes possible due to a special conspiracy of a large number of particles which can move flow collectively without any friction.

[4] From our argument, we obtain $v_c = c$. This does, however, take not into account that also superconducting whirls, so-called vortices, can be emitted which can lead to a somewhat smaller critical velocity.

2 Quantization of Light

The history of quantum mechanics started with the description of light. When Planck tried to understand the radiation from a black body as a function of temperature, he introduced in 1900 for the first time Planck's constant. In 1905 Einstein explained the photoelectric effect by postulating that light consists of discretized objects – the photons. Also the quantum properties of atoms were discovered by investigating how they absorb and emit light. Quantum electro dynamics, QED, the quantum theory of light and its coupling to matter became later arguably the most successful and most precisely tested theory in physics. It describes almost all phenomena around us with the exception of gravity and effects like like radioactivity involving nuclear forces.
As the quantum theory of light has also to describe how photons are generated and destroyed, it is naturally formulated in the language of second quantization.

2.1 Quantization in Coulomb gauge

Our starting point is the classical theory of electrodynamics, the Maxwell equations. In Gauss units they take the form

$$\begin{aligned} \nabla \vec{E} &= 4\pi\rho \qquad & \nabla \times \vec{B} - \frac{1}{c}\frac{\partial \vec{E}}{\partial t} &= \frac{4\pi}{c}\vec{j} \\ \nabla \vec{B} &= 0 \qquad & \nabla \times E + \frac{1}{c}\frac{\partial \vec{B}}{\partial t} &= 0 \end{aligned} \tag{2.1}$$

where ρ is the charge density and $\vec{j}$ the current density.
The two equations in the second line are solved by introducing the **scalar potential** Φ and the **vector potential** $\vec{A}$, which plays an important role in the quantum mechanical description of electromagnetic phenomena. They are defined by

$$\vec{B} = \nabla \times \vec{A} \qquad \vec{E} = -\vec{\nabla}\Phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

These two equations do not fix $\vec{A}$ and Φ uniquely. The are only defined up to a **gauge transformation**

$$\Phi \rightarrow \Phi - \frac{1}{c}\frac{\partial}{\partial t}\varphi \quad ; \vec{A} \rightarrow \vec{A} + \vec{\nabla}\varphi$$

which leaves $\vec{E}$ and $\vec{B}$ invariant (check this!). Here $\varphi(\vec{r},t)$ is an arbitrary function. In classical electrodynamics the introduction of the vector potential appears as a mathematical trick and gauge invariance seems to be just an extra complication. In the context of quantum mechanics and quantum field theory, however, gauge invariance turns out to be a central phenomenon as we will discuss later in some detail.
For the moment, however, the gauge invariance complicates somehow the formulation of a quantum theory of light and, indeed, quantization in the presence of gauge invariance can be complicated due to "unphysical" gauge degrees of freedom. We will avoid these complications by using only one specific gauge by adding one more equation to determine $\vec{A}$

$$\text{Coulomb gauge: } \vec{\nabla}\,\vec{A} = 0$$

This has two main disadvantages: the Coulomb gauge is not Lorentz invariant and we lost gauge invariance, i.e. the freedom to switch from one gauge to the next. But there are also two advantages: we do not have to worry about changes of the vector potential which describe only changes of the gauge but have no physical consequences and, second, the Coulomb interaction becomes simple.
To see this, we study the first Maxwell equation

$$\vec{\nabla}\,\vec{E} = -\vec{\nabla}^2\Phi - \underbrace{\frac{1}{c}\frac{\partial}{\partial t}\vec{\nabla}\vec{A}}_{=0 \text{ choice of gauge}} = 4\pi\rho$$

This is solved directly by

$$\Phi\left(\vec{r},\,t\right) = \int \frac{\rho\left(\vec{x},\,t\right)}{|\vec{r}-\vec{x}|}\,\mathrm{d}\vec{x}$$

The potential Φ is in this gauge therefore exactly fixed by the charge and no further quantization is required for this field. All effects of photons and the quantum nature of the electric field will be described by $\vec{A}$ instead.
To simplify the problem, we will now consider free space in the absence of charges and currents, $\rho = 0$, $\vec{j} = 0$. Therefore also Φ vanishes and we obtain

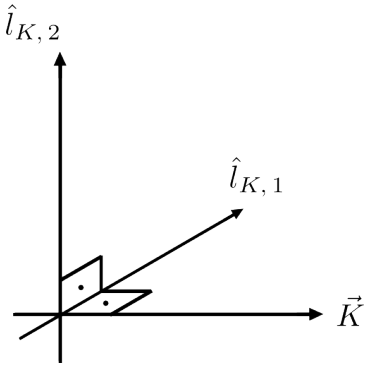
$$\vec{\nabla}\times\vec{B} = \vec{\nabla}\times\left(\vec{\nabla}\times\vec{A}\right) = \underbrace{\vec{\nabla}\left(\vec{\nabla}\vec{A}\right)}_{=0 \text{ choice of gauge}} - \vec{\nabla}^2\vec{A}, \qquad \frac{\partial\vec{E}}{\partial t} = -\frac{1}{c}\frac{\partial^2\vec{A}}{\partial t^2}$$

Therefore the second of Maxwell's equation takes the simple form

$$\Box\vec{A} = \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \vec{\nabla}^2\right)\vec{A} = 0$$

As the solutions of this wave equation are just plane waves, it is useful to expand $\vec{A}$ in plane waves, while taking into account the gauge condition $\nabla\vec{A} = 0$
In these variables the vector potential has the form

$$\begin{aligned}\vec{A}(\vec{x},\,t) &= \frac{1}{\sqrt{V}}\sum_{\vec{K}} e^{i\vec{K}\vec{x}}\,\vec{A}_{\vec{K}}(t)\\ \vec{\nabla}\vec{A} &= 0 \Rightarrow \vec{K}\cdot\vec{A}_K = 0\end{aligned}$$



The last equation is implemented by defining two unit vectors perpendicular to $\vec{K}$, $\hat{e}_{\vec{K},\,1} \perp \hat{e}_{\vec{K},\,2} \perp \vec{K}$, $|\hat{e}_{K,\lambda}| = 1$ and, furthermore, $\hat{e}_{-\vec{K},\lambda} = \hat{e}_{\vec{K},\lambda}$. Later we will see that $\hat{e}_{k,1/2}$ describes two polarization directions of light. As $\vec{A}_{\vec{K}}$ is perpendicular to $\vec{K}$, we can write it in the form $\vec{A}_{\vec{K}} = \hat{e}_{K,\,1}\,q_{\vec{K},1} + \hat{e}_{K\,2}\,q_{\vec{K},2}$ where $q_{\vec{K},1}$ and $q_{\vec{K},2}$ are some complex coefficients.

$$\vec{A}(\vec{x},\,t) = \frac{1}{\sqrt{V}}\sum_{\vec{K},\,\lambda=1,2} e^{i\vec{K}\vec{x}}\,\hat{e}_{\vec{K},\,\lambda}\,q_{\vec{K},\,\lambda}(t)$$

From the condition $\vec{A}(\vec{x},\,t) = \vec{A}^*(\vec{x},\,t)$ follows $q_{-\vec{K},\,\lambda} = q^*_{\vec{K},\,\lambda}$. From the equation of motion $\Box\vec{A} = 0$, we obtain the frequency ω_K describing the oscillations of the two modes

$$\ddot{q}_{K,\,\lambda} + (kc)^2\,q_{K,\,\lambda} = 0 \quad \Rightarrow \quad \omega_K = c|K|$$

It is instructive to rewrite also the energy in terms of the variables $q_{\vec{K},1}$ and $q_{\vec{K},2}$. In our units the energy is given by $E = \frac{1}{8\pi}\int\left(\vec{E}^2 + \vec{B}^2\right)\mathrm{d}^3x$. Using

$$\begin{aligned}&\vec{E} = -\frac{1}{c}\frac{\partial\vec{A}}{\partial t}, \qquad \hat{e}_{K,\,1}\,\hat{e}_{K,\,2} = 0, \qquad \left(\vec{K}\times\hat{e}_{K,\,\lambda}\right)\left(\vec{K}\times\hat{e}_{K,\,\lambda'}\right) = \delta_{\lambda\,\lambda'}K^2\\ &\vec{B} = \vec{\nabla}\times\vec{A} = \frac{1}{\sqrt{V}}\sum_{\vec{K},\,\lambda=1,2} i\left(\vec{K}\times\hat{e}_{K,\,\lambda}\right)e^{i\vec{K}\vec{x}}\,q_{K,\,\lambda}\end{aligned}$$

one can rewrite the electromagnetic energy in the vacuum

$$E = \frac{1}{2}\sum_{K,\,\lambda}\frac{\dot{q}_{K,\,\lambda}\dot{q}_{-K,\,\lambda}}{4\pi c^2} + \frac{(|K|c)^2}{4\pi c^2}\,q_{K,\,\lambda}\,q_{-K,\,\lambda} \tag{2.2}$$

with $q_{K,\,\lambda}\,q_{-K,\,\lambda} = |q_{K,\,\lambda}|^2 = (\mathrm{Re}\;q_{K,\,\lambda})^2 + (\mathrm{Im}\;q_{K,\,\lambda})^2$.

What we have achieved is a *classical* description of the electromagnetic waves in vacuum using for each momentum two relevant degrees of freedom $q_{\vec{K},1}$ and $q_{\vec{K},2}$ describing oscillations int the two polarization directions of electromagnetic waves given by $\hat{e}_{k,1}$ and $\hat{e}_{k,1}$, respectively.

Now we will quantize this classical theory. Here it is useful to realize that Eq. (2.2) looks almost like the energy of a harmonic oscillator. Luckily, we already know how to write a harmonic oscillator in terms of operators which have exactly the properties of creation

and annihilation operators. The classical energy of an harmonic oscillator can be written as $E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2$, the corresponding Hamiltonian written in terms of new variales $a^\dagger$ and a with

$$x = \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right), \qquad p = i\sqrt{\frac{\hbar m\omega}{2}}\left(a^\dagger - a\right)$$
$$\left[a,\, a^\dagger\right] = 1 \;\Leftrightarrow\; [x,\, p] = \frac{i\hbar}{2}\left[a + a^\dagger,\, a^\dagger - a\right] = \frac{i\hbar}{2}(1+1) = i\hbar \tag{2.3}$$

has the form $H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$.
We will use precisely this construction in the following. By comparing (2.2) to $E = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\omega^2 x^2$, the energy of the harmonic oscillator, we can identify for each fixed $\vec{K}$

$$m \mathrel{\hat{=}} \frac{1}{4\pi c^2}\,, \quad \omega \mathrel{\hat{=}} |K|c = \omega_K$$

In close analogy to the harmonic oscillator we therefore define

$$q_{\vec{K},\lambda} = \sqrt{\frac{\hbar 4\pi c^2}{2c|K|}}\left(a^\dagger_{\vec{K},\lambda} + a_{-\vec{K},\lambda}\right) \tag{2.4}$$

such that $q_{-K,\lambda} = q^\dagger_{K,\lambda}$. We postulate canonical commutation relations for the new operators and get

$$\vec{A}\,(\vec{x}) = \sqrt{\frac{2\pi\hbar c^2}{V}}\sum_{\vec{K},\lambda}\frac{\hat{e}_{\vec{K},\lambda}}{\sqrt{c|K|}}\left(e^{-i\vec{K}\vec{x}}a^\dagger_{\vec{K},\lambda} + e^{+i\vec{K}\vec{x}}\,a_{\vec{K},\lambda}\right) \tag{2.5}$$

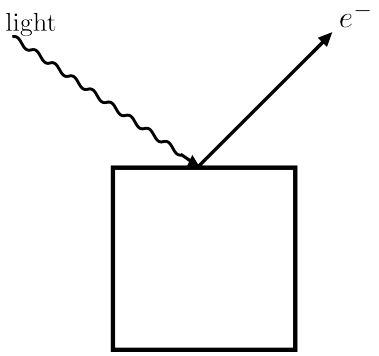
with: $\left[a_{\vec{K},\lambda},\, a^\dagger_{\vec{K}',\lambda'}\right] = \delta_{\lambda\lambda'}\,\delta_{K,K'}, \quad \left[a^\dagger,\, a^\dagger\right] = [a,\, a] = 0$

Thus we have quantized light. The new operator $a^\dagger_{\vec{K},\lambda}$ creates a photon with momentum $\hbar\vec{K}$ and polarisation $\hat{e}_{\vec{K},\lambda}$.
As all formulas are the same as for the harmonic oscillator we obtain for the Hamiltonian

$$\text{in vacuum:}\quad H_{\text{photon}} = \sum_{\vec{K},\lambda}\hbar\omega_K\left(a^\dagger_{\vec{K},\lambda}\,a_{\vec{K},\lambda} + \frac{1}{2}\right) \qquad \text{with:}\;\; \omega_K = |K|c \tag{2.6}$$

As a side remark, we note that the factor 1/2 in the energy (2.6) would imply that the vacuum itself has an enormous energy density. While adding a constant to the energy has no effects within quantum electrodynamics, we know from general relativity, that it leads to a curvature of space. As this is not observed, the factor 1/2 is either unphysical or cancelled with extremely high precision by another term. At least partially such a cancellation is reached in extensions of the standard model of particle physics which are based on "supersymmetry" – a postulated symmetry of bosons and fermions. Here each

This already explains the basic observation of the photoelectric effect (Einstein 1905). As the counting operator $a^\dagger_{\vec{K},\lambda}\, a_{\vec{K},\lambda}$ is always an integer, the energy of light of a given wavelength $\lambda = 2\pi/K$ is quantized in "chunks" of energy $\hbar|K|c$. Therefore a minimal value of $\vec{K}$ is required to kick out an electron of a solid. The total energy current of light of a given wavelength determines only the photon density, not the energy of a given photon. It therefore determines the number of emitted electrons but not their energy. All this cannot be understood in terms of a classical description of light.



boson is accompanied by a new – not yet discovered – particle which is a fermion. The partner of the photon, for example, is called „photino". These fermions come with a contribution to the energy of $-\frac{1}{2}\hbar\omega_K$ per mode, therefore helping to solve this problem. One main goal of the LHC at Cern is to search for signatures of supersymmetry – up to now with no success.

It is now easy to construct also the **Hilbert space of photons**. We just postulate the existence of a vacuum $|0\rangle$ state with $a_{K,\lambda}\ |0\rangle = 0$. The we build the Fock-space by applying $a^\dagger_{K,\lambda}$.

In vacuum, the Heisenberg equations of motion take the form

$$i\hbar\frac{\partial}{\partial t}a^\dagger_{K,\lambda} = \left[a^\dagger_{K,\lambda},\, \hbar\omega_K a^\dagger_{K,\lambda}a_{K,\lambda}\right] = \hbar\omega_K\, a^\dagger_{K,\lambda} \quad \text{in vacuum}$$

solved by

$$a^\dagger_{K,\lambda}(t) = e^{i\omega_K t}\, a^\dagger_{K,\lambda}(0)$$

In the Heisenberg picture the time dependent electric and magnetic fields **in vacuum** can now easily be obtained from the formula for the vector potential (2.5)

$$\vec{B}(r,t) = \vec{\nabla}\times\vec{A} = \sqrt{\frac{2\pi\hbar c^2}{V}}\sum_{K,\lambda}\frac{i\vec{K}\times\hat{e}_{K,\lambda}}{\sqrt{c|K|}}\left(e^{i\vec{K}\vec{r}}\, a_{K,\lambda}(t) - e^{-i\vec{K}\vec{r}}\, a^\dagger_{K,\lambda}(t)\right)$$

only in the absence of matter: (2.7)

$$\vec{E}(\vec{r},t) = \vec{E}_\perp(\vec{r},t)$$
$$= -\frac{1}{c}\frac{\partial\vec{A}}{\partial t} = \sqrt{\frac{2\pi\hbar}{V}}\sum_{K,\lambda} i\sqrt{c|K|}\,\hat{e}_{K,\lambda}\left(e^{i\vec{K}\vec{r}}\, a_{K,\lambda}(t) - e^{-i\vec{K}\vec{r}}\, a^\dagger_{K,\lambda}(t)\right)$$

The formula for $\vec{E}$ is only valid in the absence of matter for two reasons. First, in the presence of charges there is an extra contribution $\vec{E} = -\nabla\Phi$ and, second, the time dependence

of the the operators is modified by interactions and one has to compute $\vec{E}_\perp = \vec{E} + \nabla\Phi$ from $\left[\dot{\vec{A}} = -\frac{i}{\hbar}\left[\vec{A},\, H\right]\right]$.
At equal times, we obtain for the commutators of electric and magnetic field

$$\begin{aligned}\left[E_i(r),\, E_j(r')\right] &= \left[B_i(r),\, B_j(r')\right] = 0\\ \left[E_i(\vec{r}),\, B_j(\vec{r}')\right] &= i\; 4\pi\hbar c\; \epsilon_{ijk} \frac{\partial}{\partial r_K} \delta^3\left(\vec{r} - \vec{r}'\right)\end{aligned}$$

This implies an uncertainity relation for E and B fields: they can in principle not be measured simultaneously.

2.2 Coherent states and classical electromagnetic fields

After we have found the quantum description of fields, we will now consider again the classical limit. More precisely, we ask for which quantum states one obtains the classical fields as expectation values of the quantum operators, $\vec{E}_c = \left\langle \vec{E} \right\rangle$. As the electromagnetic fields $\vec{E}$ and $\vec{B}$ always change the photon number by $\pm$ one photons, their expectation value $\langle\Psi|\, \vec{E}\, |\Psi\rangle = \langle\Psi|\, \vec{B}\, |\Psi\rangle = 0$ vanishes for each wave function $|\Psi\rangle$ with *fixed* number of photons and therefore for each basis state of our Fock space.
In vacuum a *classical* electromagnetic wave has the form

$$\vec{E}_c(x,t) = \vec{E}_0\, \sin\left(\vec{K}_0\vec{x} - \omega_0 t\right) \qquad \vec{B}_c(x,t) = \vec{B}_0\, \sin\left(\vec{K}_0\vec{x} - \omega_0 t\right)$$

with $\omega_0 = c|K_0|$, $\vec{B}_0 = i\vec{K}_0 \times \vec{E}_0$ and $E_0,\, B_0 \perp K_0$.
Comparing this with the formula (2.7) for the operator, we see that this can only be achieved for

$$\begin{aligned}\langle a_{K,\lambda}\rangle &= \delta_{K,K_0}\, \delta_{\lambda,\lambda_0}\, \alpha e^{i\varphi}\, \sqrt{V}\,, \quad \alpha,\ \varphi \in \mathbb{R}\\ \left\langle a^\dagger_{K,\lambda}\right\rangle &= \delta_{K,K_0}\, \delta_{\lambda,\lambda_0}\, \alpha e^{-i\varphi}\, \sqrt{V}\end{aligned}$$

With this one finds

$$\begin{aligned}\left\langle \vec{E}(r,t)\right\rangle &= \sqrt{2\pi\hbar\, c\, |k_0|}\, \hat{e}_{\vec{K}_0,\,\lambda_0}\, 2\alpha \sin\left(\vec{k}_0\vec{r} - \omega_0 t - \varphi\right)\\ \left\langle \vec{B}(r,t)\right\rangle &= \sqrt{2\pi\hbar\, c\, |k_0|}\, \vec{K}_0 \times \hat{e}_{\vec{K}_0,\,\lambda_0}\, 2\alpha \sin\left(\vec{k}_0\vec{r} - \omega_0 t - \varphi\right)\end{aligned}$$

We obtained previously states with a finite expectation value of a creation operator: Bose Einstein condensates. A classical plane indeed shares some similarities with a BEC: the analogy works best when a laser is used as a light source. There are, however, two main differences: the electromagnetic plane wave is not a state in thermal equilibrium and it is not a superfluid.

Eigenstates of the annihilation operator, so called **coherent states** have the desired property .

$$\text{coherent state} = \text{eigenstate of } a_{\vec{K}_0,\lambda_0}$$

As we discuss also in the problem sets of this lecture, the equation $a_{K_0,\,\lambda_0}\,|\Psi\rangle = Z\,|\Psi\rangle$ with $Z = \sqrt{V}\alpha e^{i\varphi} \quad \in \mathbb{C}$ is solved by

$$|\Psi\rangle = c\,\exp\Big(z a^\dagger_{K_0,\,\lambda_0}\Big)\,|0\rangle$$

Here we just check this result

$$\begin{aligned} a\,e^{za^\dagger}\,|0\rangle &= a\sum \frac{z^n}{n!}\left(a^\dagger\right)^n|0\rangle = \sum \frac{z^n}{n!} n\left(a^\dagger\right)^{n-1}|0\rangle \\ &= z\sum \frac{z^{n-1}}{(n-1)!}\left(a^\dagger\right)^{n-1}|0\rangle = z\,e^{za^\dagger}\,|0\rangle \end{aligned}$$

where we used that

$$\begin{aligned} a\left(a^\dagger\right)^n = \left(a^\dagger\right)^{n-1} + a^\dagger a\left(a^\dagger\right)^{n-1} = \left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^2 a\left(a^\dagger\right)^{n-2} = \\ \cdots = n\left(a^\dagger\right)^{n-1} + \left(a^\dagger\right)^n a \end{aligned}$$

The importance of coherent states arises as they describe best classical states of matter. As such they can also be used to describe a particle in a simple harmonic oscillator. They are also the starting point for describing a BEC or a laser.

2.3 Interactions of photons & matter

2.3.1 Hamiltonian

To describe the coupling of the electromagnetic waves to matter, we use that for the chosen Coulomb gauge the only new aspect is that the vector potential is now written in terms of photon creation and annihilation operators. The electric potential, in contrast, and therefore the interaction energies of ions and electrons are not modified for this gauge choice.[1] We can therefore just use the previously obtained Hamiltonian (1.11) and replace vector potential and magnetic field by the quantized operators. The total Hamiltonian is then given by

$$H = H_{\text{photon}} + H_{\text{matter}}[\vec{A}] \qquad \text{with:} \quad H_{\text{photon}} = \sum \hbar\omega_K a^\dagger_{K,\,\lambda} a_{K,\,\lambda} \tag{2.8}$$

This Hamiltonian describes accurately all relevant properties of light bulbs, solar cells, the human eye[2], the laser at the supermarket and many more things.

[1] For other gauge choices the Coulomb interaction is described by the virtual exchange of photons.

[2] The motion of nuclei needed for description of most biological processes, which is missing in (1.11), can easily be added.

In the following, we will focus on a simple but important example: the coupling of light to a single atom. As most of the readers are probably still more familiar with 1st instead of 2nd quantization, we describe for this example the electrons is the language of first quantization. This implies that for an atom with N electrons we introduce N coordiates r_1, r_2, $\dots$, r_N and N spin operators $\vec{S}_1$, $\vec{S}_2$, $\dots$, $\vec{S}_N$. The light, however, has to be described in second quantization. The total Hilbert space is given by $\mathbb{H} = \underbrace{\mathcal{F}_{\text{photons}}}_{\text{Fock-space}} \otimes \underbrace{\mathbb{H}_{\text{atom}}}_{N-\text{electrons}}$.
Using this mixed 1st/2nd quantization language, the Hamiltonian is given by

$$H = \sum_{\vec{K},\lambda} \hbar c |K| a^{\dagger}_{K,\lambda} a_{K,\lambda} + \sum_{i=1}^{N} \frac{\left(\vec{p}_i - \frac{e}{c}\vec{A}\left(\vec{r}_i\right)\right)^2}{2m} + V\left(\vec{r}_i\right) - 2\mu_B \vec{B}\left(\vec{r}_i\right)\vec{S}_i$$

It is worthwhile to consider the mathematical structure of, $\vec{A}(\vec{r}_i)$ and $\vec{B}(\vec{r}_i)$. They are operators acting on the photon Fock space $\mathcal{F}_{\text{photons}}$ as they are expressed in terms of creation and annihilation operators, Eqs. (2.5) and (2.7). The coordinate r_i is, however, an operator acting on the atomic Hilbert space $\mathbb{H}_{\text{atom}}$. Therefore this operator connects the two parts of $\mathbb{H}$.

2.3.2 Absorption & Emission in perturbation theory

In practically all cases (exceptions are strong lasers or atoms in extremely good cavities made from almost perfect mirrors) the coupling of atoms to light can be described by perturbation theory. The reason for this is (as we will also see in our chapter on relativistic quantum theory) that the parameter describing the strength of the coupling of light and matter, the fine-structure constant $\alpha = e^2/(\hbar c)$ turns out to be very small

$$\alpha = \frac{e^2}{\hbar\, c} \approx 0.00729735256 \approx \frac{1}{137} \ll 1 \tag{2.9}$$

We therefore split the Hamiltonian in a large part H_0 and a small correction H'

$$H = H_0 + \underbrace{H'}_{\text{small}}$$
$$H_0 = H_{\text{photon}} + H_{\text{matter}}\left(\vec{A} = 0\right), \qquad H' = H'_1 + H'_2 + H'_3$$
$$H'_1 = -\sum_{i=1}^{N} \frac{e}{c\, m}\vec{p}_i\,\vec{A}, \qquad H'_2 = -\frac{e\,\hbar}{2m\,c}\sum_i \vec{\sigma}_i \vec{B}\left(\vec{r}_i\right), \qquad H'_3 = \sum_i \frac{e^2}{2m\,c^2}\left(\vec{A}\left(\vec{r}_i\right)\right)^2$$

where we used for H'_1 that in the Coulomb gauge, $\nabla\vec{A} = 0$, one has $\vec{p}_i\vec{A}(r_i) = \vec{A}(r_i)\vec{p}_i$ as $\vec{p}_i = -i\hbar\vec{\nabla}_{r_i}$.
In the following we will focus our discussion on **one-photon processes** where a single photon is either emitted or absorbed. To formulate perturbation theory, we first need the eigenstates of H_0 which we denote as

$$|\alpha\rangle = |\underbrace{\mu}_{\substack{\text{quantum number}\\ \text{of atom}}}, \underbrace{n_{K,\lambda}}_{\substack{\text{occupation of}\\ \text{photon mode}}}\rangle$$

$$H_0|\alpha\rangle = E_\alpha|\alpha\rangle \qquad \text{with} \quad E_\alpha = \underbrace{E_\mu^A}_{\substack{\text{energy of}\\ \text{atomic state}}} + \hbar c|K| n_{K,\lambda}$$

For our discussion of one-photon processes only a single photon mode is important, therefore a single integer describes the last argument of $|\alpha\rangle$ in the following.
In leading order perturbation theory, we will use an important result, derived and discussed in all quantum mechanics text books in the chapter on time-dependent perturbation theory. "Fermi's golden rule" states that the transition rate from a quantum state $|\alpha\rangle$ to the state $|\alpha'\rangle$ due to the perturbation H' is given by

$$\Gamma_{\alpha',\alpha} = \frac{2\pi}{\hbar}\left|\langle\alpha'|H'|\alpha\rangle\right|^2 \delta\left(E_\alpha - E'_\alpha\right) \tag{2.10}$$

where for single-photon processes we consider only $|\alpha\rangle = |\mu, n_{K,\lambda}\rangle$ in combination with $|\alpha'\rangle = |\mu', n_{K,\lambda} \pm 1\rangle$.
As we need the matrix element $\langle\alpha'|H'|\alpha\rangle$, we evaluate it for $H' = H'_1 + H'_2 + H'_3$. The first contribution arises from

$$\begin{aligned}\langle\alpha'|H'_1|\alpha\rangle = -\sum_{K,\lambda=1,2}\frac{e}{cm}\sqrt{\frac{2\pi\hbar c^2}{V}}\frac{1}{\sqrt{c|K|}}\Big\langle \mu',\, n_{K,\lambda\pm1}\Big|\hat{e}_{K,\lambda}\vec{p}_i\Big(e^{-i\vec{K}\vec{r}_i}\,a^\dagger_{K,\lambda} + \dots \\ \dots + e^{i\vec{K}\vec{r}_i}\,a_{K,\lambda}\Big)\Big|\mu,\, n_{K,\lambda}\Big\rangle \\ = -\frac{e}{cm}\sqrt{\frac{2\pi\hbar c}{V|K|}}\cdot\begin{cases}F_e^{(1)}\sqrt{n_{K,\lambda}+1} & \text{emission}\\ F_a^{(1)}\sqrt{n_{K,\lambda}} & \text{absorption}\end{cases}\end{aligned}$$

$$F_{e/a}^{(1)} = \Big\langle\mu'\Big|\sum_{i=1}^{N}\hat{e}_{K,\lambda}\vec{p}_i e^{\pm i\vec{K}\vec{r}_i}\Big|\mu\Big\rangle \qquad \text{atomic matrix element}$$

In analogy, the second contribution is given by

$$\langle\alpha'|H'_2|\alpha\rangle = \frac{i\,e}{cm}\sqrt{\frac{2\pi\hbar c}{V|K|}}\cdot\begin{cases}F_e^{(2)}\sqrt{n_{K,\lambda}+1} & \text{emission}\\ F_a^{(2)}\sqrt{n_{K,\lambda}} & \text{absorption}\end{cases}$$

$$F_{e/a}^{(2)} = \Big\langle\mu'\Big|\frac{1}{2}\sum_{i=1}^{N}\hat{e}_{K,\lambda}\left(\hbar\vec{K}\times\vec{\sigma}_i\right)e^{\pm i\vec{K}\vec{r}_i}\Big|\mu\Big\rangle \tag{2.11}$$

As we consider only processes where one photon is absorbed or emitted, there is not contribution from $H'_3 \propto A^2 \propto a^\dagger a^\dagger + a^\dagger a + aa$.
Combining both contributions we obtain

$$\Gamma_{\alpha'\alpha} = \frac{2\pi}{\hbar}\left(\frac{e}{c\,m}\sqrt{\frac{2\pi\hbar c}{V|K|}}\right)^2 \delta\big(E^A_\mu - \big(E^A_{\mu'} \pm \hbar|K|c\big)\big) \times \left|F^{(1)}_{e/a} - iF^{(2)}_{e/a}\right|^2 \begin{cases} n_{K,\lambda}+1 & \text{emission} \\ n_{K,\lambda} & \text{absorption} \end{cases} \tag{2.12}$$

When there was not photon in the initial state, $n_{K,\lambda} = 0$, obviously an absorption process, where the energy of the electron rises, is not possible. An excited state can, however, decay by emitting one photon, thus lowering its energy. This is far from obvious: in classical physics, a transition from one stationary state to another would not be possible in the absence of some external stimulation by light. **Spontaneous emission**, i.e. emission starting from $n_{K,\lambda} = 0$, becomes possible only due to quantum fluctuations. The groundstate of an atom is its only stable state: for an atom in vacuum all excited states ultimatively decay.

The absorption rate of a single atom is in perturbation theory proportional to the number of photons consistent with the observation, e.g., in the context of the photoelectric effect. Remarkably, also the emission rate increases when more photons are present in a given mode. This phenomenon, called **stimulated emission**, is the working principle behind a laser. Excited atoms tend to emit more and more photons into a given mode of a cavity if this mode is already occupied. This results in intensive single-mode laser light.

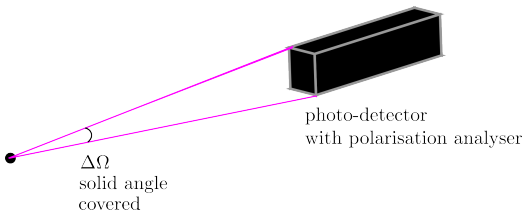
2.3.3 Decay rate of excited atoms

Absorption and emission of light atoms and molecules can be measured in various ways. Most importantly, one can measure the absorption or emission spectrum. The emission spectrum is measured by first exciting atoms (e.g., by heating up a gas or shining light on it) and then measuring the energy of emitted photons. One usually observes sharp peaks in the spectrum. The position of the peak is determined by the energy difference $E^A_\mu - E^A_{\mu'}$. If at time $t = 0$ a large number N_0 of atoms is excited, the number of excited atoms in state μ will decay exponentially, $N_\mu(t) \approx N_0 e^{-\Gamma_\mu t}$ where the total decay rate is obtained by summing over all possible final states

$$\Gamma_\mu = \sum \Gamma_{\alpha'\alpha}$$

with initial state $|\alpha\rangle = |\mu, 0\rangle$. One of the goals of this chapter will be to calculate the decay rate. Such decay rates also determine the line width observed in the spectrum.

One can also use a photo detector to record the number of photons which have been emitted in a certain direction. An (idealized) photon detector counts all photons of a given energy and polarization emitted into a given solid angle, see figure.



To calculate the signal in the detector, we need to add up all processes which emit photons with polarization λ into a given solid angle $\Delta\Omega$. To do this, we use polar coordinates for the wave vector $\vec{k}$ of the emitted photon. We define

$$\frac{d\Gamma_{\mu',\lambda\mu}}{d\Omega_k} = V\int \frac{k^2 dk}{(2\pi)^3}\Gamma_{\alpha'\alpha}$$

This is the decay rate per solid angle of the atomic level μ to the level μ' by emitting a for photon with polarization λ into a given direction $\hat{k}$. The initial state is an atom in state μ without any extra photons, $|\alpha\rangle = |\mu, 0\rangle$. In the final state $|\alpha'\rangle = \left|\mu', \lambda\vec{k}\right\rangle$ the atom is in state μ' and a photon wavevector $\vec{k} = k\hat{k}$ and polarization λ. The total decay rate can be obtained by simply summing over all angles, all possible final states μ' and the two polarization directions

$$\Gamma_\mu = \int d\Omega_k \sum_{\mu',\lambda} \frac{d\Gamma_{\mu'\lambda,\mu}}{d\Omega_k}$$

where we used that $\sum_{\vec{k}} ... = \frac{V}{(2\pi)^3}\int d^3\vec{k}... = V\int \frac{k^2 dk}{(2\pi)^3}\int \underbrace{d\Omega_k}_{angles}$

From Eq. (2.12) we therefore obtain

$$\frac{d\Gamma_{\mu',\lambda\mu}}{d\Omega_k} = V\int \frac{k^2 dk}{(2\pi)^3}\Gamma_{\alpha'\alpha} = \int \frac{k^2 dk}{(2\pi)^3}\frac{e^2}{m^2c^2}\frac{2\pi}{\hbar}\frac{2\pi\hbar c}{|k|}\delta\left(\hbar c\,|k| - \left(E^A_\mu - E^A_{\mu'}\right)\right)\left|F_e^{(1)} - iF_e^{(2)}\right|^2$$

With the help of the δ function, the k integral is easily evaluated

$$\frac{d\Gamma_{\mu',\lambda\mu}}{d\Omega_k} = \frac{|k|\,e^2}{2\pi\hbar c^2 m^2}\left|F_e^{(1)} - iF_e^{(2)}\right|^2 = \frac{\alpha}{2\pi}\frac{mc^2}{\hbar}\frac{\hbar k}{mc}\frac{\left|F_e^{(1)} - iF_e^{(2)}\right|^2}{(mc)^2} \tag{2.13}$$

$$\text{with}\quad k = \frac{1}{\hbar c}\left(E^A_\mu - E^A_{\mu'}\right) > 0 \tag{2.14}$$

Note that we have expressed the result in terms of the relativistic rest energy mc^2 of the electron and the fine structure constant $\alpha = \frac{e^2}{\hbar c}$, see Eq. (2.9). In general, it is useful to use consistently relativistic units

energy mc^2, momentum mc, length $\frac{\hbar}{mc}$, time $\frac{\hbar}{mc^2}$

which are then multiplied by powers of $\alpha \approx 1/137$.
For example, one obtains for Bohr's radius $a_B = \frac{\hbar}{mc}\frac{1}{\alpha}$ and for the binding energy of the electron in a hydrogen atom 1 Rydberg $= mc^2\frac{\alpha^2}{2}$. Therefore the typical velocity of an

electron in a hydrogen atom is $v \sim \alpha c \ll c$, a fact which will be come important when we develop later a relativistic quantum theory.
These qualitative considerations are also very useful when computing the matrix elements $F_e^{(1)}$ and $F_e^{(2)}$. The first was defined as

$$F_e^{(1)} = \left\langle \mu' \left| \sum_i \hat{e}_{\vec{k}\lambda} \vec{p_i} e^{i\vec{k}\vec{r}_i} \right| \mu \right\rangle$$

To estimate the size of the factor $\vec{k}r_i$, we can use that the emitted light has an energy of the order of $\alpha^2 mc^2$ and therefore the typical size of k is of the order of $\alpha^2 mc$. The typical size of r_i is given by Bohr's radius $\frac{\hbar}{mc}\frac{1}{\alpha}$ and therefore $\vec{k}\vec{r}_i$ is of the order of α only. In other words, the wavelength of light is much larger than the atomic radius because α is so small. We can therefore just use a Taylor expansion in $\vec{k}$ when computing F_e^1 or F_e^2. To leading order in powers of α we approximate

$$F_e^{(1)} \approx \hat{e}_{k\lambda} \left\langle \mu' \left| \sum_{i=1}^{N} \vec{p_i} \right| \mu \right\rangle (1 + O(\alpha))$$

Using that $[\vec{r_i}, H_0] = \left[r_i, \frac{p_i^2}{m}\right] = i\hbar\frac{\vec{p_i}}{m}$ one can rewrite

$$\left\langle \mu' \left| \vec{p_r} \right| \mu \right\rangle = \frac{m}{\hbar i} \left\langle \mu' \left| \vec{r_i} H_0 - H_0 \vec{r_i} \right| \mu \right\rangle = \frac{m}{\hbar i} \left(E_\lambda^A - E_{\lambda'}^A\right) \left\langle \mu' \left| \vec{r_i} \right| \mu \right\rangle$$

Therefore the matrix element $F_e^{(1)}$ is determined to leading order in α by the **dipole operator** $\vec{r} = \sum_{i=1}^{N} \vec{r_i}$

$$\begin{aligned} F_e^{(1)} &= i\, mc|k| \cdot \hat{e}_{\vec{k}\lambda} \left\langle \mu' \left| \vec{r} \right| \mu \right\rangle \\ \frac{d\Gamma_{\mu'\lambda\mu}}{d\Omega_k} &= \frac{\alpha}{2\pi} \frac{(|k|\, c)^3}{c^2} \left| \hat{e}_{\vec{k}\lambda} \left\langle \mu' \left| \vec{r} \right| \mu \right\rangle \right|^2 \end{aligned} \tag{2.15}$$

The corresponding radiation is named **electrical dipole radiation**. It has the typical angular distribution known from a dipole antenna in classical physics oriented in the direction of $\langle \mu' | \vec{r} | \mu \rangle$. Note that the matrix element $\langle \mu' | \vec{r} | \mu \rangle$ is finite only when certain selection rules are fulfilled, $\Delta l = \pm 1$, $\Delta m = 0, \pm 1$, $\Delta\sigma = 0$.
To calculate the total decay rate for dipole radiation, we use $\sum_\lambda e_{k\lambda}^{\vec{i}} e_{k\lambda}^{\vec{j}} = \delta_{ij} - \hat{k}_i \hat{k}_j$, $\int d\Omega_k = 4\pi$ and $\int d\Omega_k \hat{k}_i \hat{k}_j = \delta_{ij}\frac{4\pi}{3}$. Therefore we obtain $\int d\Omega_k \sum_\lambda e_{k\lambda}^{\hat{i}} e_{k\lambda}^{\hat{j}} = \delta_{ij}\left(4\pi - \frac{4\pi}{3}\right) = \delta_{ij}\frac{8\pi}{3}$ and

$$\Gamma_{tot}^{dipole} = \sum_{\mu'} \frac{4\alpha}{3} \frac{\omega_{\mu'\mu}^3}{c^2} \left| \left\langle \mu' \left| \vec{r} \right| \mu \right\rangle \right|^2 \qquad \text{with} \quad \omega_{\mu'\mu} = \frac{E_\mu^A - E_{\mu'}^A}{\hbar} > 0 \tag{2.16}$$

To obtain an order-of-magnitude estimate of the decay rate, we use that $\omega_{\mu'\mu} \propto \alpha^2$ and a typical value for $\vec{r}$ is $r \sim a_B \propto \frac{1}{\alpha}$. Therefore

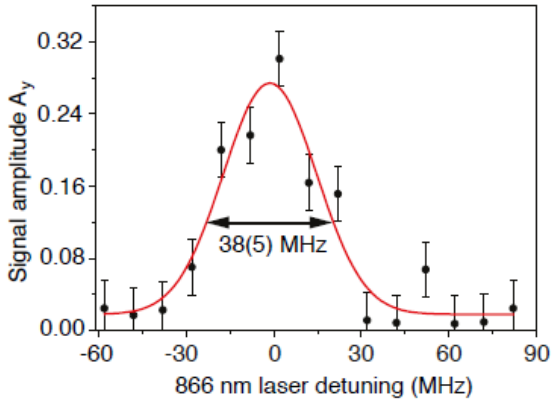


Figure 2.1: Intrinsic linewidth of the $D_{3/2} \rightarrow P_{1/2}$ dipole transition in a Ca^+ ion taken from C. Hempel *et al.*, Nature Photonics **7**, 630 (2013). The linewidth of about 38 MHz is about a factor of $1.1 \times 10^{-7} \approx 0.3\,\alpha^3$ smaller than the frequency of the emitted light, consistent with the estimate (2.17). To avoid broadening effects from collisions and the motion of atoms, such precision measurements can be performed on single atoms captured in the harmonic potential of a Paul trap.

$$\Gamma_{tot} \sim \frac{mc^2}{\hbar}\alpha^5 \ll \frac{E^A_\mu - E^A_{\mu'}}{\hbar} \sim \frac{mc^2}{\hbar}\alpha^2 \tag{2.17}$$

The decay rate is smaller by the factor α^3 than the energy of the emitted light, see Fig. (2.1). The finite decay rate also influences the energy distribution of the emitted photons. As $Im\left[\int e^{i\left(E^A_\gamma - E^A_{\gamma'}\right)\frac{t}{\hbar}} e^{-\Gamma^{tot}t} e^{-i\omega t} dt\right] = \frac{\frac{\Gamma}{\pi}}{\left(\omega - \frac{\Delta E}{\hbar}\right)^2 + \Gamma^2}$, the energy distribution measured by analyzing the emitted light by a spectrometer has the form of a Lorentz distribution, see Fig. (2.1). Due to the tiny total decay rate, one obtains extremely sharp Lorentzian peaks when the emission spectra of atoms are measured. Note, however, that we have calculated the photon emission only for a single atom at rest. In real experiments, the line width is further broadened by several mechanisms. When atoms move in the diluted gas, they have different velocities, some moving towards, some away from the observer. Due to the Doppler effect (a shift of the frequency due to this velocity), the spectrum obtains an extra broadening. Also collisions of atoms can lead to a decay of the excited state without emitting photons (a non-radiative decay) which also contributes to a broadening of the spectral lines.

The small decay rate also proves that our approach to use perturbation theory only is valid. This is also the reason that higher powers of $\vec{k}\vec{r}_i$ which lead, e.g., to electric quadrupole or magnetic dipole radiation can typically be ignored as they are suppressed by factors of α^2 if a dipole transition is possible. They have, however, to be considered if all dipole transitions are forbidden by selection rules.

Also the contribution from $F_e^{(2)}$, defined in Eq. (2.11), is small. Here one has to calculate the matrix elements of the spin operator, $\Gamma \sim \alpha k^3 \left|\langle \mu' \left|\vec{\sigma}\right| \mu \rangle\right|^2$. Here it is important to take

spin-orbit coupling into account (discussed later), which leads to an energy splitting of states with different spin of the order of $E^A_\mu - E^A_{\mu'} \sim \alpha^4 mc^2$. As k therefore is of order α^4, the total decay rate is of the order of $\Gamma \sim \alpha^{13}$ and therefore a factor α^9 reduced compared to the frequency of the emitted light.
The fact that some excited states decay extremely slowly is the basis for the extreme precision of atomic clocks. Relative accuracies of up to 10^{-15} can be reached with atomic clocks. Therefore the second is nowadays defined by the duration of 9,192,631,770 periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the Caesium 133 atom.

2.4 Cavity QED and Rabi oscillator

In modern physics, the manipulation of quantum states plays a more and more important role. In this area quantum optics is probably the most advanced field. Powerful experimental techniques have been developed to manipulate with light the quantum states of atoms. One can cool atoms down to the microkelvin regime, capture single atoms or can control the quantum state of the electrons and the nuclear spin. Similarly, one can use interactions with matter to manipulate the quantum states of photons. This has lead to a number of important applications – and many more can be expected for the future. An important example is the atomic clock which is even used to define the second as mentioned above. Without such high precision clocks, the GPS system would, for example, not work. Quantum states of light are used for quantum encryption which allows to send messages which by the laws of physics cannot be eavesdropped without being detected. Other interesting areas include research on quantum simulators and future quantum computers. As cavities, i.e., the standing waves of light between two mirrors play an important role in most experiments where one manipulates the quantum states of light by coupling it to matter, the field is called "cavity quantum electrodynamics" or, shorter, cavity QED.
The 2012 Nobel Prize in Physics was awarded to Serge Haroche and David J. Wineland *for ground-breaking experimental methods that enable measuring and manipulation of individual quantum systems*. This chapter is mainly motivated by a famous paper[3] by Haroche and coworkers on *Quantum Rabi Oscillation: A Direct Test of Field Quantization in a Cavity* from 1996 which describes the probably most simple setup where quantized light is coupled to the internal states of an atom.
An atom in an excited Rydberg state flies through a cavity where a standing electromagnetic wave can form between two almost perfect superconducting mirrors (a photon can be reflected $\mathrm{Q} = 10^8$ times before it gets lost), see Fig. 2.2. In the experiment the transition between two highly excited states (so-called Rydberg states) of a Rb atom with quantum number $n = 50$ and $n = 51$ has been used. The energy difference $\Delta E = h \cdot 51.1\mathrm{GHz}$ can

[3] M. Brune, F. Schmidt-Kaler, A. Maali, J. Dreyer, E. Hagley, J. M. Raimond, and S. Haroche, Phys. Rev. Lett. **76**, 1800 (1996)

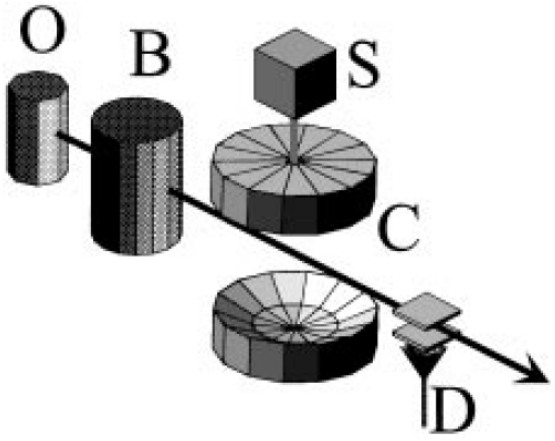


Figure 2.2: Schematic setup of the experiment (from M. Brune *et al.*, Phys. Rev. Lett. **76**, 1800 (1996)). An atom flies through a cavity formed by two mirrors (C) along the arrow. The internal state of the atom is measured in D by ionizing the excited atomic state and the time Δt between the preparation of the atom in B and the detection in D is recorded to calculate the velocity of the atom. From this, the time t spent in the cavity can be determined.

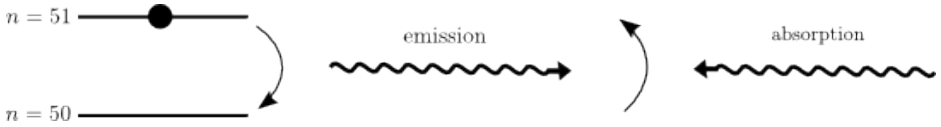


Figure 2.3: Due to the smallness of the matrix element, only resonant processes have to be taken into account, which are the emission of a cavity photon for the transition from the $n = 51$ to the $n = 50$ state of the Rb atom and the absorption during the reverse transition.

be tuned by an electric field (Stark effect) to match the energy of the photon captured between the two mirrors. This energy corresponds to a wavelength of $\lambda = 5.9\,\mathrm{cm}$, therefore the mirrors have approximately the distance $\frac{\lambda}{2}$.
The Hamiltonian describing the coupling of the internal state of the atom to the photon mode in the cavity is given by

$$H = \underbrace{\hbar\,\omega_0\,a^\dagger a}_{\substack{\text{1 photon mode}\\ \text{in cavity}}} + \sum \underbrace{E_n c_n^\dagger c_n}_{\substack{\text{energy levels}\\ \text{of the atom}}} + \sum g_{n,m} \underbrace{\left(a + a^\dagger\right) c_n^\dagger c_m}_{\substack{\text{dipol transsition}\\ \text{of level } m \to n}} + \underbrace{\text{h.c.}}_{\substack{\text{the hermitian}\\ \text{conjugate (h.c.)}\\ \text{describes the}\\ \text{reverse process.}}}$$

As we have seen, the dipole matrix element which determines the size of $g_{n,m}$ is extremely small. Therefore only resonant processes are relevant, i.e. transitions where $|E_m - E_n \pm \hbar\,\omega_0|$ is also small, $|E_m - E_n \pm \hbar\,\omega_0| \lesssim |g_{n,m}|$. Therefore from all atomic levels, only two will contribute, see Fig. 2.3. These two relevant internal states, one can describe by a spin degree of freedom, where $\uparrow$ ($\downarrow$) describes the state with higher (lower) energy. As for the transition from $\uparrow$ to $\downarrow$ energy will be released, a photon has to be emitted. In contrast,

the process where a photon is absorbed during the transition from $\uparrow$ to $\downarrow$ can safely be neglected as it is far off-resonance, $|E_\uparrow - E_\downarrow + \hbar\omega_0| \gg |g_{n,m}|$.
After these (very precise) approximations, one obtains the famous Jaynes-Cummings model

$$H = \underbrace{\frac{\hbar\omega}{2}\sigma_z}_{\substack{2 \text{ atomic} \\ \text{state}}} + \underbrace{\hbar\omega_0\, a^\dagger a}_{\text{photon energy}} + \hbar g \underbrace{\left(a^\dagger\sigma^-\right.}_{\substack{\text{resonant} \\ \text{emission}}} + \underbrace{\left.a\sigma^+\right)}_{\substack{\text{resonant} \\ \text{absorption}}} \tag{2.18}$$

where $\hbar\omega = E_n - E_{n'}$ is the energy difference of the two atomic levels, $g = g_{n,n'}$ the corresponding matrix element and $\hbar\omega_0$ the energy of the photon in the cavity. The two levels in the atom and their transitions are described just by Pauli matrices, $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ for the energy levels, $\sigma^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$ for the transition from the higher- to the lower energy state and $\sigma^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ for the reverse process.
The Hamiltonian (2.18) can be simplified even more by realizing that from the infinite number of states $|\uparrow, n\rangle$ and $|\downarrow, n\rangle$ only pairs of two couple (here n is the number of photons in the cavity). For example, the state $|\uparrow, n-1\rangle$, an excited atom with $n-1$ photons can only couple to $|\downarrow, n\rangle$, the deexcited atom with n photons but not to any other state. Using that

$$a^\dagger\sigma^- \,|\uparrow, n-1\rangle = \sqrt{n}\,|\downarrow, n\rangle \quad \text{and} \quad a\sigma^+ \,|\downarrow, n\rangle = \sqrt{n}\,|\uparrow, n-1\rangle$$

we can therefore write in this subspace

$$H = \hbar \begin{pmatrix} \frac{\Delta}{2} & \sqrt{n}\,g \\ \sqrt{n}\,g & -\frac{\Delta}{2} \end{pmatrix} + E_0\,\mathbb{1} \tag{2.19}$$

with $\hbar\Delta = \dfrac{\hbar\omega}{2} + \hbar\omega_0(n-1) - \left(-\dfrac{\hbar\omega}{2} + \hbar\omega_0\, n\right) = \hbar\omega - \hbar\omega_0$.
An especially interesting point is obtained directly at resonance, i.e., for

$$\omega = \omega_c \quad \Leftrightarrow \quad \Delta = 0$$

which is considered in the following. In this case the eigenvalues of H are given by $E_{s/a} = E_0 \pm \sqrt{n}g$ with eigenvectors $|s/a, n\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\left(|\uparrow, n-1\rangle \pm |\downarrow, n\rangle\right)$.
As a first example, let us consider an excited atom flying into the cavity. At $t = 0$ the initial state is given by $|\uparrow, n-1\rangle$. As $(1,0) = ((1,1)/\sqrt{2} + (1,-1)/\sqrt{2})/\sqrt{2}$, the time

dependent wave function is

$$|\Psi(t)\rangle = \left(e^{-iE_{s/\hbar}t}\ |s,\, n\rangle\ +\ e^{-iE_{a/\hbar}t}\ |a,\, n\rangle\right)\ \frac{1}{\sqrt{2}}$$

$$= \left(\cos\left(\sqrt{n}gt\right)\ |\uparrow,\, n-1\rangle - i\sin\left(\sqrt{n}gt\right)\ |\downarrow,\, n\rangle\right) e^{-iE_0 t/\hbar}$$

In the experiment the time is determined by the time the atom flies through the cavity.

- Consider an initial state where the atom is in a superposition of the two states while there is no photon in the cavity, $|\Psi(0)\rangle = (\alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle)\ |0\rangle$. Then after a time $t = \pi/g$ the wave function is given by $\left|\Psi\left(\frac{\pi}{g}\right)\right\rangle = |\downarrow\rangle\left(\beta\,|0\rangle - i\,\alpha\,|1\rangle\right)$. The atom is in its low-energy state while the photon is now in a superposition state. One has therefore transfered the quantum state from the atom to the photon, a useful element for any quantum logic.

- Entangled state, i.e. states which cannot be written as the product of two wave function, are the basis of practically all applications of quantum information theory, including quantum computing and quantum encryption. Starting from the initial state $|\Psi(0)\rangle = |\uparrow,\, 0\rangle$, which is a simple "product state" without any entanglement of one obtains an entangled state of light and matter by waiting the time $\pi/(2g)$ as $\left|\Psi\left(\frac{\pi}{2g}\right)\right\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow,\, 0\rangle - i\ |\downarrow, 1\rangle\right)$ which turns out to be a so-called "Bell pair", a maximally entangled state.

One can also use the cavity to measure directly the statistics of the photons in the cavity. To achieve this, we start from an excited atom and a cavity filled with a certain photon state $|\Psi(0)\rangle = |\uparrow\rangle \sum_n \underbrace{\alpha_n\,|n\rangle}_{\text{light filling}}$. Our goal is to determine $|\alpha_n|^2$, the probability that n photons are in the cavity. After the time t the wave function is given by

$$|\Psi(t)\rangle = \sum \alpha_n \left[|\uparrow,\, n\rangle \cos\left(\sqrt{n+1}\,gt\right) + |\downarrow, n+1\rangle\left(-i\,\sin\left(\sqrt{n+1}\,gt\right)\right)\right]\ e^{-i\,E_0 t/\hbar}$$

By measuring whether the atom is after the time t in its $\downarrow$ state and by repeating the experiment over and over again, one can determine $P_\downarrow(t)$, the probability that the atom is in this state after the time t with

$$P_\downarrow(t) = \sum |\alpha_n|^2 \sin^2\left(\sqrt{n+1}\,gt\right) \tag{2.20}$$

A simple Fourier transformation of $P_\downarrow(t)$ allows to determine the $|\alpha_n|^2$. The corresponding experiment is shown in Fig. 2.4.
In the experiment, the coherent light of a "maser" (Microwave Amplification by Stimulated Emission of Radiation), the low-frequency brother of a laser (Light Amplification by Stimulated Emission of Radiation) was used described by the coherent states discussed in

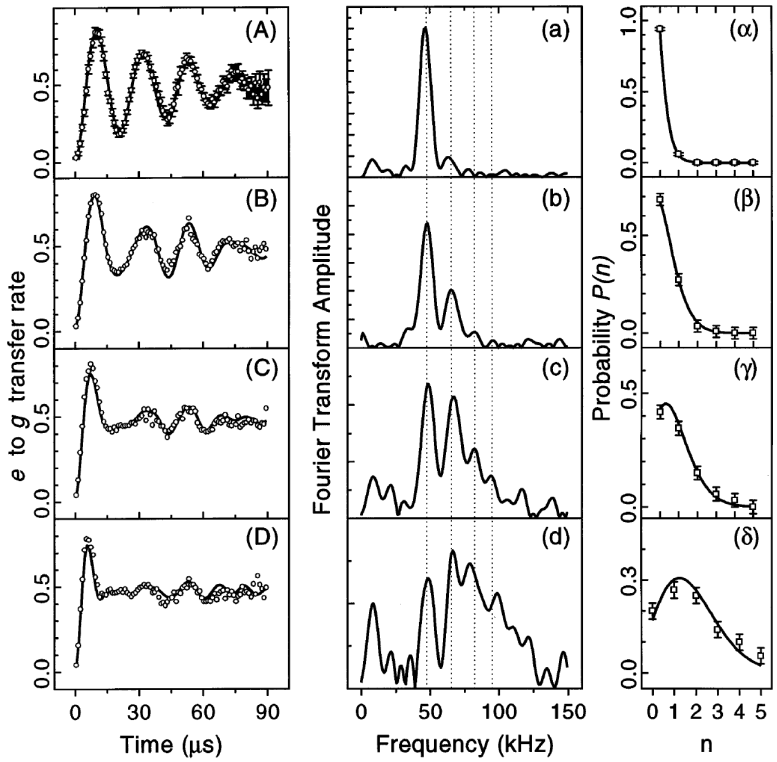


Figure 2.4: Measurements from M. Brune *et al.*, Phys. Rev. Lett. **76**, 1800 (1996) for coherent light with 4 different intensities (A-D) filling the cavity. Left: $P_\downarrow(t)$. Middle: the Fourier transform is peaked at frequencies $\omega = \sqrt{n+1}\,g$. From this one can determine the probabilites $|\alpha_n|^2$ that n photons are in the cavity shown in the right panels.

Sec. 2.2, $|z\rangle = e^{-|z|^2}\, e^{z\,a^\dagger}\, |0\rangle$ where $\alpha_n = \frac{z^n}{\sqrt{n!}}$ as $\left(a^\dagger\right)^n |0\rangle = \sqrt{n!}\, |0\rangle$. Therefore we obtain

$$P_-(t) = e^{-|z|^2} \sum_n \frac{\left(z^2\right)^n}{n!} \sin^2\left(\sqrt{n+1}\, g\, t\right) \tag{2.21}$$

which is plotted in Fig. (2.5) for $z = 20$. Clear oscillations are observed at short times, which decay however, after a few oscillations. Then the signal is constant for a long time but suddenly the oscillations grow again.

To understand this surprising behavior, we first need to understand the distribution of photonic states. From $a\,|z\rangle = z\,|z\rangle$ we find that the average photon number $\bar{n}$ is $\bar{n} = \langle z|\, a^\dagger a\, |z\rangle = |z|^2$. Similiarly, we can calculate the typical size Δn of the fluctuations of the photon number

$$\begin{aligned}(\Delta n)^2 &= \langle z|\left(a^\dagger a - \bar{n}\right)^2 |z\rangle = \langle z|\, a^\dagger a\, a^\dagger a - 2\bar{n}\, a^\dagger a + \bar{n}\, |z\rangle \\ &= \langle z|\, a^\dagger a^\dagger a a + a^\dagger a - 2\bar{n}\, a^\dagger a + \bar{n}\, |z\rangle = |z|^4 + |z|^2 - 2\,|z|^4 + |z|^4 = |z|^2 = \bar{n}\end{aligned}$$

Therefore $\Delta n = \sqrt{\bar{n}}$. For large $\bar{n}$, the photon distribution is therefore peaked at $\bar{n}$. From

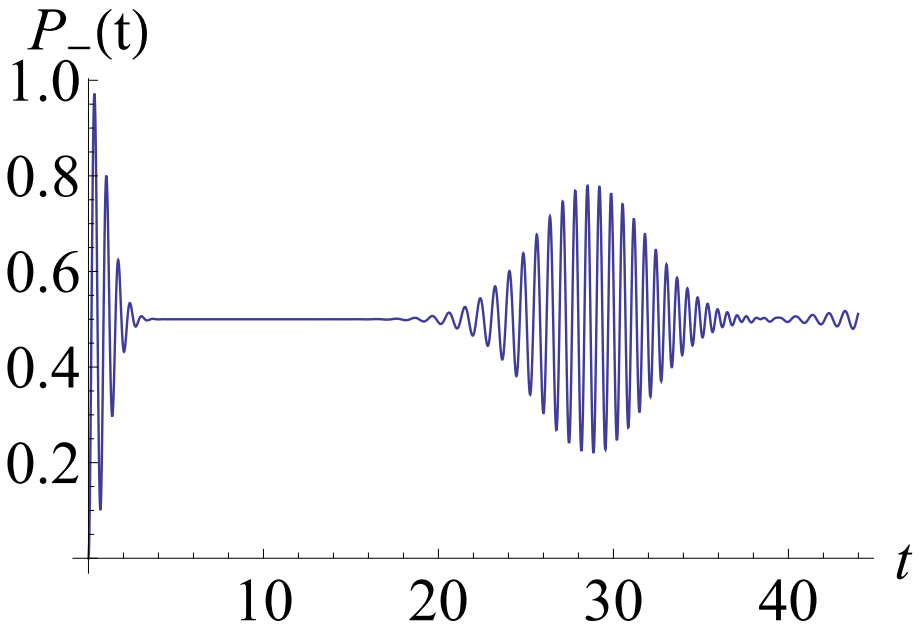


Figure 2.5: Plot of $P_\downarrow(t)$ obtained from Eq. (2.21) for $z = \sqrt{20}$, i.e., for a cavity occupied with coherent light and an average photon number of $\bar{n} = |z|^2 = 20$. After a collapse of the oscillating signal after about $2\sqrt{\bar{n}}$ oscillations, a revival of the signal occurs after about $\bar{n}$ oscillation periods.

Eq. (2.20) we therefore expect pronounced oscillations (so-called "Rabi-oscillations") of $P_\downarrow(t)$ with the frequency $\omega = 2\sqrt{\bar{n}}g$ (the factor of 2 comes from the $\sin^2 x = (1-\cos 2x)/2$). But as the photon number has a spread around $\bar{n}$, the oscillations will decay as there are multiple frequencies, $\bar{\omega} \pm \Delta\omega = 2\sqrt{\bar{n} \pm \sqrt{\bar{n}}} = \bar{\omega} \cdot \left(1 \pm \frac{1}{2\sqrt{\bar{n}}}\right)$. The oscillating signal does therefore decay after about $\sqrt{\bar{n}}$ oscillations as observed in Fig. 2.5. But why is there a recovery of the signal? This arises as only discreet frequencies contribute to Eq. (2.21). For example $\cos(\omega_1 t) + \cos(\omega_2 t)$ will interfere constructively whenever $(\omega_2 - \omega_1)t = 2\pi n$, i.e., first after the time $2\pi/(|\omega_1 - \omega_2)$. In our example, the difference of two neighboring frequencies in Eq. (2.21) is given at the peak of the photon distribution function by $\Delta\omega = 2g(\sqrt{\bar{n}+1} - \sqrt{\bar{n}}) \approx \frac{g}{\sqrt{\bar{n}}}$. Therefore the revival is expected after the time $2\pi/\Delta\omega = 2\pi\sqrt{\bar{n}}/g$ or after about $2\bar{n}$ periods. This explains the observation in Fig. (2.21). A little bit of the revival physics is also seen in Fig. (2.5) but as $\bar{n} < 2$ in this experiment, this effect is not very pronounced.

This chapter on cavity QED was supposed to give a first impression on how one can manipulate the quantum states of light and of atoms and actively control both light and matter on the quantum level.

3 Relativistic Quantum Mechanics

Einstein's theory of special relativity changed our notion of space and time in a profound way. The formulation of a relativistic quantum theory was a difficult challenge. A main reason for that is that the single-particle approach fails in a profound way for relativistic theories. According to Einstein's famous formula, $E = mc^2$, particles can be converted into energy as it occurs when, for example, an electron and a positron annihilate with each other. Therefore a meaningful formulation of relativistic quantum mechanics is only possible using the language and concepts of second quantization where one can describe processes where particles are created and annihilated.

3.1 Special theory of relativity

This section is a brief reminder on some aspects of the theory of special relativity. It assumes that the reader has seen this before, e.g., in a course on classical electrodynamics. Special relativity builds on two main principles

- Principle of relativity: all inertial frames are equivalent
- Principle of the invariant speed of light:
  c is constant and identical in all inertial frames

Therefore a transformation exists from one frame of reference to another one moving with constant velocity v such that c is constant. These are the so-called Lorentz boosts.

$$x \to x' = \frac{x + v \cdot t}{\sqrt{1 - \left(\frac{v}{c}\right)^2}} \qquad ct \to ct' = \frac{ct + \frac{v}{c}x}{\sqrt{1 - \left(\frac{v}{c}\right)^2}} \tag{3.1}$$

To show that the speed of light is constant, we have to calculate $x'^2 - (ct')^2$ which indeed gives $x^2 - (ct)^2$.
By introducing the notation $x^\mu = \left(x^0,\, x^1,\, x^2,\, x^3\right) = (ct,\, \vec{x})$ we emphasize that space and time are treated equivalently. Together they form the 4-dimensional space-time. Defining $\beta = \frac{v}{c}$ and $\gamma = \frac{1}{\sqrt{1-\beta^2}}$, we can rewrite Eq. (3.1)

$$x^{1'} = \gamma\left(x^1 + \beta x^0\right) \quad ;\; x^{0'} = \gamma\left(x^0 + \beta x^1\right) \tag{3.2}$$

The essential property that the speed of light is constant, leads to a metric in space-time which is identical in each inertial frame. The distance s of two points x_1^μ and x_2^μ in the 4-dimensional space-time with $\Delta x^\mu = x_1^\mu - x_2^\mu$ is defined as

$$s^2 = (c\Delta t)^2 - (\Delta\vec{x})^2 = g_{\mu\,\nu}\,\Delta x^\mu\,\Delta x^\nu = \Delta x_\mu\,\Delta x^\mu$$

where we introduce the metric tensor

$$g_{\mu\,\nu} = g^{\mu\,\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}$$

and defined $x_\mu = g_{\mu\,\nu}x^\nu = (ct,\, -\vec{x})$ using Einstein's summation convention that one always sums over double indices. Here Greek letters are typically denote space-time indices, i.e. the summation is from 0 (the time component) up to 3.
Events in space-time with distance $s^2 = 0$ can be connected by light-rays. For $s^2 > 0$, $c\Delta t$ is larger than the distance in space and therefore the earlier event can influence the later event. This is not possible for $s^2 < 0$, where the distance in space is larger than $c\Delta t$: As no signal can travel faster than the speed of light, the two events cannot influence each other. In this case, the question whether one event is earlier or later than the other depends on the frame of reference as can directly be seen by computing $\Delta t'$ using Eq. (3.1).
Lorentz transformations between inertial frames are those transformations which leave s^2 and therefore the speed of light,c, invariant. They have the form

$$x^{\mu'} = \Lambda^\mu{}_\nu\, x^\nu + \underbrace{a^\mu}_{\text{shift in space-time}}$$

From the condition that s^2 remains unchanged, $s^2 = g_{\mu\,\nu}\,\Delta x^\mu\,\Delta x^\nu = g_{\tilde{\mu}\,\tilde{\nu}}\,\Delta x^{\tilde{\mu}'}\,\Delta x^{\tilde{\nu}'}$, we obtain that

$$g_{\mu\,\nu} = g_{\tilde{\mu}\,\tilde{\nu}}\,\Lambda^{\tilde{\mu}}{}_\mu\,\Lambda^{\tilde{\nu}}{}_\nu \quad \Leftrightarrow \quad g = \Lambda^T\,g\,\Lambda \quad \Leftrightarrow \quad \Lambda^{-1} = g\,\Lambda^T\,g \tag{3.3}$$

We will later discuss that matrices which fulfilling this condition form a group, the so-called Lorentz group, $O(1,3)$. We have already discussed one matrix which has the property, the Lorentz boost in the x-direction:

$$\Lambda^\mu{}_\nu = \begin{pmatrix} \gamma & \beta\gamma & 0 & 0 \\ \beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{3.4}$$

We will use a few definitions and useful properties:

- We call all 4-tuples a^μ which transform like x^μ according to $a^\mu \to \Lambda^\mu_\nu\, a^\nu$, **contravarian 4-vectors** and we use an upper Greek index in this case.

- Similarly, **covariant 4-vectors**, denoted by lower indices, $a_\mu = g_{\mu\nu} a^\nu$ transforms in the same way as x_μ with $a_\mu \to \Lambda_\mu{}^\nu \, a_\nu$. Here one defines with: $\Lambda^\nu_\mu = g_{\mu\,\alpha} \, \Lambda^\alpha_\beta \, g^{\nu\,\beta}$. Let us check this result: $x'_\mu = g_{\mu\,\alpha} x'^\alpha = g_{\mu\,\alpha} \, \Lambda^\alpha_\beta \, x^\beta = \underbrace{g_{\mu\,\alpha} \, \Lambda^\alpha{}_\beta \, g^{\beta\,\gamma}}_{\Lambda_\mu{}^\gamma} \, x_\gamma$

- The combination $a^\mu \, b_\mu = a^0 \, b^0 - \vec{a}\,\vec{b} = a^\mu \, g_{\mu\,\nu} \, b^\nu$ is Lorentz invariant due to our definition of Λ.

- We will also need derivatives and define

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \left(\frac{1}{c} \frac{\partial}{\partial t}, \vec{\nabla} \right) \quad \text{covariant}$$
$$\partial^\mu = \frac{\partial}{\partial x_\mu} = \left(\frac{1}{c} \frac{\partial}{\partial t}, -\vec{\nabla} \right) \quad \text{contravariant}$$

  Let us check whether ∂^μ transforms indeed like x^μ and is therefore a contravariant vector by performing a Lorentz transformation. We get $\frac{\partial}{\partial x'_\mu} = \frac{\partial x_\nu}{\partial x'_\mu} \frac{\partial}{\partial x_\nu}$ with $\frac{\partial x_\nu}{\partial x'_\mu} = \underbrace{\left(\underbrace{(g \, \Lambda \, g)^{-1}}_{\Lambda^T} \right)^T}_{\substack{g=\Lambda^T g \Lambda \\ \mathbb{1}=\Lambda^T g \Lambda g}} \underbrace{=}_{} \Lambda$

Immediately, a few very useful applications follow.

- The combination $\partial_\mu \, \partial^\mu = \frac{\partial^2}{c^2 \, \partial t^2} - \vec{\nabla}^2 = \Box$ (the d' Alembert operator) has to be invariant under Lorentz-transformations. This implies that equations like $\partial_\mu \, \partial^\mu \, \Phi = 0$ will be the same in all inertial frames of reference.

- An important result (which we will not proof) is that the scalar and vector potential of electromagnetism form together a 4-vectors $A^\mu = (\varphi, \vec{A})$. The transformation properties of the electromagnetic fields, $\vec{E} = -\nabla\varphi - \frac{1}{c} \frac{\partial}{\partial t} \vec{A}$ and $\vec{B} = \vec{\nabla} \times \vec{A}$ are more complicated. In the relativistic context it is useful to combine them into the so-called **field strength tensor**

$$F^{\mu\,\nu} = \partial^\mu A^\nu - \partial^\nu A^\mu = \begin{pmatrix} 0 & E_x & E_y & E_z \\ -E_x & 0 & B_z & -B_y \\ -E_y & -B_z & 0 & B_x \\ -E_z & B_y & -B_x & 0 \end{pmatrix} \tag{3.5}$$

  The 6 independent components of this antisymmetric tensor describe all electromagnetic field. It can, for example, be used to read off the transformation properties of the electromagnetic fields. From the transformation rules for ∂^μ and A^μ we find directly for any moving coordinate system

$$F'^{\mu\,\nu} = \Lambda^\mu{}_{\mu'} \, \Lambda^\nu{}_{\nu'} \, F^{\mu'\,\nu'}$$

- Also energy and momentum can be combined to a 4-vector:

$$\Pi^\mu = \left(\frac{E}{c}, \vec{p}\right) \tag{3.6}$$

Later we will want to identify (according to the correspondence principle of quantum mechanics) $i\hbar\partial^\mu$ with Π^μ. In the coordinate system where a particle is at rest, one has $\Pi^\mu = (m_0 c, 0, 0, 0)$ where m_0 is the (rest) mass of the particle. We can immediately conclude that $\Pi_\mu \Pi^\mu = \frac{1}{c}\left(E^2 - p^2c^2\right) = \text{const.} = m_0^2 c^2$ has to be a constant in any intertial frame of reference and we obtain the famous energy-momentum relation of Einstein

$$E^2 = \left(m_0 c^2\right)^2 + (pc)^2 \tag{3.7}$$

- The **continuity equation** $\partial_t \varrho + \vec{\nabla}\vec{j} = 0$ for any conserved density ϱ can be written as

$$\partial_\mu j^\mu = 0$$

if we define $j^\mu = (c\,\varrho, \vec{j})$. As the continuity equation is valid in any coordinate system, we can conclude that j^μ has to transform like a contravariant vector.

3.2 Lorentz group

As mentioned above, the set of all Lorentz tranformations Λ, which leave the distance measure s invariant form a group called $O(1,3)$. As discussed in Eq. (3.3), the 4x4 matrices Λ are defined by the property that they leave the metric tensor $g^{\mu\nu}$ invariant

$$O(1,3) = \left\{\Lambda \in \mathbb{R}^{4\times 4} \,\middle|\, \Lambda^T g\, \Lambda = g\right\}$$

The notation $O(1,3)$ refers to the fact that one entry in $g^{\mu\nu}$ is $+1$, while 3 entries are -1. It is useful to compare this to the group $O(3) = O(3,0) = O(0,3)$, the group of rotations, mirror symmetries and inversion, which leave distances in space $(\Delta\vec{x})^2$, or – equivalently – the matrix $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ invariant.

The group $O(1,3)$ has three discrete elements. They are (i) the inversion of space, usually called **parity P** defined by $\vec{x} \to -\vec{x}$, $t \to t$, (ii) **time reversal T** defined by $\vec{x} \to \vec{x}$, $t \to -t$, and (iii) **PT** is the combined transformation of time-reversal and parity. The

corresponding matrices are therefore given by

$$\Lambda_P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \Lambda_T = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \Lambda_{PT} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{3.8}$$

If one considers only the continuous symmetries, i.e. Lorentz boosts, rotations and combinations thereof one obtains the so-called proper Lorentz group $SO^+(1,3)$ defined by

$$SO^+(1,3) = \left\{ \Lambda \in \mathbb{R}^{4\times 4} \,\middle|\, \Lambda^T\, g\, \Lambda = g\,,\ \det\Lambda = 1\,,\ \Lambda^{00} > 0 \right\}$$

Note that from the equation $\Lambda^T\, g\, \Lambda = g$ one can immediately conclude that $(\det\Lambda)^2 = 1$. Furthermore from the 00 component of the equation one finds that $1 = \Lambda^{00\,2} - \Sigma_{i=1,2,3}\Lambda^{0i\,2}$ and therefore $\Lambda^{00\,2} \geq 1$. By multiplying elements of $SO^+(1,3)$ with Λ_P, Λ_T and Λ_{PT} one can switch the sign of the determinant and the sign of Λ^{00} thus obtaining all elements of $O(1,3)$.

The group of rotations, $SO(3)$, is generated by 3 generators characterized by the commutation relations $[L_m,\, L_n] = i\epsilon_{mnk}L_k$. For example, rotations around the x,y and z axis are generated by L_1, L_2, L_3 with

$$L_1 = i\begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \qquad L_2 = i\begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \qquad L_3 = i\begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

A finite rotation is obtained by $e^{i\sum_i \phi_i L_i}$. For example a rotation around the z axis is described by

$$e^{i\varphi L_3} = \lim_{N\to\infty}\left(\mathbb{1} + i\frac{\varphi}{N}\,L_z\right)^N = \sum_n \frac{(i\phi L_z)^n}{n!} = \begin{pmatrix} \cos(\varphi) & -\sin(\varphi) & 0 \\ \sin(\varphi) & \cos(\varphi) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

.

Similarly $SO^+(1,3)$ can be built up from three generators of rotations J_1, J_2, J_3 and three generators of Lorentz boosts denoted by K_1, K_2, K_3 for boosts in x, y and z direction. Here we use a slightly different convention than above and include the factor i in the definition of the generators. Therefore the rotations are written as $e^{\sum_{i=1,2,3}\phi_i J_i}$ with

$$J_k = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & & & \\ 0 & & iL_k & \\ 0 & & & \end{pmatrix}$$

The generator for a boost in x direction can be obtained by expanding the transformation matrix for a finite boost (3.4) for small velocities. One finds that the boosts are generated by the matrices

$$K_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad K_2 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \qquad K_z = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}$$

To check the result, let us calculate $e^{\varphi K_x} = \sum \frac{\varphi^n}{n!} K_n^x$. As $K_x^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$

one finds $K_x^0 = \mathbb{1}$, $K_x^{2n} = K_x^2$ for $n \geq 1$ and $K_x^{2n+1} = K_x$. Using this, the exponential series can be summed up to obtain

$$e^{K_x} = \sum_{n=0}^{\infty} \frac{\varphi^n}{n!} K_x^n = (\cosh(\varphi) - 1)K_x^2 + \sinh(\varphi K_x) + \mathbb{1} = \begin{pmatrix} \cosh\varphi & \sinh\varphi & 0 & 0 \\ \sinh\varphi & \cosh\varphi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

consistent with Eq. (3.4) for $\sinh(\varphi) = \beta\gamma$ and $\cos(\varphi) = \gamma = \frac{1}{\sqrt{1-\beta^2}}$. As a check, note that $1 = \cosh^2(\varphi) - \sinh^2(\varphi) = \frac{1}{1-\beta^2} - \frac{\beta^2}{1-\beta^2} = 1$.

Using the definitions given above, one can easily work out the **algebra** of the generators of $SO(1,3)$ which is given by

$$[J_i,\, J_j] = \epsilon_{ijk}\, J_k, \quad [K_i,\, J_j] = \epsilon_{ijk}\, K_k, \quad [K_i,\, K_j] = -\epsilon_{ijk}\, J_k \tag{3.9}$$

3.3 Klein Gordon Equation

After the Schrödinger equation had been found, an important challenge was to find a relativistic generalization of this equation. For guessing the form of the Schrödinger equation, the **correspondence principle**, $E \to\ i\hbar\partial_t$ and $\vec{p} \to -i\hbar\vec{\nabla}$ was a very useful approach. In relativistic notation this reads

$$p^\mu = \left(\frac{E}{c}, \vec{p}\right) \ \to\ i\hbar\partial^\mu = \left(i\hbar\frac{\partial}{c\partial t}, -i\hbar\vec{\nabla}\right)$$

Can we use the correspondence to derive a relativistic version of the Schrödinger equation starting from $E = \sqrt{(m_0c^2)^2 + (pc)^2}$? It is tempting to 'guess' the equation $i\hbar\partial_t\Phi(\vec{r},t) = \sqrt{(mc^2)^2 + \left(-ci\hbar\vec{\nabla}\right)^2}\,\Phi(\vec{r},t)$. But this is not a good idea as space and time are treated very differently and a Taylor expansion in the second term leads to arbitrary high powers of ∇.

Instead, one can try to start directly from the squared equation: $E^2 = \left(m_0c^2\right)^2 + (cp)^2$. Using the correspondence principle, one obtains $(i\hbar\partial_t)^2\,\Phi - \left(m_0c^2\right)^2\Phi - (-i\hbar\nabla)^2\,\Phi = 0$. This is the **Klein-Gordon Equation:**. In relativistic notation it takes the form

$$\left(\partial_\mu\,\partial^\mu + \frac{m_0^2c^2}{\hbar^2}\right)\Phi = 0 \tag{3.10}$$

Two versions of the Klein-Gordon equations exist, both with imporant applications: Φ can either be a real or complex field. We will discuss in the following primarily the complex case.

The solutions of this equation are obviously plane waves

$$\Phi(\vec{x},t) = \exp(i\frac{\vec{p}\vec{x} - Et}{\hbar}) = e^{-i\frac{p_\mu x^\mu}{\hbar}} \qquad \text{(both sign, positiv \& negativ energies)}$$

with $p^\mu p_\mu = (m_0c)^2$, or, equivalently, $E = \pm\sqrt{(m_0c)^2 + (pc)^2}$. Interestingly, **both** signs of the energy appear to be allowed.

But what is the physical interpretation of this equation? In the case of the Schrödinger equation the key was to realize that $|\Psi|^2$ can be interpreted as a probability. Does in this case also exist a quantity which can be interpreted as a probability? An important property of any probability is that the total probability is conserved and normalized to 1, $\int |\Psi|^2\,d^3r = 1$. A first important step is therefore to ask whether the Klein-Gordon equation also has a conserved quantity. Does a local quantity ϱ (a conserved density) and a current $\vec{j}$ exist which fulfills a continuity equation $\dot{\varrho} + \vec{\nabla}\vec{j} = 0$? In relativistic notation one defines the 4-vector $j^\mu = (c\varrho, \vec{j})$ and the continuity equation has the form

$$\partial_\mu j^\mu = 0$$

Using that $\Phi^*\underbrace{\left(\partial_\mu\partial^\mu + \frac{m_0^2c^2}{\hbar^2}\right)}_{=0}\Phi - \left[\left(\partial_\mu\partial^\mu + \frac{m_0^2c^2}{\hbar^2}\right)\Phi^*\right]\Phi = 0$, we can show directly that $\partial_\mu j^\mu = 0$ where

$$j^\mu = ic\,(\Phi^*\partial^\mu\Phi - (\partial^\mu\Phi^*)\Phi)$$

describes the conserved density

$$\varrho = j^0/c = i\left(\Phi^*\left(\frac{\partial\Phi}{\partial t}\right) - \left(\frac{\partial\Phi^*}{\partial t}\right)\Phi\right) \tag{3.11}$$

with the associated current density $\vec{j} = ic\left(\Phi^*\vec{\nabla}\Phi - \left(\vec{\nabla}\Phi^*\right)\Phi\right)$. As $\int \varrho\, d^3r = const.$, one can ask the question whether ϱ can be interpreted as a probability density, similar to $|\Psi|^2$ in the non-relativistic limit. The answer is negative: as ϱ can be negative it cannot be a probability!

When the Klein-Gordon equation was first found, the interpretation of it had several properties which at that time seemed to make it completely useless to describe the properties of nature. First, the natural conserved density ρ could be both positive and negative and there was not quantity which could be interpreted as a probability. Second, arbitrarily large negative energies were allowed which seemed to contradict the stability of matter and the fact that one cannot generate infinite amounts of energy out of the vacuum. And finally, the equation was not describing the spin of the electron.

After the formalism of second quantization had been found, the solution to all questions given above is known: the Klein Gordon equation describes not only positively charged particles but simultaneously negatively charged antiparticles. The conserved quantity ρ thereby is the total charge density which can be positive or negative. The negative energy solutions describe antiparticles with positive energy (see below). While the Klein-Gordon equation does not describe the properties of electrons, it is the correct theory for particles with spin 0. It has many applications and can be used to describe the Higgs particle and plays, e.g., an important role in the theory of superconductivity.

We will not discuss the Klein-Gordon equation in much detail but just describe briefly how the theory can be quantized and interpreted. One way to obtain the correct quantization rules is to rewrite the equation in the Hamiltonian formalism. Then one obtains the quantized theory by replacing Poisson brackets by commutators following the example that the Poisson brackets for position and momentum, $\{x,\, p\} = 1$, correspond to $[x,\, p] = i\hbar$ in the quantum world.

Here we will not follow this route but just give the final result, especially as it turns out to be very similar to the quantization rules of the vector potential in Coulomb gauge described in chapter 2.1. This arises as the equation for the vector potential $\partial_\nu \partial^\mu \vec{A} = 0$ is up to the mass term identical to the Klein-Gordon equation.

The most important point is that Φ and $\Phi^\dagger$ are not fields but field operators which create and destroy bosons and their antiparticles. Using the notation $K^\mu = \left(\frac{\omega_K}{c},\, \vec{K}\right)$ where we define $\omega_K = +\frac{1}{\hbar}\sqrt{(m_0c^2)^2 + (\hbar\vec{K}c)^2}$ always larger than 0, we can identify $\Phi^\dagger$ with a field operator

$$\Phi^+(r,\,t) = \frac{\sqrt{\hbar}}{\sqrt{V}} \sum_{\vec{K}} \frac{1}{\sqrt{2\,\omega_K}} \Big(\underbrace{e^{i\omega_K t - i\vec{K}\vec{r}}\, c_K^\dagger}_{\substack{\text{positiv energy} \,\hat{=}\, \\ \text{creation of particle}}} + \underbrace{e^{-i\omega_K t + i\vec{K}\vec{r}}\, b_K}_{\substack{\text{negative energy} \,\hat{=}\, \\ \text{destruction of anti-particle}}} \Big) \tag{3.12}$$

with besonic commutation relations: $\left[c_K,\, c_K^\dagger\right] = \delta_{K\,K'} = \left[b_K,\, b_K^\dagger\right]$

$[b,\, c] = \left[b^\dagger,\, c\right] = [b,\, b] = [c,\, c]\left[b,\, c^\dagger\right] = 0$

Obviously this field operator satisfies the Klein-Gordon equation. $c_k^\dagger$ creates a boson with momentum k while b_k destroys a different type of particle which turns out to have opposite charge: it is the antiparticle. When one replaces in the above equation b_k by c_k one obtains a quantum field with $\Phi^\dagger = \Phi$ providing a solution for the Klein-Gordon equation for a real-valued field, which corresponds to a quantum theory where the particle is its own antiparticle (this is exactly the situation for photons).

The form of the Hamiltonian we can read off from the time dependence of the operators evident from Eq. (3.12): $c_{K'}^\dagger(t) = e^{i\omega_K t}\, c_K(0)$ and $b_K(t) = e^{-i\omega_K t}\, b_K(0)$. This implies that the Hamiltonian has the form

$$H = \sum_K \hbar\omega_K \left(c_K^\dagger c_K + b_K^\dagger b_K\right) + \text{const.} \tag{3.13}$$

Note that this implies that both particle and antiparticle have positive energies $\hbar\omega_K \geq 0$. There is no problem with negative energy solutions.

As we will discuss in the problem set accompanying the lecture, the Hamiltonian can be rewritten as

$$H = \int \Pi^\dagger(x)\,\Pi(x) + c^2(\nabla\Phi^\dagger)(\nabla\Phi) + \frac{m_0 c^2}{\hbar}\Phi^\dagger\Phi$$

with $\quad \Pi = \partial_t\,\Phi^\dagger$

and $\quad \left[\Phi(\vec{x}),\, \Pi(\vec{x}')\right] = i\hbar\delta\left(\vec{x} - \vec{x}'\right)$

To obtain the charge of the particles we evaluate ϱ defined in Eq. (3.11) using Eq. (3.12).

$$\begin{aligned} Q = \int \varrho(\vec{r},\, t)\,\mathrm{d}^3\vec{r} &\underbrace{=}_{\rho = j^0/c} i\int \Phi^+\partial_t\Phi - (\partial_t\Phi^+)\Phi\mathrm{d}^3\vec{r} \\ &\underbrace{=}_{\frac{1}{V}\int e^{i(K-K')r} = \delta_{K\,K'}^K} \hbar\sum_K i\left(c_K^+\frac{-i\omega_K}{2\omega_K}\,c_K + b_K\frac{i\omega_K}{2\omega_K}\,b_K^\dagger + b_K\frac{-i\omega_K}{2\omega_K}\,c_K e^{-2i\omega_K t} + \right. \\ &\qquad \left. + c_K^+\frac{i\omega_K}{2\omega_K}\,b_K^+ e^{2i\omega_K t}\right) + \text{h.c.} \end{aligned}$$

The last two terms cancel after the hermitian conjugate has been added and we find for the total charge

$$Q = \hbar \sum_K \left(c_K^+ c_K - b_K^+ b_K \right) \tag{3.14}$$

Thus $c_K^\dagger$ creates a particle with momentum K and energy ω_K (according to Eq. (3.13)) and charge $\hbar$. That its charge turns out to be „$\hbar$“ is only an artifact of our conventions: obviously one can redefine the Q operator by multiplication with a constant. Independent of the convention is, however, that $b_K^\dagger$ creates a particle with the same momentum and energy but the opposite charge: it is the creation operator of the antiparticle.
This chapter gave a brief overview of some of the most essential ideas of relativistic quantum field theory (which we will discuss in more detail for the Dirac equation, describing electrons and positrons): relativistic quantum theory can only be interpreted in the context of second quantization. A remarkable feature is that the presence of antiparticles is enforced by its mathematical structure.

3.4 Gauge invariance

One of the most successfull concepts in physics is the notion of Gauge invariance: it describes not only electrodynamics, but also weak and strong interactions in elementary particle physics. In this context, Gauge invariance is postulated as a fundamental principle – a root which we will also follow here. But in modern solid state theory, we also know that in some situations Gauge theories are 'emergent' which means that they naturally arise when one describes the low-energy long-distance properties of some states of matter which on a microscopic level is *not* described by a Gauge theory.
In this section we will discuss the coupling of matter to the electromagnetic field using the Klein-Gordon equation as an example. The arguments used here can equally be applied to the Schrödinger equation and, in the following chapters, to the Dirac equation.
Probably the single most important postulate of quantum mechanics is that states are described by complex amplitudes while only their modulus squared – a probability – can be measured. That implies that multiplying all amplitudes simultaneously by a phase factor, $e^{i\varphi}$ has no effect. As the group of multiplication by such phase factors is called $U(1)$ (the unitary 1×1 matrices, one calls this property a global $U(1)$ symmetry.
Surprisingly, it turns out that a much stronger postulate is at the heart of electromagnetism: physics is invariant when one multiplies wavefunctions or field operators by an arbirary *space- and time-dependent phase factor*

$$\Phi(x) \to \; e^{i\varphi(x)}\, \Phi(x)$$

where $\varphi(x)$ is an arbitrary real function of $x = x^\mu = (x^0, x^1, x^2, x^3)$, i.e. of space and time[1]. This is called a gauge transformation.

[1] Sometimes we use either x^μ or x to denote the dependence of time and space.

On first glance, this appears to be a postulate contradicting the basic fact that relative phases and interference are an imporant part of quantum mechanics. Furthermore, the Schrödinger, Klein-Gordon and Dirac equations are all formulated in terms of derivatives of fields. Applying a derivative to the transformed field, $\partial^\mu \left(e^{i\varphi(x)}\,\Phi(x)\right) = e^{i\varphi}\left(i\left(\partial^\mu\varphi\right) + \partial^\mu\right)\Phi(x)$, one obtains an extra term proportional to $\partial^\mu\varphi$.
Here the most important insight is that there is an other place in physics, where an unobservable function $\varphi(x)$ shows up: electromagnetic fields are not modified when one changes the vector potential by $A^\mu(x) \to A^\mu(x) + \partial^\mu\tilde{\varphi}(x)$. Within Maxwell's theory this was just a result of a simple mathematical trick (see discussion in chapter 2.1). In the context of quantum mechanics and quantum field theory it became on the deepest observations: multiplying quantum fields by a phase factor and redefining vector potential is actually the same and $\varphi(x)$ and $\tilde{\varphi}(x)$ are proportional to each other. If one can guarantees that all derivatives arise in a linear combination with vector potentials, the factors $\partial^\mu\varphi$ can cancel with each other.
When formulating the **postulate of gauge invariance** , we have to take both transformations into account

Gauge invariance:
All physical observables are invariant under the gauge transformation

$$\Phi(x) \to \exp\left(i\frac{q}{\hbar c}\varphi(x)\right)\,\Phi(x) \quad , \; A^\mu(x) \to A^\mu(x) - \partial^\mu\varphi(x) \tag{3.15}$$

Here $q/(\hbar c)$ is a factor of proportionality relating the two transformations. q can later be identified with the charge of the particle described by the field $\Phi(x)$ (which can also be 0 in some cases).
The postulate of Gauge invariance *enforces* that the Hamiltonian and all observables have a specific structure: all derivatives of fields *have to* be accompanied by a vector-potential term written as

$$D^\mu = \partial^\mu + \tfrac{iq}{\hbar c}\,A^\mu$$

This also implies that we can easily 'guess' how the coupling electromagnetic field couples to a give quantum theory: in each term we just replace ∂^μ by D^μ. This procedure is called **minimal coupling**. As the name indicates, other gauge invariant couplings are also possible in general[2] but this is certainly the simplest 'minimal' solution
Let us check how a gauge transformation affects the combination $D^\mu\Phi$.

$$\begin{aligned} D^\mu\Phi \to & \left(\partial^\mu + \frac{iq}{\hbar c}\left(A^\mu - \partial^\mu\varphi\right)\right)\left(\exp\left(i\frac{q}{\hbar c}\varphi(x)\right)\Phi\right) \\ & = \exp\left(i\frac{q}{\hbar c}\varphi(x)\right)\left(\partial^\mu + \frac{iq}{\hbar c}\,A^\mu\right)\Phi = \exp\left(i\frac{q}{\hbar c}\varphi(x)\right)\,D^\mu\,\Phi \end{aligned}$$

[2] An example are intraband transitions in solids induced by light which cannot be derived from general principles of gauge invariance without knowledge of the detailed wave functions.

In an Hamiltonian, the remaining multiplicative phase cancels with the corresponding phase factor for $\Phi^\dagger$; in the equations of motions it can just be divided out.
Therefore, the Klein-Gordon equation which describes also the coupling to the electromagnetic field is simply given by

$$\left(D_\nu\, D^\mu + \tfrac{m_0^2 c^2}{\hbar^2}\right) \Phi = 0$$

which by construction is gauge invariant. Adding Maxwells equation one can derive that q is indeed the charge of the particle created by $c_k^\dagger$ in this context.
Up to the factor q, the charge of the created particle, the principle of gauge invariance can be used to fix the coupling of the electromagnetic field to matter! This is an extremely powerful concept which also works for weak and strong interactions. It is probably fair to say, that much of our understanding of the world around us and of its quantum properties comes from this basic principle.
Historically, the importance of the concept of gauge invariance has first been recognized in the context of general relativity. Therefore also the name gauge invariance (in German Eichinvarianz) refer to a change of the scale of measurement.

3.5 Dirac equation

As a straightforward interpretation of the Klein-Gordon equation along the lines of the Schrödinger equation was not possible, Dirac was searching for a relativistic equation which like the Schrödinger equation is linear in ∂_t. Now assuming that time and space have to be treated similarly in any relativistic setup, he concluded that the equation should also be linear in space-derivatives, $\vec{\nabla}$.
The lead to the following ansatz for a relativistic version of the Schrödinger equation

$$i\hbar\partial_t\Psi = \left(c\vec{\alpha}\vec{p} + \beta m_0 c^2\right)\Psi = H_D\Psi \tag{3.16}$$

where $\vec{p} = -i\hbar\vec{\nabla}$. This equation should fulfill the relativistic energy-momentum relation, $E^2 = \left(m_0c^2\right)^2 + (pc)^2$, with E to be replaced by $i\hbar\partial_t$. To achieve this, one has to take one more derivative

$$E^2\Psi \hat{=} -\hbar^2\partial_t^2\Psi = H_D^2\Psi = \left(c\vec{\alpha}\vec{p} + \beta m_0 c^2\right)^2 \stackrel{!}{=} \left((m_0c^2)^2 + (pc)^2\right)\Psi$$

This leads to the condition

$$\begin{aligned}\left(c\vec{\alpha}\vec{p} + \beta m_0 c^2\right)^2 &= \beta^2(m_0c^2)^2 + \frac{c^2}{2}\sum_{i\,j}(\alpha_i\alpha_j + \alpha_j\alpha_i)p_i\,p_j + \sum_i(\alpha_i\beta + \beta\alpha_i)p_i\,m_0c^2 \\ &\stackrel{!}{=} \left((m_0c^2)^2 + (pc)^2\right)\Psi\end{aligned}$$

or, equivalently

$$\beta^2 = 1, \quad (\alpha_i\alpha_j + \alpha_j\alpha_i) = 2\delta_{ij}, \quad (\alpha_i\beta + \beta\alpha_i) = 0 \tag{3.17}$$

Obviously, this set of equation does not have any solution for $\alpha_i, \beta \in \mathbb{C}$. But Dirac realized that solutions do exist when α_i and β are Hermitian matrices.
More convenient than α_i and β are the so-called γ**-matrices** defined by $\gamma^0 = \beta$, $\gamma^i = \beta\alpha^i$ with $i = 1, 2, 3$). From this definition we obtain $(\gamma^i)^2 = \beta\alpha_i\beta\alpha_i \underbrace{=}_{\alpha_i\beta=-\beta\alpha_i} -\alpha_i\beta\beta\alpha_i = -\mathbb{1}$. All conditions from Eq. (3.17) can be combined in the compact equation

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\,\nu}\ \mathbb{1} \tag{3.18}$$

where – as before – we define $\{A, B\} = AB + BA$.
The smallest possible matrices which fulfill these equations are 4×4 matrices. One can, for example, choose the following solution

$$\gamma^0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \quad \gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix} \quad (i = 1, 2, 3)$$

with the Pauli matrices $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$.
It is also useful to define

$$\gamma^5 = i\gamma^0\,\gamma^1\,\gamma^2\,\gamma^3 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$$

Note that also other representations are possible. If one redefines $\gamma^\mu \rightarrow M\gamma^\mu M^{-1}$ with arbitrary unitary matrices M, physics will not change (only some observables have also to be redefined).
As the γ matrices are 4×4 matrices, it is clear that the wave function must have also 4 components. It is called a **spinor** , $\Psi = \begin{pmatrix} \Psi_1(x) \\ \Psi_2(x) \\ \Psi_3(x) \\ \Psi_4(x) \end{pmatrix}$. For the moment we will pretend that the components are complex functions, $\Psi_i(x) \in \mathbb{C}$ but later we will see that they are actually field operators. A **warning** is appropriate in this context: while $\Psi(x)$ has 4 compents it is, nevertheless, **not** a covariant or contravariant 4-vector. The transformation properties of Ψ are completely different and will be discussed in chapter 3.6.
Now we can rewrite (3.16) by multiplying it with $\frac{\gamma^0}{c}$ to obtain the **Dirac equation**

$$(-i\hbar\gamma^\mu\partial_\mu + m_0 c)\Psi = 0 \tag{3.19}$$

As discussed in chapter 3.4, the coupling to the electromagnetic field can be obtained simply by replacing ∂_μ by $D_\mu = \partial_\mu - \frac{e}{c}A_\mu$ and one obtains

$$(-i\hbar\gamma^\mu D_\mu + m_0 c)\,\Psi = 0 \quad \Leftrightarrow \quad \left(-i\hbar \not{D} + m_0 c\right)\Psi = 0 \tag{3.20}$$

where we introduced as a short-hand notation the so-called Feynman slash notation (sometimes also called the Feynman dagger): $\not{a} = \sum_{\mu=0,\ldots 3} \gamma^\mu a_\mu$ defines a 4×4 matrix.
Historically, it was a goal of Dirac to find an equation where a positive quantity, $\Psi^\dagger\Psi$ can be interpreted as a probability. Later we will see that such an interpretation is *not* possible. $\rho = \Psi^\dagger\Psi$ describes instead the charge density. As this is an important quantity, we will derive its continuity equation. From the Dirac equation in the form $i\hbar\partial_t\Psi = H_D\Psi$ with $H_D = i\hbar c\vec{\alpha}\vec{\nabla} + \beta m_0 c^2$ we obtain by Hermitian conjugation conjugation $-i\hbar\partial_t\Psi^\dagger = (H_D\Psi)^\dagger = -i\hbar c(\nabla_i\Psi^\dagger)\alpha_i + m_0 c^2\Psi^\dagger\beta$. Therefore

$$\begin{aligned}
\dot{\rho} &= \Psi^\dagger\partial_t\Psi + \left(\partial_t\Psi^\dagger\right)\Psi \\
&= \frac{1}{i\hbar}\left(\Psi^\dagger\gamma^0\left(i\hbar c\gamma^i\nabla_i\right)\Psi + \Psi^\dagger\gamma^0 m_0 c^2\Psi + \left(i\hbar c\left(\nabla_i\Psi_i^\dagger\right)\gamma^0\gamma^i\Psi - \Psi^\dagger\gamma^0 m_0 c^2\Psi\right)\right) \\
&= -c\nabla_i\left(\Psi^\dagger\gamma^0\gamma^i\Psi\right) = -\vec{\nabla}\vec{j}
\end{aligned}$$

We therefore obtain the conserved 4-current

$$j^\mu = (c\rho, \vec{j}) = c\bar{\Psi}\gamma^\mu\Psi \quad \text{with} \quad \partial_\mu j^\mu = 0 \;\Leftrightarrow\; \partial_t\rho + \vec{\nabla}\vec{j} = 0 \tag{3.21}$$

where we introduced $\overline{\Psi}$ defined by

$$\overline{\Psi} = (\gamma^0\Psi)^\dagger = \Psi^\dagger\gamma^0 = \left(\Psi_1^\dagger, \Psi_2^\dagger, -\Psi_3^\dagger, -\Psi_4^\dagger\right)$$

For complex functions $\Psi_i(x)$ we have $\Psi_i^\dagger = \Psi_i^*$, but for field operators it is important to use instead $\Psi_i^\dagger(x)$.

3.6 Lorentz covariance of the Dirac equation

If the Dirac equation is a valid relativistic equation, it should have the same form in all frames of reference. This we will show in this chapter. This will also help us later to find and understand the solutions of the Dirac equation.
We consider the Lorentz transformation, $x^\mu \;\rightarrow\; \tilde{x}^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu$, or, equivalently, without indices in a matrix notation

$$x \rightarrow \tilde{x} = \Lambda\, x + a$$

In the new frame of reference the Dirac equation has to have the form

$$\left(-i\gamma^\mu \frac{\partial}{\partial \tilde{x}^\mu} + m\right) \tilde{\Psi}(\tilde{x}) = 0 \tag{3.22}$$

where we have used units with $c = \hbar = 1$ and have set $m = m_0$. We have now to find out how $\tilde{\Psi}$ and Ψ are related. We set

$$\tilde{\Psi}(\tilde{x}) = S_\Lambda \Psi(x) = S_\Lambda \Psi\left(\Lambda^{-1}(\tilde{x} - a)\right) \tag{3.23}$$

where the (yet unknown) 4×4-matrix S_Λ, acts on the spinor index only.
Using $\frac{\partial}{\partial \tilde{x}^\mu} = \Lambda_\mu{}^\nu \frac{\partial}{\partial x^\nu}$ we obtain from Eq. (3.22)

$$\left(-i\gamma^\mu \Lambda_\mu{}^\nu \partial_\nu + m\right) S_\Lambda \Psi(x) \quad \underbrace{\Rightarrow}_{S^{-1}\cdot\ldots} \quad \Big(- i \underbrace{S_\Lambda^{-1} \gamma^\mu \Lambda_\mu{}^\nu S_\Lambda}_{\stackrel{!}{=}\gamma^\nu} \partial_\nu + m\Big)\Psi(x) = 0$$

Therefore $S_\Lambda^{-1}\gamma^\mu S_\Lambda \Lambda_\mu{}^\nu = \gamma^\nu$ or, equivalently

$$S_\Lambda^{-1}\gamma^\mu S_\Lambda = \Lambda^\mu{}_\nu \gamma^\nu \tag{3.24}$$

Below, we will see that S_Λ does exist and therefore we have shown that the Dirac equation is indeed Lorentz invariant, i.e., it looks the same way in all coordinate systems when the transformation

$$\begin{aligned} x \to \tilde{x} &= \Lambda\, x + a \\ \Psi(x) \to \tilde{\Psi}(\tilde{x}) &= S_\Lambda \Psi(x) = S_\Lambda \Psi(\Lambda^{-1}(\tilde{x} - a)) \end{aligned} \tag{3.25}$$

is considered.
To construct S_Λ it is useful to investigate first only infinitesimal transformations

$$\Lambda = \mathbb{1} + \underbrace{\Delta\omega}_{\text{small}}, \qquad S = \mathbb{1} + \underbrace{\Delta\tau}_{\text{small}}$$

where both $\Delta\omega$ and $\Delta\tau$ are small (!) 4×4 matrices. As $S^{-1} = \mathbb{1} - \Delta\tau + \mathcal{O}(\Delta\tau^2)$, we obtain from Eq. (3.24) $-\Delta\tau\gamma^\mu + \gamma^\mu \Delta\tau = \Delta\omega^\mu{}_\nu \gamma^\nu$ which is solved by

$$\Delta\tau = -\frac{i}{4}\Delta\omega^{\mu\nu}\sigma_{\mu\nu} = \frac{1}{8}\Delta\omega^\mu{}_\nu\, g_{\mu\nu'}\,[\gamma^{\nu'}, \gamma^\nu], \qquad \text{with} \quad \sigma_{\mu\nu} = \frac{i}{2}\,[\gamma_\mu\,,\,\gamma_\nu]$$

Let us see, how we can use this equation to find out how spinors are rotated. A rotation

around the z axis is described by the matrix

$$\Lambda = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\varphi) & -\sin(\varphi) & 0 \\ 0 & \sin(\varphi) & \cos(\varphi) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \Rightarrow \quad \Delta\omega = \varphi \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Therefore only $\Delta\omega_{12} = -\varphi$ and $\Delta\omega_{21} = \varphi$ are finite and therefore

$$\begin{aligned} \Delta\tau &= -\frac{i}{4}\left(-\varphi\sigma_{12} + \varphi\sigma_{21}\right) = \frac{i}{2}\varphi\sigma_{12} = -\frac{\varphi}{4}\left(\gamma_1\gamma_2 - \gamma_2\gamma_1\right) \\ &= -\frac{\varphi}{2}\begin{pmatrix} 0 & \sigma_x \\ -\sigma_x & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_y \\ -\sigma_y & 0 \end{pmatrix} = +\frac{i\varphi}{2}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix} \end{aligned}$$

Therefore we find that for small rotation angles, S_Λ is given by $S = \mathbb{1} + \frac{i}{2}\varphi \begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}$. From this we can easily construct S for a finite rotation by an angle φ by considering N rotations by the angle φ/N.

$$S(\varphi) = \left(S\Big(\frac{\varphi}{N}\Big)\right)^N = \lim_{N\to\infty}\left(\mathbb{1} + \frac{i\varphi}{2N}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}\right)^N = \exp\left(i\frac{\varphi}{2}\begin{pmatrix} \sigma_z & 0 \\ 0 & \sigma_z \end{pmatrix}\right)$$

As similar formulas hold for rotations around the y and z axis with σ_z replaced by σ_x and σ_y, respectively, we can conclude that

the generator of rotation of spinors is given by $\vec{S} = \frac{\hbar}{2}\begin{pmatrix} \vec{\sigma} & 0 \\ 0 & \vec{\sigma} \end{pmatrix}$

The prefactor $\hbar$ appears here as a convention: a finite rotation is described by $e^{i\vec{\varphi}\vec{S}/\hbar}$. To describe the full rotation of a spinor wave function, $\Psi \to \tilde{\Psi}$ with $\tilde{\Psi}(\tilde{x}) = S_\Lambda\Psi(x)$, we have to take into account that also the coordinate system has been transformed, $x \to \tilde{x}$, see Eq. (3.25). As the generator of rotation in space is given by the angular momentum, $\vec{L} = \vec{r}\times\vec{p} = \vec{r}\times(-i\hbar\vec{\nabla})$, we obtain that a rotated wavefunction $\tilde{\Psi}(x)$ is obtained from

$\tilde{\Psi}(x) = e^{i\vec{\varphi}\vec{J}/\hbar}\Psi(x)$ with the total angular momentum $\vec{J} = \vec{L} + \vec{S}$,

which is the generator of rotations involving both real and spin space.
While in a relativistic theory neither $\vec{L}$ nor $\vec{S}$ is conserved separately, the statement that the physics is identical in a rotated coordinate system implies that

$$\Big[\vec{J},\ H_D\Big] = \Big[\vec{L} + \vec{S},\ H_D\Big] = 0,$$

the total angular momentum is conserved.

We can repeat the discussion given above without any problem also for boosts. A boost in x-direction is described for a small $\eta \approx v/c \ll 1$ by

$$\Lambda = \begin{pmatrix} \cosh(\eta) & -\sinh(\eta) & 0 & 0 \\ -\sinh(\eta) & \cosh(\eta) & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \approx \mathbb{1} + \eta \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \mathbb{1} + \Delta\omega$$

Following exactly the same steps as in the case of the rotation described above one finds that the corresponding transformation of the spinor is obtained by the 4×4 matrix $S = \exp\left(-\frac{\eta}{2}\begin{pmatrix} 0 & \sigma_x \\ \sigma_x & 0 \end{pmatrix}\right)$. We conclude that in general

boosts of spinors are generated by $\frac{1}{2}\begin{pmatrix} 0 & \vec{\sigma} \\ \vec{\sigma} & 0 \end{pmatrix}$

.

We have therefore determined how the continuous group elements affect spinors. What is missing are the discreet transformation, P, T and PT. We just give the result.

The inversion transformation P of a spinor is described by

$$S_P = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} = \gamma^0$$

More complicated is time reversal, at it is not a linear operator but also involves complex conjugation using that $i\hbar\partial_t = -i\hbar\partial_{-t}$. One obtains that

time reversal is described by

$$t \to -t \quad , \vec{r} \to \vec{r} \quad , i \to -i, \qquad \Psi(t, \vec{r}) \to i\gamma^1\gamma^3\Psi^*(-t, r)$$

The combined transormation PT is obtained by multiplying both transformations $\Psi(t, \vec{r}) \to i\gamma^0\gamma^1\gamma^3\Psi^*(-t, -r)$.

It is important to note that S_Λ turns out to be not a unitary transformation but instead one finds for proper Lorentz transformation (excluding time-reversal which is special)

$$S^\dagger\gamma^0 = \gamma^0 S^{-1}.$$

This implies that not $\Psi^\dagger$ but only $\bar{\Psi}$ has simple transformation properties.

$$\overline{\Psi} = \Psi^\dagger\gamma^0 \;\to\; (S\Psi)^\dagger\gamma^0 = \Psi^\dagger S^\dagger\gamma^0 = \Psi^\dagger\gamma^0 S^{-1} = \overline{\Psi}S^{-1}$$

Therefore it is not surprising, that physical observables are often expressed in terms of $\bar{\Psi}$ and Ψ. For example, we have found for the conserved 4-current, that $j^\mu = \overline{\Psi}\gamma^\mu\Psi$. Let us check how j^μ transforms under a Lorentz transformation

$$j^\mu = \overline{\Psi}\gamma^\mu\Psi \;\to\; \tilde{\Psi}\, S^{-1}\, \gamma^\mu\, S\, \Psi = \Lambda^\mu{}_\nu\, j^\nu$$

where we used Eq. (3.24). As expected, j^μ transforms like any covariant 4-vector.
Similarly, $\overline{\Psi}\Psi$ has to be a Lorentz scalar, it does not change under a Lorentz transformation $\overline{\Psi}\Psi \;\rightarrow\; \overline{\Psi}\, S^{-1} S\, \Psi = \overline{\Psi}\Psi$.
The matrices S_Λ have to form a group. This group is, however, *not* identical to SO(1,3). This is very similar to the situation known from the group of rotations: rotating of a spin by 2π leads to a minus sign in the wave function, therefore SU(2), describing rotation of spins, and SO(3) are not identical. The group of Lorentz transformations acting on spinors is called spin$(1,3)$ which turns out to be identical to the group $SL(2,\mathbb{C})$, the group of complex 2×2-matrices M with $\det M = 1$ which is also parametrized by 6 real variables. For completeness, we mention one more important symmetry transformation, C, of the Dirac fields, which is obtained by considering the complex-conjugated version of the Dirac equation. The symmetry is called charge conjugation (hence the letter C) or – more precisely – particle-antiparticle transformation as this transformation turns out to transform an electron to a positron and vice versa (c.f. chapter 3.8). It is given by

charge conjugation C: $\Psi \rightarrow C\bar{\Psi}^T$ with $C = i\gamma^2\gamma^0$

3.7 Solution of the Dirac equation

In this chapter we will solve the Dirac equation in the absence of electromagnetic fields as a differential equation in the absence of fields. These solutions will also be the building block of the quantized theory. We want to solve

$$(-i\hbar\partial\!\!\!/ + m_0 c)\,\Psi = 0$$

We first determine the zero-momentum solution of a particle at rest. We therefore set the spatial derivative to zero, $\frac{\partial}{\partial\vec{r}}\Psi = 0$

$$\left(-i\frac{\hbar}{c}\frac{\partial}{\partial t}\begin{pmatrix}1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1\end{pmatrix} + m_0 c\,\mathbb{1}\right)\Psi = 0 \quad \Rightarrow \quad i\hbar\partial_t\Psi = m_0c^2\cdot\begin{pmatrix}1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1\end{pmatrix}\Psi$$

This $4x4$ matrix equation has 4 solutions

$$\Psi_i^{(+)}(x) = e^{-im_0c^2t/\hbar}u_i(0) \qquad \Psi_i^{(-)}(x) = e^{+im_0c^2t/\hbar}v_i(0)$$

$$\text{with} \quad u_1(0) = \begin{pmatrix}1\\0\\0\\0\end{pmatrix}, \quad u_2(0) = \begin{pmatrix}0\\1\\0\\0\end{pmatrix}, \quad v_1(0) = \begin{pmatrix}0\\0\\1\\0\end{pmatrix}, \quad v_2(0) = \begin{pmatrix}0\\0\\0\\1\end{pmatrix}$$

The two + solutions have an obvious interpretation: they describe electrons at rest with energy m_0c^2. As we have determined the spin-operator to be $\vec{S} = \frac{\hbar}{2}\begin{pmatrix}\vec{\sigma} & 0\\ 0 & \vec{\sigma}\end{pmatrix}$, we also know

that $\Psi_1^{(+)}$ and $\Psi_2^{(+)}$ describe electrons with $\uparrow$ and $\downarrow$ spins, respectively. The interpretation of the solution with negative energy is unclear at the moment, later we will use these solutions to describe the antiparticle of the electron, the positron.
To obtain solutions of the Dirac equation at finite momentum one can just perform a Lorentz transformation to a coordinate system moving with velocity $-\vec{v}$ such that the particle at rest obtains the velocity $+\vec{v}$. This is left as an exercise. Here we just derive the solution starting from a straightforward plane-wave ansatz

$$\Psi_i^{(+)} = u_i(K)e^{-iK_\mu x^\mu}, \qquad \Psi_i^{(-)} = v_i(K)e^{+iK_\mu x^\mu}$$

From the Dirac equation one finds directly

$$\left(\not{K} - \frac{m_0 c}{\hbar}\right) u_i(K) = 0, \qquad \left(\not{K} + \frac{m_0 c}{\hbar}\right) v_i(K) = 0$$

We have therefore just to determine the eigenvectors of some 4×4 matrix with eigenvalue 0. This is simplified by a trick: $\not{K}\not{K} = K_\mu \gamma^\mu K_\nu \gamma^\nu = \frac{K_\mu K_\nu}{2} \{\gamma^\mu, \gamma^\nu\} = K_\mu K_\nu g^{\mu\nu} \mathbb{1} = K_\mu K^\mu \mathbb{1}$. Therefore we find

$$\left(\not{K} - \frac{m_0 c}{\hbar}\right)\left(\not{K} + \frac{m_0 c}{\hbar}\right) = K_\mu K^\mu \mathbb{1} - \left(\frac{m_0 c}{\hbar}\right)^2 \mathbb{1} \stackrel{!}{=} 0$$

From this we can directly read off the relativistic energy-momentum relation

$$E = c\hbar K_0 = +\sqrt{(m_0 c^2)^2 + (\hbar K c)^2}$$

Using this K^μ, we also find that $u_i(K) = \alpha\left(\not{K} + \frac{m_0 c}{\hbar}\right) u_i(K = 0)$ solves the desired equation $\left(\not{K} - \frac{m_0 c}{\hbar}\right) u_i(K) = 0$ where the normalization constant α is chosen to be $\alpha = \frac{\hbar c}{\sqrt{(2m_0 c^2 (m0c^2 + E))}}$, see discussion below.
Finally, we obtain

$$u_i(K) = \alpha\left(\not{K} + \frac{m_0 c}{\hbar}\right) u_i(K=0) = \begin{pmatrix} \left(\frac{(E+m_0c^2)}{2m_0c^2}\right)^{1/2} \chi_i \\ \frac{\hbar c \vec{\sigma}\vec{K}}{\sqrt{((2m_0c^2)(m_0c^2+E))}} \chi_i \end{pmatrix}$$

$$v_i(K) = \alpha\left(\not{K} + \frac{m_0 c}{\hbar}\right) v_i(K=0) = \begin{pmatrix} \frac{\hbar c \vec{\sigma}\vec{K}}{\sqrt{((2m_0c^2)(m_0c^2+E))}} \chi_i \\ \left(\frac{(E+m_0c^2)}{2m_0c^2}\right)^{1/2} \chi_i \end{pmatrix} \qquad (3.26)$$

where $\chi_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\chi_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$.
The normalization constant α has been chosen such that $\overline{u}_i u_j = u_i^\dagger \gamma^0 u_j = \delta_{ij}$ and $\overline{v}_i v_j = v_i^\dagger \gamma^0 v_j = -\delta_{ij}$. Here we used that the combination $\overline{\Psi}\Psi$ is Lorentz invariant. This guarantees that the solutions at different $\vec{K}$ can be obtained from Lorentz transformations.

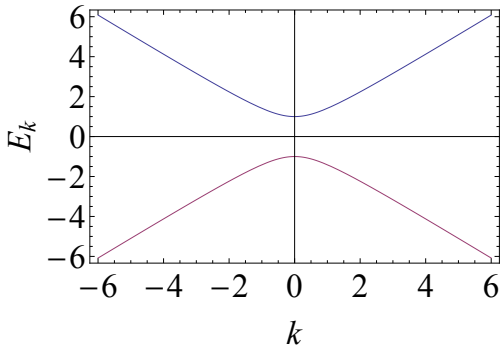


Figure 3.1: Apparently, the Dirac equations has solutions with positive and negative energies, $\pm\sqrt{(m_0c^2)^2+(pc)^2}$. Dirac used as an interpretation, that all states with negative energy are occupied.

Note that in general the solutions at finite $\vec{K}$ are *not* eigenstates of $S_z = \frac{\hbar}{2}\begin{pmatrix}\sigma_z & 0\\ 0 & \sigma_z\end{pmatrix}$. This reflects that the direction of the spin changes when we switch to a moving coordinate system. An exception is the case when $\vec{K}$ is in the z direction.
It is instructive to calculate the charge density of our solutions

$$\overline{\Psi}\gamma^0\Psi = \Psi^\dagger\Psi = \frac{E+m_0c^2}{2m_0c^2} + \frac{\left(c\hbar\vec{K}\right)^2}{(E+m_0c^2)\,(2m_0c^2)} = \frac{1}{2m_0c^2}\left(E+m_0c^2+\underbrace{\frac{E^2-(m_0c^2)^2}{E+m_0c^2}}_{E-m_0c^2}\right)$$

$$= \frac{E}{m_0c^2} = \frac{1}{\sqrt{1-(\frac{v}{c})^2}}$$

where we used that $\chi_i^\dagger(\vec{K}\vec{\sigma})^2\chi_i \underbrace{=}_{\sigma_i\sigma_j=\delta_{ij}+i\epsilon^{ijk}\sigma_k} \vec{K}^2+0$ While the charge density depends on the frame of reference, this is not the case for the total charge $Q = \int \mathrm{d}^3r\rho(\vec{r})$ which is Lorentz invariant as from $r' = \dfrac{r-vt}{\sqrt{1-(\frac{v}{c})^2}}$ we obtain $\mathrm{d}r = \sqrt{1-(\frac{v}{c})^2}\,\mathrm{d}r$ which cancels the change of the charge density discussed above. We will use the above derived result again and therefore remember

$$\overline{u}_i\gamma^0u_j = \delta_{ij}\frac{E}{m_0c^2} = \overline{v}_i\gamma^0v_j \tag{3.27}$$

3.8 Interpretation of Dirac equation

As we have already seen in the case of the Klein Gordon equation, the energy of excitations described by the Dirac equation, $E = \pm\sqrt{(m_0c^2)^2+(\hbar Kc)^2}$, can – apparently – be not only positive but also negative. Clearly something which does not occur in nature. Dirac found a solution to this problem: he argued that all states with negative energy have to

be already occupied even in the vacuum. This state is called the "Dirac sea" . The Pauli principle ensures that this state is stable. An electron at rest, for example, cannot gain extra energy by by moving to a negative energy state as such processes are forbidden by the Pauli principle. One might ask the question whether the infinite negative charge of the vacuum is a problem. The answer is that the negative charge is canceled by the positively charged Dirac sea of other particles (e.g. the protons or, more precisely, the quarks building up the proton). A more tricky (and presently unresolved) question is whether the nominally infinite negative energy density of the Dirac sea exists which can couple to gravity. Is this contribution (almost) exactly canceled by a positive energy density arising from bosonic modes (see discussion in Sec. 2.1)?
Dirac realized, that his interpretation also implies that there is a new type of excitation: removing one of the negative energy states costs a positive amount of energy,

$$E - E_{\text{vacuum}} = +\sqrt{(m_0c^2)^2 + (\hbar Kc)^2}.$$

The excitation therefore has exactly the same mass as the electron. But as one negatively charged electron is missing, this excitation has a *positive* charge. Based on this interpretation, Dirac predicted in 1928 the positron, which was experimentally discovered by C.D. Anderson in 1932, when he investigated how particles coming from cosmic rays are deflected by a magnetic field. Due to their opposite charge positrons and electrons are deflected in opposite directions.
From a modern point of view, the Dirac construction is a valid point of view. A more flexible approach is, however, to define from the beginning the vacuum and the field operator in such a way that negative energy states never arise. We have seen that such a procedure works also to interpret the negative energy states of the Klein Gordon equation, which describes Bosons (therefore Pauli's principle, an important element of Dirac's construction, is not applicable).
To obtain a valid quantization of the Dirac field, we proceed in three steps. First, we expand $\Psi(x)$ in the four plane wave solutions $\Psi_{1/2}^{(+/-)}$. Second, we rewrite the energy of the system in terms of the corresponding expansion coefficients. And, third, we replace the expansion coefficients by creation and annihiliation operators such that the Hamiltonian has the expected structure, $H = \sum_k E_k n_k$, with $E_k = \sqrt{(m_0c^2)^2 + (\hbar kc)^2}$ being the relativistic energy-momentum relation and n_k an operator counting the number of particles. We will now follow this program. To simplify notations at a later stage, let us first define two new functions, $w_1(k) = v_2(k)$, $w_2(k) = -v_1(k)$ (this is actually a part of a particle-hole transformation, see Eq. (1.12) in Sec. 1.4.5). We therefore write

$$\Psi(x) = \sum_{K,\,\sigma=1,2} \alpha_K \left(b_{\sigma,K} u_\sigma(K) e^{-iK_\mu x^\mu} + d^*_{\sigma,K} w_\sigma(K) e^{iK_\mu x^\mu} \right) \tag{3.28}$$

where $\alpha_K \in \mathbb{R}$ is a normalization factor to be determined later and $b_{\sigma K}, d_{\sigma K} \in \mathbb{C}$ are

some complex expansion coefficients. As the $b_{\sigma\, K}, d_{\sigma\, K}$ will later become operators, we will keep track of their ordering during the following calculations and instead of $d^*_{\sigma,\, K}$ we will write $d^\dagger_{\sigma,\, K}$.

As a next step, we need a formula for the energy, or better, the 4-vector describing both energy and momentum $p^\mu = \left(\frac{E}{c}, \vec{p}\right)$. Starting point is the correspondence principle which (in first quantization) identifies p^μ with $i\hbar\partial^\mu$ plus the requirement of Lorentz invariance. Both requirements are fulfilled by

$$p^\mu = \int d^3\vec{x}\, \Psi^\dagger i\hbar\, \partial^\mu \Psi = i\hbar \int d^3\vec{x}\, \overline{\Psi}\gamma^0 \partial^\mu \Psi \tag{3.29}$$

The extra γ^0 is needed to compensate for the Lorentz contraction of d^3r. Now we plug (3.28) into (3.29) and obtain

$$\begin{aligned} p^\mu = i\hbar \int \mathrm{d}^3\vec{x} \sum_{\substack{K\ \sigma \\ K'\ \sigma'}} \alpha_K \alpha_{K'} \Big(b^\dagger_{\sigma'\, K'} \overline{u}_{\sigma'}(K') e^{iK'_\mu x^\mu} + d_{\sigma'\, K'} \overline{w}_{\sigma'}(K') e^{-iK'_\mu x^\mu} \Big) \\ \cdot \gamma^0 \Big(-iK^\mu b_{\sigma\, K} u_\sigma(K) e^{-iK_\mu x^\mu} + iK^\mu d^\dagger_{\sigma\, K} w_\sigma(K) e^{+iK_\mu x^\mu} \Big) \end{aligned}$$

We can now perform the integration using $\int e^{iK'_\mu x^\mu} e^{-iK_\mu x^\mu}\, \mathrm{d}^3x = \delta_{K\, K'} V$ and $\int e^{iK'_\mu x^\mu} e^{iK_\mu x^\mu} = \delta_{K\, -K'} V \cdot e^{2iK^0 tc}$. With $E_K = c\hbar K^0 = \sqrt{(m_0c^2)^2 + (\hbar Kc)^2}$ and copy from Eq. (3.27) the relations $\overline{u}_\sigma \gamma^0 u_{\sigma'}(K) = \frac{E_K}{m_0c^2}\, \delta_{\sigma\, \sigma'} = \overline{w}_\sigma(K)\gamma^0 w_{\sigma'}(K)$. We obtain

$$p^\mu = \sum_{K,\, \sigma} \alpha_K^2 \frac{E_K}{m_0c^2}\, V\hbar K^\mu \left(b^\dagger_{\sigma\, K} b_{\sigma\, K} - d_{\sigma\, K} d^\dagger_{\sigma\, K} \right)$$

As this equation should have the form $\hbar K^\mu$ times an occupation number we set

$$\alpha_K = \sqrt{\frac{m_0c^2}{E_K V}}$$

such that

$$p^\mu = \sum_{K,\, \sigma} \hbar K^\mu \left(b^\dagger_{\sigma\, K} b_{\sigma\, K} - d_{\sigma\, K} d^\dagger_{\sigma\, K} \right)$$

The Hamiltonian is therefore given by

$$H = cp^0 = \sum_{K\, \sigma} E_K \left(b^\dagger_{\sigma\, K} b_{\sigma\, K} - d_{\sigma\, K} d^\dagger_{\sigma\, K} \right)$$

Now, we want to interpret $b_{\sigma\, K}$ and $d_{\sigma\, K}$ as operators. now: $b_{\sigma\, K}$ $d_{\sigma\, K}$ become creation and annihiliation operators. Due to the $-$ sign, a interpretation in terms of *bosonic* operators is *not* possible as in this case an accelerating particle would gain more and more energy, clearly unphysical. We conclude that

The Dirac equation can only be quantized with fermionic creation and annihilation operators

to avoid negative energies.
We therefore postulate that

$$\left\{d_{\sigma\,K},\, d^\dagger_{\sigma'\,K'}\right\} = \delta_{\sigma\,\sigma'}\,\delta_{K\,K'}, \qquad \left\{b_{\sigma\,K},\, b^\dagger_{\sigma'\,K'}\right\} = \delta_{\sigma\,\sigma'}\,\delta_{K\,K'} \tag{3.30}$$

while all other anticommutators vanish, $0 = \{d,\, b\} = \{d^\dagger,\, b^\dagger\} = \{d, b^\dagger\} = \{d^\dagger,\, b\}$.
The Hamiltonian can therefore be written as

$$H = \sum_{K,\,\sigma} E_K \Big(\underbrace{b^\dagger_{\sigma\,K} b_{\sigma\,K}}_{\#\text{ of electrons}} + \underbrace{d^\dagger_{\sigma\,K} d_{\sigma\,K}}_{\#\text{ of positrons}} - 1 \Big) \tag{3.31}$$

$\Psi(x)$ and $\Psi^\dagger(x)$ are now field operators with

$$\Psi(x) = \sum_{K,\sigma} \sqrt{\frac{m_0 c}{E_K V}} \left(b_{\sigma\,K} u_\sigma(K) e^{-iK_\mu x^\mu} + d^\dagger_{\sigma\,K} w_\sigma(K) e^{iK_\mu x^\mu} \right) \tag{3.32}$$

One can easily check that the time dependence of the field $\Psi(x)$ is consistent with the Heisenberg equations of motions. According to the Hamiltonian (3.31) one has $b_{K_0}(t) = e^{-iE_K t/\hbar} b_{K\,\sigma}$ and $d^\dagger_K(t) = e^{+iE_K t/\hbar} d^\dagger_{K\,\sigma}$ reproducing the terms $e^{-iK^0 ct}$ and $e^{iK^0 ct}$ in Eq. (3.32). Expressed in these quantum fields, the Hamiltonian (3.31) can also be written as

$$H = \int d^3\vec{x}\, \bar{\Psi}\gamma^0 i\hbar\partial_t \Psi = \int d^3\vec{x} \sum_{i=1,2,3} \bar{\Psi}(-i\hbar c\gamma^i \partial_i + mc^2)\Psi \tag{3.33}$$

The first equality was our original ansatz for the energy, the second equality follows directly from the Dirac equation.
To define the Hilbert space, one start from the vacuum state $|0\rangle$ which is defined by

$$b_{\sigma\,K}\,|0\rangle = 0, \qquad d_{\sigma\,K}\,|0\rangle = 0$$

All other basis states of the Hilbert space are created by applying products of creation operators to $|0\rangle$.
To find the correct interpretation for $b_{\sigma\,K}$ and $d_{\sigma\,K}$ one can repeat the calculation sketched above to show that the momentum is given by $\vec{p} = \sum_{K\,\sigma} \hbar\vec{K} \left(b^\dagger_{\sigma\,K} b_{\sigma\,K} + d^\dagger_{\sigma\,K} d_{\sigma\,K} \right)$ and the total charge by

$$\begin{aligned} Q &= q \int \overline{\Psi}\gamma^0 \Psi = q \int \Psi^\dagger \Psi = q \sum \left(b^\dagger_{\sigma\,K} b_{\sigma\,K} + d_{\sigma\,K} d^\dagger_{\sigma\,K} \right) \\ &= q \sum_{K\,\sigma} \left(b^\dagger_{\sigma\,K} b_{\sigma\,K} - d^\dagger_{\sigma\,K} d_{\sigma\,K} \right) + \text{const.} \end{aligned}$$

where an overall prefactor q is a convention.
Based on these formulas, we can conclude that

$b^\dagger_{K\,\sigma}$: creates an electron with energy E_K and charge $q = e$
$d^\dagger_{K\,\sigma}$: creates an positron with energy E_K and charge $-q = -e$

In conclusion, we have shown that the quantization of the Dirac equation naturally leads to a description of an electron with a spin 1/2 which is a fermion. It also predicts the presence of its antiparticle, the positron. Exactly the same equation can be used to describe other fermions, including the proton and the neutron (or the quarks, the constituents of proton an neutron). Using our prescriptions for minimal coupling, we can also immediately describe the coupling to the electromagnetic field and therefore also the coupling of protons and electrons.

We finish this section by calculating the commutator of our quantum fields using the commutation relations (3.30). For **equal times** one has to compute

$$\left\{\Psi_\alpha(\vec{r}),\, \Psi^\dagger_\beta(\vec{r}\,')\right\} = \sum_{\vec{K}\,\vec{\sigma}} \frac{m_0 c^2}{E_K V} \left(e^{i\vec{K}(\vec{r}-\vec{r}\,')} u_{\sigma\,\alpha}(K) u^*_{\sigma\,\beta}(K) + w_{\sigma\,\alpha}(K) w^*_{\sigma\,\beta}(K) e^{-i\vec{K}(\vec{r}-\vec{r}\,')}\right)$$

To simplify this expression one needs the relation $\sum_\sigma u_{\sigma\,\alpha}\overline{u}_{\sigma\,\beta} = \left(\frac{\not{K}+m_0 c}{2m_0 c}\right)_{\alpha\,\beta}$ and $\sum_\sigma w_{\sigma\,\alpha}\overline{w}_{\sigma\,\beta} = \left(\frac{\not{K}-m_0 c}{2m_0 c}\right)_{\alpha\,\beta}$ which are easy to check. One finds the expected anticommutation relations

$$\left\{\Psi_\alpha(\vec{r}),\, \Psi^\dagger_\beta(\vec{r}\,')\right\} = \delta_{\alpha\,\beta}\; \delta^3(\vec{r}-\vec{r}\,')$$

Note that the commutation relations for fields at different times are much more complicated even in the absence of interactions. But one always has the property that $\left\{\Psi_\alpha(r,\,t),\, \Psi^\dagger_\beta(r',\,t')\right\} = 0$ for $|r-r'| > c|t-t'|$, such that no information can propagate from r to r'.

3.9 Graphene as a Dirac material

In recent years, the Dirac equation and variants thereof have found remarkable applications in the description of the properties of actual materials. In this section we discuss briefly a by now famous example in two spatial dimensions: the physics of graphene. Graphene is a single layer of graphite, where the carbon atoms form a honeycomb lattice. For our purpose, the best way to view the honeycomb lattice is to split it into two sublattices, A and B, both formed by carbon atoms, see Fig. 3.2. Using the two basis vectors

$$\vec{a}_1 = a(1,0), \qquad \vec{a}_2 = a\left(\cos\frac{\pi}{3}, \sin\frac{\pi}{3}\right) = a\left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right) \tag{3.34}$$

the A-sublattice is spanned by the vectors

$$\vec{R}_{\vec{n}} = n_1\vec{a}_1 + n_2\vec{a}_2, \qquad n_1, n_2 \in \mathbb{Z}.$$

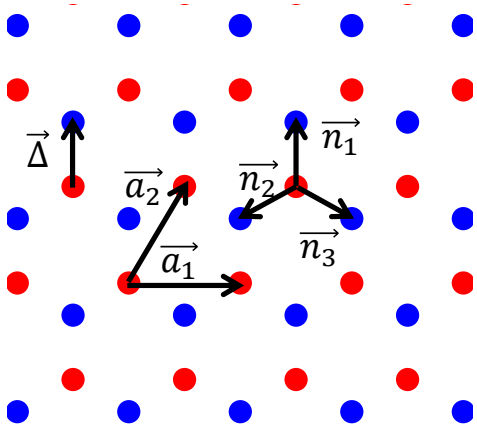


Figure 3.2: In graphene carbon atoms are located on a hexagonal lattice. The hexagonal lattice splits into two sublattices, A and B, shown in red and blue.

Similarly, the B-sublattice is spanned by $\vec{R}_{\vec{n}} + \vec{\Delta}$, with

$$\vec{\Delta} = a\left(0, \frac{1}{\sqrt{3}}\right). \tag{3.35}$$

We want to describe electrons hopping from one site of the graphene lattice to a neighboring site. We therefore introduce creation operators, $c^\dagger_{A,\vec{n}}$ and $c^\dagger_{B,\vec{n}}$, which creates electrons at the graphene atom located at $n_1\vec{a}_1 + n_2\vec{a}_2$ and $n_1\vec{a}_1 + n_2\vec{a}_2 + \vec{\Delta}$, respectively, with $\vec{n} = (n_1, n_2)$. To be precise, the operators create an electron in the p_z orbital of the respective carbon atoms but this detail is not really important for the following discussion. The physics is simply that atoms tunnel from one carbon atom to the neighboring carbon atom with a rate t. Thus the Hamiltonian is simply given by

$$H = -t \sum_{\langle \vec{n}, \vec{n}' \rangle} c^\dagger_{A,\vec{n}} c_{B,\vec{n}'} + c^\dagger_{B,\vec{n}'} c_{A,\vec{n}} \tag{3.36}$$

where $\langle \vec{n}, \vec{n}' \rangle$ means that the sum only extends to nearest neighbors. This means that within our approximation (which can easily be improved), we only consider the tunneling from one atom to each three neighboring atoms. As an atom on the A sublattice is surrounded by three atoms on the B sublattice, we have always tunneling between A and B sides. The sign of the prefactor, $t > 0$, is not obvious but turns out to come out when one calculates the tunneling rate.

In the following, we will need the vectors pointing from an atom on the A side to its three nearest neighbors. They are simply given by the vector $\vec{\Delta}$ introduced above and by

rotating this vector by the angle $2\pi/3 = 120°$ and $4\pi/3 = 240°$,

$$\vec{n}_1 = \vec{\Delta} = a\left(0, \frac{1}{\sqrt{3}}\right), \quad \vec{n}_2 = R_{2\pi/3}\cdot\vec{n}_1 = a\left(-\frac{1}{2}, -\frac{1}{2\sqrt{3}}\right), \quad \vec{n}_3 = R_{4\pi/3}\cdot\vec{n}_1 = a\left(\frac{1}{2}, -\frac{1}{2\sqrt{3}}\right). \tag{3.37}$$

The next step in solving the problem is a simple Fourier transformation. We introduce creation operators in momentum space with

$$c^\dagger_{A,\vec{n}} = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{k}\vec{R}_{\vec{n}}} c^\dagger_{A,\vec{k}}, \qquad c^\dagger_{B,\vec{n}} = \frac{1}{\sqrt{N}}\sum_{\vec{k}} e^{-i\vec{k}(\vec{R}_{\vec{n}}+\vec{\Delta})} c^\dagger_{B,\vec{k}}. \tag{3.38}$$

We simply use this relation when evaluating H using that

$$\sum_{\langle\vec{n},\vec{n}'\rangle} e^{-i\vec{k}\vec{R}_{\vec{n}}} e^{i\vec{k}'\vec{R}_{\vec{n}'}} = \sum_{\vec{n},i=1,2,3} e^{-i\vec{k}\vec{R}_{\vec{n}}} e^{i\vec{k}'(\vec{R}_{\vec{n}}+\vec{n}_i)} = N\sum_{i=1,2,3}\delta_{\vec{k},\vec{k}'} e^{i\vec{k}\vec{n}_i}. \tag{3.39}$$

This allows to rewrite

$$H = \sum_{\vec{k}} \left(c^\dagger_{A\vec{k}}, c^\dagger_{B\vec{k}}\right) \begin{pmatrix} 0 & \alpha_{\vec{k}} \\ \alpha^*_{\vec{k}} & 0 \end{pmatrix} \begin{pmatrix} c_{A\vec{k}} \\ c_{B\vec{k}} \end{pmatrix} \tag{3.40}$$

with $\alpha_{\vec{k}} = -t\sum_{i=1,2,3} e^{i\vec{k}\vec{n}_i}$. I have skipped a 'detail' in the discussion above which concerns the question what is precisely meant by $\sum_{\vec{k}}$. The sum actually runs over the so-called 1st Brillouin zone, a concept discussed in the lecture on solid state physics but it is not directly relevant for the following discussion.

The eigenvalues of the 2×2 matrix are simply $\pm|\alpha_{\vec{k}}|$. There are two special points in momentum space, where the complex function $\alpha_{\vec{k}}$ vanishes, the so-called K-points with momentum $\vec{K}_0 = (\frac{4\pi}{3a}, 0)$ and $\vec{K}'_0 = -\vec{K}_0$. Let us Taylor expand the momenta around these points. We obtain

$$\begin{aligned} \alpha_{\vec{K}_0+\vec{q}} &= \tilde{c}(q_x - iq_y) + O(q^2) \\ \alpha_{\vec{K}'_0+\vec{q}} &= \tilde{c}(-q_x - iq_y) + O(q^2) \end{aligned} \tag{3.41}$$

where we will see that $\tilde{c} = ta\sqrt{2}/2$ will later take over the role of the speed of light in the Dirac equation.

To obtain our final result in a form which resembles the Dirac equation, we introduce the 4-component operator $\psi_{\vec{q}} = (c_{A,\vec{K}_0+\vec{q}}, c_{B,\vec{K}_0+\vec{q}}, c_{A,\vec{K}'_0+\vec{q}}, c_{B,\vec{K}'_0+\vec{q}})^T$ and the corresponding field in real-space $\psi(\vec{x}) = \frac{1}{\sqrt{N}}\sum_{\vec{q}} e^{-i\vec{q}\vec{x}}\psi_{\vec{q}}$. This field will describe our low-energy excitations using Eq. (3.41), therefore we implicitly assume that the momentum sum used in its

definition only spans small $\vec{q}$. Furthermore, we introduce two 4×4 matrices

$$\alpha_x = \begin{pmatrix} \sigma_x & \mathbf{0} \\ \mathbf{0} & -\sigma_x \end{pmatrix}, \qquad \alpha_y = \begin{pmatrix} \sigma_y & \mathbf{0} \\ \mathbf{0} & \sigma_y \end{pmatrix}. \tag{3.42}$$

Finally, we are able to rewrite the low-energy excitations of graphene in a from strongly resembling the massless Dirac equation

$$\begin{aligned} H &= \tilde{c} \sum_{\vec{q}} \psi^\dagger_{\vec{q}} (q_x \alpha_x + q_y \alpha_y) \, \psi_{\vec{q}} \\ &= \tilde{c} \int d^2\vec{x} \; \psi^\dagger(\vec{x}) (-i\hbar\partial_x \alpha_x - i\hbar\partial_y \alpha_y) \psi(\vec{x}). \end{aligned} \tag{3.43}$$

Thus, we have shown that the low-energy excitations in graphene are really described by a two-dimensional variant of the massless Dirac equation. In other materials, one can also realize the three-dimensional version.

There are many reasons why materials following the Dirac equation are interesting. First, one can use them to realize some of the effects which have been previously known for the Dirac equation in a solid state context. For example, in 1929 the physicist Oscar Klein studied potential scattering in the context of the Dirac equation and found that electrons could tunnel through a high barrier with essentially no reflection from the barrier. This effect is called Klein paradox (or Klein tunneling). This effect can easily be observed in graphene (and turns out to be a major problems as it complicates the creation of electronic devices from graphene). But more generally, the properties of materials like graphene turned out to have many interesting properties due to their intrinsically linear dispersion and vanishing density of state. For example, the react much stronger to magnetic fields, allowing to observe the quantum Hall effect at room temperatures.

3.10 Non-relativistic limits

We now come back to the 'real' Dirac equation where c is the speed of light. In most situations occuring on earth, electrons are much smaller than the speed of light, $v \ll c$, and therefore relativistic effects are small. To quantify this statement, we can use the discussion of Sec. 2.3.3 where we already observed that the fine structure constant $\alpha \approx \frac{1}{137}$ controls velocities and energies with

$$\frac{v}{c} \approx \alpha \qquad \text{binding energy} \sim m_0 v^2 \sim m_0 c^2 \alpha^2$$

We can therefore expect that all relativistic connection, typically of order $\mathcal{O}((\frac{v}{c})^2) \approx \mathcal{O}(10^{-4})$ are indeed small. Nevertheless, they play an important role. For example, they lift some degeneracies. This becomes of technological importance for magnetic memories: due to relativistic effects, there is no spin rotation invariance and one can build devices where the magnetization aligns along preferential directions. Quantitatively, relativistic

effects are large in all materials with heavy elements. The reason is that electrons are flying faster in such elements. We can make a naive estimate of this effect (assuming that only a single electron is present): the Coulomb potential of a nucleus with Z protons is obtained by replacing e^2 with Ze^2. Therefore one can view this as a replacement of α by $Z\alpha$ (e.g., $Z = 79$ in gold). Quantitatively, this naive estimate cannot be applied due to the influence of all the other electrons but one can in general expect sizable relativistic effects mainly in heavy elements.

The goal of this chapter is to derive relativistic corrections to the Schrödinger equation. It turns out, that it is possible to derive the leading terms without using the language of second quantization. As this approach is slightly more easy and as most books use this approach, we will also follow this historical route in this chapter. We start from the Dirac equation in the presence of a vector potential A^μ)

$$(-i\hbar \not{D} + m_0 c)\Psi = 0$$

and read it as a wave equation. Our goal is to obtain a systematic expansion in powers of $\alpha \ll 1$ in situations where one electron is present. We therefore focus on the solution with positive energies,

$$\Psi = e^{-iE\,t/\hbar}\,\Psi(\vec{r})\,,\ E > 0.$$

Positrons are assumed to be absent, or, more precisely, they will only occur as virtual quantum fluctuations during the calculation.

To order $\mathcal{O}(\alpha^0)$, we can neglect the motion of the particle completely, $v = 0$, and obtain $E = m_0 c^2$ and therefore

$$\left(-m_0 c^2 \cdot \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} + m_0 c^2\, \mathbb{1} \right) \Psi(\vec{r}) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} m_0 c^2\, \Psi(\vec{r}) = 0$$

The upper two components $\Psi_A = \begin{pmatrix} \Psi_{A\uparrow} \\ \Psi_{A\downarrow} \end{pmatrix}$ of the spinor $\Psi = \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix}$ play therefore a completely different role than the lower two comonents, $\Psi_B = \begin{pmatrix} \Psi_{B\uparrow} \\ \Psi_{B\downarrow} \end{pmatrix}$. To $\mathcal{O}(\alpha^0)$, Ψ_B (describing positrons) vanishes while Ψ_A can be arbitrarily large. In the non-relativistic limit, we can therefore view Ψ_A as **large** while Ψ_B is **small**.

We can rewrite the Dirac equation in terms of $\Psi_a\,,\ \Psi_b$ using the notation

$$\vec{\Pi} = \vec{p} - \frac{e}{c}\,\vec{A}.$$

As in our convention we have $\gamma^i = \begin{pmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{pmatrix}$ we obtain $\gamma^i \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix} = \begin{pmatrix} \sigma_i \Psi_B \\ -\sigma_i \Psi_A \end{pmatrix}$. One

therefore can rewrite the 4-component Dirac equation as two 2-component equations

$$\vec{\sigma}\,\vec{\Pi}\cdot\Psi_B = \frac{1}{c}(E - e\phi - m_0c^2)\Psi_A$$
$$\vec{\sigma}\,\vec{\Pi}\cdot\Psi_A = \frac{1}{c}(E - e\phi + m_0c^2)\Psi_B$$

The second equation is solved by

$$\Psi_B = c\,\frac{1}{E + m_0c^2 - e\phi}\,\vec{\sigma}\,\vec{\Pi}\Psi_A \tag{3.44}$$

We can plug this result into the first equation. Using the definition of a non-relativistic energy, $E_{NR} = E - m_0c^2$ we find

$$\vec{\sigma}\,\vec{\Pi}\cdot\frac{c^2}{2m_0c^2 + E_{NR} - e\phi}\,\vec{\sigma}\,\vec{\Pi}\cdot\Psi_A = (E_{NR} - e\phi)\Psi_A$$

This 2-component equation is exact and contains all the physics of the Dirac equation. It is, however, non-linear in the energy E_{NR}. We can easiliy find an approximation to this equation using a simple Taylor expansion based on $E_{NR} \ll m_0c^2$.
To obtain the leading contribution, we approximate $2m_0c^2 + E_{NR} - e\phi \simeq 2m_0c^2 + \mathcal{O}(\alpha^2)$ in the denominator of Eq. (3.45) and obtain directly the **Pauli equation**

$$\text{to } \mathcal{O}(\alpha^2): \quad E_{NR}\Psi_A = \left(\frac{(\vec{\sigma}\,\vec{\Pi})^2}{2m_0} + e\phi\right)\Psi_A$$

To rewrite the Pauli equation in terms of the equivalent Schrödinger equation we use $\sigma^i\sigma^j = \delta_{ij} + i\epsilon_{ijk}\sigma^k$ and

$$i\epsilon^{ijk}\Pi^i\Pi^j = i\epsilon^{ijk}\frac{1}{2}\left[\Pi^i,\,\Pi^j\right] \underbrace{=}_{\substack{[p^i,p^j]=0\\ [A^i,A^j]=0}} \frac{e}{c}\hbar\epsilon^{ijk}\left[\partial^i, A^j\right] = \frac{e\hbar}{c}(\vec{\nabla}\times\vec{A})_K$$

(as $[\partial_x,\, f(x)]g(x) = \partial_x(f(x) - f(x)\partial_x)g(x) = (\partial_x f)g$) and obtain therefore

$$E_{NR}\Psi_A = \left(\frac{(\vec{p} - \frac{e}{c}\vec{A})^2}{2m_0} + e\phi - g\mu_B\vec{S}\,\vec{B}\right)\Psi_A$$

with $\vec{S} = \hbar\frac{\vec{\sigma}}{2}$ and Bohr's magneton $\mu_B = \frac{e}{2m_e}$. Most importantly, we obtain the prefactor of the coupling of spin and magnetic field

$$g = 2$$

Before Dirac's equation, the so-called g-factor was only known experimentally. While the coupling of the angular momentum to the B-field is given by $-\mu_B \vec{L}\vec{B}$, the electron spin has the extra factor $g = 2$. This factor is exact within the pure Dirac theory, but if quantum fluctuations of the light are included, one obtains a small correction to this value, $g \approx 2 + \frac{\alpha}{\hbar} + \mathcal{O}(\alpha^2) = 2.0041$. Obtaining the correct value for the g factor was an important success of Dirac's theory.

To obtain the relativistic correction to the Dirac equation arising to $O(\alpha^4)$, we just have to expand our equations one order higher. Before doing so, we have, however, to consider the normalization of the wave function. Using the total charge to normalize our wave function for a single electron we demand

$$\int \Psi_A^\dagger \Psi_A + \Psi_B^\dagger \Psi_B = 1$$

where it turns out to be sufficient to determine Ψ_B from (3.44) expanded to leading order in α, $\Psi_B \approx \frac{\vec{\sigma}\vec{\Pi}}{2m_0 c}\Psi_A$.

$$\int \mathrm{d}^3x\, \Psi_A^\dagger \left(1 + \left(\frac{\vec{\sigma}\,\vec{\Pi}}{2m_0 c}\right)^2\right) \Psi_A \stackrel{!}{=} 1$$

For a Schrödinger equation (with relativistic corrections), we do, however, want to have the standard normalization $\int |\Psi|^2 \mathrm{d}^3x = 1$. Therefore we define

$$\Psi = \Omega \Psi_A$$
$$\Omega \approx \sqrt{1 + \left(\frac{\vec{\sigma}\,\vec{\Pi}}{2m_0 c}\right)^2} \approx 1 + \frac{(\vec{\sigma}\,\vec{\Pi})^2}{8m_0^2 c^2} + \mathcal{O}(\alpha^4), \qquad \Omega^{-1} \approx 1 - \frac{(\vec{\sigma}\,\vec{\Pi})^2}{8m_0^2 c^2} + \mathcal{O}(\alpha^4)$$

Furthermore, we approximate now to next-to-leading order $\frac{c^2}{2m_0c^2 + E_{NR} - e\phi} \simeq \frac{1}{2m_0} - \frac{E_{NR} - e\phi}{4m_0^2 c^4}$ and obtain after multiplication of Eq. (3.45) from the left side by Ω

$$\Omega(E_{NR} - e\phi)\Omega^{-1}\,\Psi = \Omega\,\vec{\sigma}\,\vec{\Pi}\,\left(\frac{1}{2m_0} - \frac{E_{NR} - e\phi}{4m_0^2 c^4}\right)\,\vec{\sigma}\,\vec{\Pi}\,\Omega^{-1}\,\Psi$$

With the above found approximation for Ω this is the desired equation. After collecting various terms (which takes a few more steps) one obtains

$$E_{NR}\,\Psi = H\Psi \quad \text{with} \quad H = H_0 + H_1 + H_2 + H_3 + \mathcal{O}(\alpha^6)$$

where

$$H_0 = H_{\text{pauli}} = \frac{\left(\vec{p} - \frac{e}{c}\vec{A}\right)^2}{2m_0} - 2\mu_B \vec{B}\vec{S} + e\phi$$

as before. In the following we give the formulas for the relativistic corrections only for

$\vec{A} = 0$ (results for finite magnetic fields can, e.g., be found in the book of Schwabl). One obtains

$$H_1 = -\frac{p^4}{8m_0^3c^2} \tag{3.45}$$

$$H_2 = -\frac{e\hbar\vec{\sigma}(\vec{E}\times\vec{p})}{4m^2c^2} \tag{3.46}$$

$$H_3 = \frac{e\hbar^2}{8m_0^2c^2}\nabla^2\phi(r) \tag{3.47}$$

The first term, H_1, has a simple interpretation as it just arises from the Taylor expansion of the relativistic energy momentum relations in powers of the momentum, $\sqrt{(m_0c^2)^2+(pc)^2} \approx m_0c^2 + \frac{p^2}{2m} - \frac{p^4}{8m_0^2c^2} + \ldots$. More interesting is the second term, H_2, the **spin-orbit coupling**. One way to understand at least qualitatively, where it is coming from is to perform a Lorentz transformation to a frame of reference comoving with the electron with a velocity p/m. In this frame of reference, an existing electric field in the original frame of reference will produce a magnetic field which couples directly to the spin. This argument does not reproduce the numerical prefactor but otherwise gives the correct dependence of $\vec{E}$, $\vec{\sigma}$, m_0 and $\vec{p}$. H_3 is called the Darwin term. For a $1/r$ Coulomb potential it gives a contribution at the origin and affects therefore only affects only s electrons with vanishing angular momentum.

The most important term is by far the spin orbit coupling, H_2 as it links the spin orientation, the motion of the electron and electric fields. It can be used to fix the orientation of the magentization in magnetic memory, allows for an electric control of the spin orientation (important for the field of *spintronics* which studies the use of the electron spin in future computers), it lifts degeneracies in the spectrum of atoms and is an important player in driven complex states of matter (e.g., topological insulators).

For a central potential, which depends only on r one can use $\vec{E} = -\vec{\nabla}\phi = -\frac{\vec{r}}{r}\frac{\partial\phi}{\partial r}$ and $\vec{L} = \vec{r}\times\vec{p}$ to rewrite the spin-orbit coupling as

$$H_2 = \frac{e}{2m_0^2c^2}\vec{S}\,\vec{L}\,\frac{1}{r}\frac{\partial\phi}{\partial r} \tag{3.48}$$

which immediately implies that the spin and the angular momentum of an atom are always coupled. More precisely, it implies that at least for a single electron spin and angular momentum are always parallel (this is part of the so-called Hundt's rule).

Let us investigate how relativistic corrections affect the hydrogen atom. We will not calculate numerical values but instead just show how such a calculation has to be performed and we will discuss the qualitative results. We first quote the well known result without relativistic correction, i.e., the result to order α^2. Here one uses that H, L^2, L_z and S_z are commuting conservation laws to introduce the quantum numbers n, l, m_z and s_z.

$S^2 = \frac{1}{2}(\frac{1}{2}+1) = \frac{3}{4}$ is also conserved but it takes for the single electron of the hydrogen atom always the same value. The eigenenergies of the bound states, $E_n = -\frac{E_0}{n^2}$, $n = 1, 2, ...$, with $E_0 = \frac{1}{2}\alpha^2 m_0 c^2$ depend only on n.[3].
As E_n is independent of the other quantum numbers, each state has the

$$\text{degeneracy to } \mathcal{O}(\alpha^2): \qquad 2\sum_{l=0}^{n-1}(2l+1) = 2n^2$$

which will be partially lifted by relativistic corrections.
To calculate the relativistic corrections to $\mathcal{O}(\alpha^4)$, we use perturbation theory (an exact solution is also possible for the hydrogen atom, but not for more complicated situations). We define the perturbation ΔH by

$$H = H_0 + \Delta H, \qquad \Delta H = H_1 + H_2 + H_3$$

In situations without degeneracy the shift of the energy of eigenstates is calculated from a formula derived in the undergraduate quantum mechanics course

$$E_\alpha = E_\alpha^0 + \langle\alpha|\,\Delta H\,|\alpha\rangle - \sum_{\alpha\neq\beta}\frac{|\,\langle\beta|\,\Delta H\,|\alpha\rangle\,|^2}{E_\beta^0 - E_\alpha^0} + \mathcal{O}(\Delta H^3) \tag{3.49}$$

As we are only interested in corrections linear in ΔH (which are of $\mathcal{O}(\alpha^4)$) it seems that the first correction is sufficient. This is, however, not correct in the presence of degeneracies as in this case the correction proportional to $(\Delta H)^2$ diverges in general as the denominator can vanish, $E_\beta^0 - E_\alpha^0 = 0$. The solution of this problem (found under 'degenerate perturbation theory' in undergraduate textbooks) is to choose a new basis $\{|\tilde{\alpha}_1\rangle, \ldots, |\tilde{\alpha}_N\rangle\}$ to describe the space spanned by all the eigenstates of H_0 with the fixed energy E_α^0, $\{|\alpha_1\rangle, \ldots, |\alpha_N\rangle\}$ with $H_0\,|\alpha_i\rangle = E_\alpha^0\,|\alpha_i\rangle$. In this basis all the problematic terms in Eq. (3.49) vanish. We have to choose $|\tilde{\alpha}_i\rangle = \sum_{j=1}^{N} c_{ij}\,|\alpha_j\rangle$ such that $\langle\tilde{\alpha}_i|\,\Delta H\,|\tilde{\alpha}_j\rangle = 0$ for $i \neq j$. Finding these states is exactly equivalent to the problem of finding eigenstates of the $N \times N$ matrix $\langle\alpha_i|\,\Delta H\,|\alpha_j\rangle$.
We therefore conclude that we have to diagonalize ΔH in the space of degenerate wave functions to obtain the leading correction linear in ΔH. Here it is very useful (especially for the interpretation of the result) to use the available symmetries to effectively reduce the dimension N of the matrix. In the case discussed below, one can actually construct the basis in which ΔH is diagonal just by a symmetry analysis (in general this is not possible). Due to the spin-orbit coupling terms, neither L_z nor S_z is conserved, $[L_z,\, H] \neq 0$, $[S_z,\, H] \neq 0$. We have, however, determined in Sec. 3.2 the generator of rotations J which has to

[3] Due to the finite mass m_p of the proton, the effective mass in the center-of-mass coordinate system is not the electron mass m_e but instead given by $m_0 = \left(\frac{1}{m_e} + \frac{1}{m_p}\right)^{-1}$

commute with H for any rotation invariant potential

$$\vec{J} = \vec{L} + \vec{S}, \qquad \left[\vec{J},\, H\right] = 0$$

The reader is encouraged to check that $\vec{J}$ indeed commutes with the spin-orbit coupling term (rewrite $\vec{S}\,\vec{L} = \frac{1}{2}\left(\left(\vec{S}+\vec{L}\right)^2 - \vec{S}^2 - \vec{L}^2\right)$).
As also $\left[L^2,\, H\right] = 0$ and $\left[J^2,\, H\right] = 0$ we obtain

commuting operators	H	L^2	$S^2 = \frac{3}{4}$	J^2	J_z
quantum number	n	l		j	m_j

with $L^2 = \hbar^2 l(l+1)$ and $J^2 = \hbar^2 j(j+1)$, $J_z = \hbar m_j$, $m_j = -j, -j+1, ..., j$. These quantum numbers are used when describing the quantum states of atoms. For example $2p_{1/2}$ describes a state with $n = 2$, $j = 1/2$ and the angular momentum $l = 1$ (s, p, d, f,... describes states with $l = 0, 1, 2, 3, ...$).
As an example, let us consider all states with $n = 3$. In the absence of relativistic corrections there are $2n^2 = 18$ degenerate states with $l = 0, 1, 2$ which we have to couple to the spin with $s_z = \pm\frac{1}{2}$. We will not discuss here the rules for the addition of angular momentum (covered in most QM textbooks) but instead just use the intuitive result that a state with angular momentum l and a spin 1/2 can either be combined to $j = l + 1/2$ or $j = l - 1/2$ with the exception of $l = 0$ which always gives a state with $j = 1/2$. We therefore obtain the following values of j and corresponding degeneracies

$l = 0$	$\Rightarrow$	$j = \frac{1}{2}$	$\Rightarrow$	degeneracy	2
$l = 1$	$\Rightarrow$	$j = 1 - \frac{1}{2} = \frac{1}{2}$	$\Rightarrow$	"	2
		$j = 1 + \frac{1}{2} = \frac{3}{2}$		"	4
$l = 2$	$\Rightarrow$	$j = 2 - \frac{1}{2} = \frac{3}{2}$	$\Rightarrow$	"	4
		$j = 2 + \frac{1}{2} = \frac{5}{2}$		"	6
					18

We recover the total number of 18 states, but have now relabeled them. To construct the corresponding eigenfunctions, $|n, l, j, m_j\rangle$ as linear combinations of the states $|n, l, m_z, s_z\rangle$, one needs the rules for the addition of angular momentum (not discussed here), for example, $\left|n, l, j = l + \frac{1}{2}, m_j = l + \frac{1}{2}\right\rangle = \left|n, l, m_z = l, s_z = \frac{1}{2}\right\rangle$.
The main advantage of the construction discussed above is that in the new basis ΔH is already diagonal, i.e., $\left\langle n', l', j', m_j'\right| \Delta H \left|n, l, j, m_j\right\rangle = 0$ if only one of the quantum number differs. Furthermore, the matrix elements have to be independent of m_j due to the rotational invariance of ΔH. Therefore one can therefore use, e.g., $m_j = j$, and calculate

$$E(n, l, j) = -\frac{E_0}{\hbar^2} + \langle n, l, j, m_j = j|\, \Delta H \,|n, l, j, m_j = j\rangle + \mathcal{O}(\alpha^5)$$

We have therefore reduced the problem to the computation of a simple matrix element. The calculation can be reduced to simple integrations over the radial direction when one

uses that for fixed j and l one has

$$\vec{S}\,\vec{L} = \frac{1}{2}\left(\left(\vec{S}+\vec{L}\right)^2 - \vec{S}^2 - \vec{L}^2\right) = \frac{1}{2}\left(j\left(j+1\right)\right) - l\left(l+1\right) - \frac{3}{4}$$

For the computation of H_3 one finds for the Coulomb potential $H_3 = \frac{e}{8m^2}\nabla^2\phi = \frac{e}{8m^2}4\pi\delta^3(r)$ which implies that this term only contribution for $l = 0$, as $\Psi(0) = 0$ for $l > 0$.
Further effects which we have not discussed is the hyperfine coupling of the electronic and the nuclear spin, an effect of $\mathcal{O}\left(\frac{m_e}{m_p}\alpha^4\right)$. Furthermore, quantum fluctuations arising from photons contribute to order $\mathcal{O}(\alpha^5\,\ln(\frac{1}{\alpha}))$ (the so-called Lamb-shift).
The most important result of this section was the formula for spin-orbit coupling. In most systems, this is the most important relativistic effect which, for example, strongly determined the properties of magnets. Due to this term, the magnetization of any crystal has preferred directions determined by the interplay of crystalline structure and spin-orbit coupling. In a cubic crystal, for example, the presence of neighboring atoms implies that a state with angular momentum directed towards the next atom or oriented in some other direction will have a different energy. By spin-orbit coupling, this information is transfered to the spin direction.

3.11 Outlook: QED, renormalization and regularization

When the Dirac equation in its second quantized form is combined with the quantized theory of electromagnetic waves one obtain **quantum electrodynamics** (QED) .
This is a very powerful theory, experimentally tested with very high precision. One can easily extend it to include the atomic nuclei. In this form it describes almost all phenomena in the world around us with only very few input parameters (the electron mass, the fine-structure constant and the masses of nuclei) including, for example, all of chemistry, all known biological processes and all of our technology with a few exceptions (like nuclear power plants) mentioned below. More precisely, a simple classical gravitation potential has to be added for many of these phenomena to QED which is easily possible. QED does not describe phenomena related to weak- and strong forces which are needed to understand radioactivity, nuclear fusion (i.e, why the sun shines), the structure of nuclei and their magnetic moments. Note that the statement that QED describes in principle a phenomenon does not imply that this helps to understand the phenomenon (e.g., how our brain works) or that one is able to solve the relevant equations. In contrast, one can obtain numerically exact answers from QED only for problems involving very few particles (e.g., one or two electrons).
The most precise experimental tests of QED come from electron-positron scattering experiments, from atomic physics and from experiments on trapped electrons (e.g., the measurement of the magnetic moment of the electron). For example, the g factor of the electron is known with a precision better than 10^{-12}. Perturbative calculations in α (for, e.g., a

single electron) can be performed with similar precision up to order α^4.
The techniques needed to perform perturbative calculations within QED and other field theories are usually covered in courses on quantum field theory. Here we want to discuss briefly an important aspect: naive perturbation theory produces notoriously not finite answers but instead one finds corrections of the form $\alpha^2 \times \infty$. When QED was developed it therefore seemed to be a useless and wrong theory for some time.
Let us illustrate this problem with an example from classical physics. We calculate the energy of a point charge. More precisely, we consider a particle with charge e and radius R and we consider the energy stored in the electric field.

$$\int E^2 \mathrm{d}^3 r = \int_R^\infty \left(\frac{e}{r^2}\right)^2 \mathrm{d}^3 r = 4\pi \int_R^\infty \frac{e^2}{r^2} \mathrm{d}r = \frac{4\pi e^2}{R} = 4\pi\alpha \frac{\hbar c}{R} \to \infty \text{ for } \; R \to 0$$

Classical physics therefore predicts an infinite energy for a single electron. It turns out that this divergence is not a problem in QED. Here quantum fluctuations induce an effective radius of the electron given by $R_{\text{eff}} = \frac{\hbar}{mc}$ and the strong divergence with $1/R$ is gone. It turns out, that it is, however, replaced by a weaker, logarithmic divergence. A field theoretical calculation of the energy (or, equivalently, the mass) of an electron at rest arising from its electric field and the absoprtion and emission of virtual photons at rest gives

$$m \approx m_0 \Big(1 + \frac{3\alpha_0}{4\pi} \underbrace{\ln\Big(\frac{\Lambda^2}{m_0^2 c^4}\Big)}_{\infty \text{ for } \Lambda = \infty}\Big) \tag{3.50}$$

where m_0 and α_0 are the mass and fine-structure constants entering the theory and we had to introduce a new parameter, Λ, usually called **cutoff**, which is the maximal possible energy (of, e.g., virtual photons). Λ plays the same role as the inverse radius $1/R$ in the classical example given above. For $\Lambda \to \infty$ the perturbative correction diverges. How can this result be interpreted?
The solution to this problem consist of two steps. In the first step, called **regularization** one has to perform a calculation for *finite* but large Λ carefully keeping track of all diverging contributions. From this calculation, one obtains a formula for some physical observable,

$$A_i = A_i(\alpha_0, m_0, \Lambda) \tag{3.51}$$

which depends not only on the 'bare' coupling constant α_0 and the 'bare' mass m_0 but also the cutoff Λ (the 'bare' parameters are the parameters entering our field theory for a given value of Λ).
The main element of the second state, **renormalization**, is to realize that m_0 and α_0 are *not* the measured mass and fine structure constant. Those have to be computed from an

extra calculation. Like for any other observable, one finds

$$m = m(\alpha_0, m_0, \Lambda), \qquad \alpha = m(\alpha_0, m_0, \Lambda) \tag{3.52}$$

While α_0, m_0 and Λ are unknown, the measured mass m and the measured strength of the Coulomb potential α are known from experiments. For a given Λ, one can solve Eq. (3.52) for α_0 and m_0 to obtain

$$m_0 = m_0(m, \alpha, \Lambda), \qquad \alpha_0 = \alpha_0(m, \alpha, \Lambda)$$

These equations can now be used in Eq. (3.51) to calculate

$$A_i = A_i(\, \alpha_0(\alpha,\, m,\, \Lambda),\, m_0(\alpha, , m,\, \Lambda),\, \Lambda) \equiv A_i(\alpha,\, m,\, \Lambda) \tag{3.53}$$

For QED one finds surprisingly that A_i expressed in this way in terms of the measured values of m and α is finite and *independet* of Λ for large Λ. Predictions for experiments can therefore be obtained from

$$A_i = \lim_{\Lambda \to \infty} A_i(\alpha, m, \Lambda) \tag{3.54}$$

Theories, which have this remarkable property that all dependence on the cutoff Λ vanish after the coupling constants are fixed with a few experiments, are called **renormalizable**. It turns out, that (in contrast to many other possible theories) Gauge theories are renormalizable. In 1999 t'Hooft and Veltman received the Nobel prize for showing that the theory of electroweak interaction (which includes QED and the Higgs mechanism) is renormalizable.

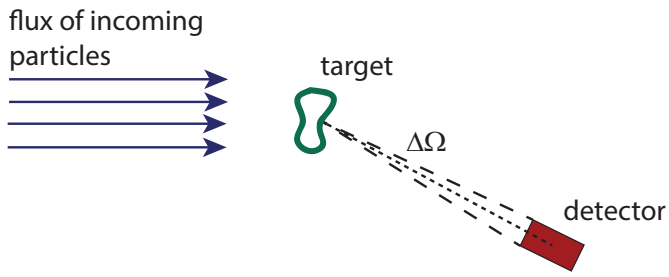
4 Scattering Theory

Scattering experiments play a decisive role in physics. Often the only way to find out what is inside a material, an atom or the atomic nucleus is to do a scattering experiment by shooting something at the object of interest. In 1911, for example, Ernest Rutherford scattered α particles from a gold foil. His amazing conclusion was that practically all of the scattering came from a tiny nucleus smaller than $10^{-14}\,m$, less than 0.01% of the the size of an atom. A more modern example are the scattering experiments at the Large Hadron Collider (LHC) at the CERN in Geneva, where protons and antiprotons are accelerated in a with a diameter of 26 km with velocities of $99.999999\%\,c$. But also phenomena in everyday life, for example the blue sky during the day and the red sunset are a consequence of an energy-dependent scattering rate of photons. Other example for scattering experiments are the use of seismic waves to investigate the properties of the core of the earth or the use of neutron scattering to investigate the properties of materials.
In this chapter we will develop methods to calculate the scattering properties of quantum particles. We thereby focus for simplicity on the scattering of electrons in the non-relativistic limit.

4.1 Scattering cross-section

A central quantity which we will use to describe the scattering from an obstacle is the **differential cross section**. Here one considers an experiment characterized by a constant flux of incoming particles (e.g., electrons). The incoming flux, I, is described by the number of incoming particles (often of a fixed energy) per area and time,

$$I = \frac{\#\text{particles}}{\text{time} \times \text{area}}$$



The scattered particles are detected with a detector located far away from the scattering target. We describe the direction in which the detector is located either by two angles θ and ϕ or by the unit vector $\hat{\Omega}$. The detector is assumed to count all particles arriving within a small opening angle $\Delta\Omega$.

ΔN is the number of detected particles during the time interval Δt. The **differential cross section** is then defined as

$$\frac{\mathrm{d}\sigma(\Theta,\varphi)}{\mathrm{d}\Omega} = \frac{\text{number of counts}}{\text{time-intervall} \times \text{incoming flux} \times \text{solid angle of detector}} = \frac{\Delta N}{\Delta t \cdot I \cdot \Delta\Omega}$$

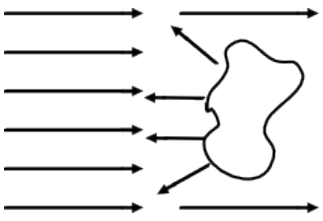
$$\text{units:} \quad \left[\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\right] = \frac{\# \times \text{time} \times \text{area}}{\# \times \text{time} \times \text{solid angle}} = \frac{\text{area}}{\text{solid angle}} \tag{4.1}$$

In general, the differential cross section will only depend on the orientation of the detector (parametrized by θ and ϕ), the direction of the incoming flux and the energy (and type) of the incoming particles. It is independent of the incoming flux (as long it is small enough to avoid non-linear effects) and of the size of the detector (as long as the angular resolution is sufficient).

The **total scattering cross section:** can be obtained by integrating the differential cross section over all directions

$$\sigma = \frac{\text{everything scattered}}{\text{time} \times \text{incoming flux}} = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\,\mathrm{d}\Omega = \int \frac{\mathrm{d}\sigma(\theta,\,\varphi)}{\mathrm{d}\Omega}\sin(\theta)\,d\theta d\varphi$$

The total cross section has the units of an area.



For the interpretation of σ, consider a flux of classical particles scattering from an obstacle. All particles hitting the obstacle are scattered. Therefore the number of scattered particles per time is given by the effective area of obstacle perpendicular to the beam of incoming particles times the incoming flux.

We therefore find that the total cross section is in this case exactly given by this area.

$$\sigma = \text{effective area of obstacle} \perp \text{to beam}$$

For a hard sphere of radius R, for example, one obtains $\sigma = \pi R^2$ in the classical limit.For scattering experiments in high-energy physics, the cross section is often measured with the unit $1\,\text{barn} = 1\,b = 100\,(\text{fm})^2 = 10^{-28}\,m^2$. The word barn refers allegedly to the saying 'as big as a barn' (in German: *so groß wie ein Scheunentor*), describing a cross section which is rather easy to detect in a typical high-energy experiment.

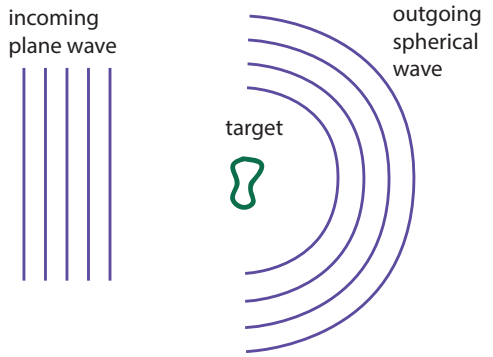
4.2 Scattering states

We will now study the quantum mechanical problem of scattering from a given potential $V(\vec{r})$ in the non-relativistic limit. We therefore search for solution of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right)\psi = E\,\psi$$

with a boundary condition which describes an **incoming plane wave**, $\Psi_{\text{in}} = e^{ik_0 z}$. Far away from the detector, we assume that the potential vanishes, $V(\vec{r} \to \infty) = 0$. In this region, the Schrödinger equation simplifies to $\left(-\frac{\hbar^2}{2m}\nabla^2 - E\right)\psi = 0$, or, after Fourier transformation $\left(\nabla^2 + k^2\right)\psi = 0$ as $E = \frac{\hbar^2 k^2}{2m}$. Far away from the scattering target, one therefore has a linear superposition of plane waves with momenta which all have the same modulus, $|\vec{k}| = k_0$.

How does the **outgoing, scattered wave** can be described far away from the scattering center?



While the incoming plane wave has the property that the current per area is a constant (more precisely, the probability current), the outgoing spherical wave comes from a point-like scattering center and far away from the scattering center it therefore has to have the property that at fixed distance r the current through a solid angle, $\int j r^2 d\Omega$, has to be independent of r. Therefore the current has to decay with $j \sim 1/r^2$ and the wave function with $1/r$.

This is precisely the property of a spherical wave (as we will check below)

$$\psi_{\text{out}} \sim \frac{1}{|\vec{r}|} e^{ik_0|\vec{r}|}$$

Such a wave can be considered as a superposition of plane waves $e^{i\vec{k}\vec{r}} = e^{ikr\cos\theta}$ with fixed $k = |\vec{k}|$ but averaged over angles.

We use these results to guess the general solution of the scattering problem for $r \to \infty$

$$\psi(|r| \to \infty) = c\left(\underbrace{e^{ik_0 z}}_{\substack{\text{incoming}\\ \text{plane wave}}} + \underbrace{f(\vartheta,\,\varphi)\frac{e^{ik_0 r}}{r}}_{\substack{\text{outgoing}\\ \text{spherical wave}}}\right) \tag{4.2}$$

To interpret this important result and check our arguments, we have to calculate the corresponding (probability-) current density

$$\vec{j} = \frac{1}{2m}\left(\psi^*(-i\hbar\vec{\nabla})\psi + \text{h.c.}\right)$$

For the incoming flux, we obtain a current into the z direction, $\vec{j}_{\text{in}} = \hat{z}\frac{\hbar k_0}{m}|c|^2$. For the calculation of the outgoing flux, we recall that $\frac{\partial}{\partial\vec{r}}h(r) = \frac{\partial r}{\partial\vec{r}}h'(r) = \hat{r}h'(r)$ as $\left(\frac{\partial}{\partial\vec{r}}\sqrt{x^2+y^2+z^2}\right) = \hat{r}$. Therefore, $\frac{\partial}{\partial\vec{r}}\frac{e^{ik_0r}}{r} = \hat{r}ik_0\frac{e^{ik_0r}}{r} + \mathcal{O}(\frac{1}{r^2})$ and the outgoing current is given by

$$\vec{j}_{\text{out}} = \frac{\hbar k_0}{m}|c|^2|f(\vartheta,\,\varphi)|^2\frac{1}{r^2} + \mathcal{O}(\frac{1}{r^3}) = |\vec{j}_{\text{in}}|\frac{|f(\vartheta,\,\varphi)|^2}{r^2}$$

Now consider a particle detector with the opening angle $\Delta\Omega$. The area where it detects a current is given by $A_d = r^2\Delta\Omega$. Therefore the total probability current into the detector (the incoming flux) is given by $I_{\text{detector}} = |j_{\text{in}}|\,|f|^2\,\Delta\Omega$ and we find for the differential cross section the important result

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\text{total flux into detector}}{\text{incoming flux / area} \times \Delta\Omega} = |f(\vartheta,\,\varphi)|^2 \tag{4.3}$$

To calculate the scattering cross section determined, we therefore only need to determine the **scattering amplitudes** $f(\vartheta,\,\varphi)$ obtained from the behavior of the scattering states for $r \to \infty$. The modulus squared of the scattering amplitudes determines the probability that particles are scattered into the direction given by ϑ and ϕ.
A remark on the interpretation of the wave function: Above, we discussed a single-particle Schrödinger equation and calculated probability currents. We did, however, not specify the normalization constant c. For scattering states, a normalization with total probability 1, $\int|\Psi|^2 = 1$, is problematic, as one cannot easily define a finite system with has boundary conditions consistent with the scattering state. We have therefore not specified c (it drops out from the final result). For a more rigorous treatment, one could, for example, build a wave packet out of the scattering solutions and normalize the wave function of this wave packet. For practical purposed, one can also choose c in such a way, that the incoming current j_{in} has nominally the units number of particles per area and time and adjust it to the experimental flux of particles. Here one should, however, not forget that we are only considering a single-particle wave function.

4.3 Scattering from central potential: phase shift

For a rotationally invariant central potential, $V(\vec{r}) = V(r)$, the determination of the differential cross section simplifies significantly as one can use angular momentum conservation. We search for simultaneous eigenfunctions of H, L^2, L_z with $E = \frac{(\hbar k)^2}{2m}$. They have the general form

$$\psi_{l,m,k}(r,\,\vartheta,\,\varphi) = \underbrace{Y_l^m}_{\substack{\text{spherical}\\ \text{harmonics}}}(\vartheta,\,\varphi)\frac{u_{kl}(r)}{r}$$

where we assume that the reader is already familiar with the spherical harmonics Y_l^m which are functions of the angles only, which have the property

$$L^2 Y_l^m = l(l+1)\hbar^2 Y_l^m \qquad , \; L_z Y_l^m = \hbar m Y_l^m \qquad m = -l, \ldots, l$$

Plugging this ansatz into the Schrödinger equation, one obtains the **radial Schrödinger equation** for $u_{kl}(r)$

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial r^2} + \frac{l(l+1)\hbar^2}{2mr^2} + V(r)\right) u_{kl}(r) = \frac{(\hbar k)^2}{2m}\, u_{kl}(r) \tag{4.4}$$
$$\text{with } u_{kl}(r=0) = 0$$

This equation has to be supplemented by a normalization condition. From $\int |\psi|^2 \, \mathrm{d}^3 r = 1$ follows the condition $\underbrace{\int |Y_l^m|^2 \, \mathrm{d}\Omega}_{=1} \int_0^\infty \mathrm{d}r \, r^2 \frac{|u|^2}{r^2} \stackrel{!}{=} 1$ and therefore $\int_0^\infty |u_{k\,l}|^2 = 1$.
Our main goal is to analyze the solution for $r \to \infty$ where $V(r) = 0$ and therefore $\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2\right) u_{k,l}(r) = 0$. Therefore for $r \to \infty$ we obtain necessarily

$$u_{k,l}(r) = A\, e^{ikr} + B\, e^{-ikr}$$

As this is a stationary state, current conservation implies that $|A|^2 = |B|^2$. Therefore we can write

$$\begin{aligned} u_{k,l}(r \to \infty) &= |A| \left(e^{ikr}\, e^{i\,\varphi_A} - e^{-ikr}\, e^{i\,\varphi_B}\right) \\ &= c \left(e^{-ikr}\, e^{i\,l\frac{\pi}{2}} - e^{ikr}\, e^{-i\,l\frac{\pi}{2}}\, e^{2\,i\,\delta_l}\right) \\ &= c' \sin\!\left(kr - \frac{l\pi}{2} + \delta_l\right) \end{aligned} \tag{4.5}$$

This equation defines the

scattering phase shifts $\delta_l(k)$

which are, in general, functions of the momentum k. The extra factors $e^{\pm i\frac{\pi}{2}\,l}$ have been chosen such that: $\delta_l = 0$ for $V(r) = 0$ as we will show below. The scattering phase shifts encode **all** information on $V(r)$ needed to describe any scattering experiment!
We can plug our result into the equation for the wave function

$$\psi_{l,m,k}(|\vec{r}| \to \infty) = -Y_l^m(\vartheta, \varphi)\Big(\underbrace{\frac{e^{-ikr}\, e^{i\,l\,\frac{\pi}{2}}}{2ikr}}_{\substack{\text{incoming} \\ \text{spherical wave}}} - \underbrace{\frac{e^{ikr}\, e^{-i\,l\,\frac{\pi}{2}}\, e^{2\,i\,\delta_l(k)}}{2ikr}}_{\substack{\text{outgoing spherical wave} \\ \text{with extra phase shift } \delta_l(k)}} \Big) \tag{4.6}$$

We will now check the limit $V = 0$.

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)\hbar^2}{2r^2 m}\right) u_{k,\,l}(r) = \frac{\hbar k^2}{2m}\, u_{k,\,l}(r)$$

$$\Leftrightarrow \quad \left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2 - \frac{l(l+1)}{r^2}\right) u_{k,\,l}(r) = 0 \quad \underset{x=k\cdot r}{\overset{\cdot\frac{1}{k^2}}{\Leftrightarrow}} \quad \left(\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 1 - \frac{l(l+1)}{x^2}\right) u_l(x) \quad = 0$$

with $u_{k,\,l}(r) = u_l(\underbrace{k\cdot r}_{x})$. This equation is solved by

$$u_{k,\,l}(r) \propto 2kr\,(\alpha\, j_l(k\,r) + \beta\, y_l(k\,r)) \tag{4.7}$$

with the spherical Bessel functions

$$j_l(x) = (-x)^l \left(\frac{1}{x}\frac{\partial}{\partial x}\right)^l \frac{\sin(x)}{x} \quad \text{first kind}$$

$$y_l(x) = -(-x)^l \left(\frac{1}{x}\frac{\partial}{\partial x}\right)^l \frac{\cos(x)}{x} \quad \text{second kind}$$

In the following, we will mainly need the asymptotic behavior of these functions which is easily obtained from their definition

$$\begin{aligned} j_l(x \to\ \infty) &= \frac{1}{x}\sin\left(x - \frac{l\,\pi}{2}\right), \qquad j_l(x \to 0) = \frac{x^l}{(2l+1)!!} \\ y_l(x \to\ \infty) &= -\frac{1}{x}\cos\left(x - \frac{l\,\pi}{2}\right), \qquad y_l(x \to 0) = -\frac{(2j-1)!!}{x^{l+1}} \end{aligned} \tag{4.8}$$

where $(2l+1)!! = (2l+1)\cdot(2l-1)\cdot(2l-3)\ldots$. As $u_{k\,l}(r=0) = 0$, we can immediately conclude that without a scattering potential, $V(r) = 0$, $u_{k\,l}(r) = 2kr\, j_l(k\cdot r)$ and therefore

$$u_{k\,l}(r \to\ \infty) = c\cdot\sin\left(kr - \frac{l\,\pi}{2}\right) = c'\left(e^{-ikr}\, e^{il\frac{\pi}{2}} \ -\ e^{ikr}\, e^{-il\frac{\pi}{2}}\right)$$

If we compare this to Eq. (4.5) we conclude that indeed $\delta_l = 0$ for $V = 0$.

4.4 Phase shifts & cross section

We have found two ways to express the wave functions of a scattering problem for $r \to \infty$, first the formula $e^{ik_0 z} + f(\vartheta,\,\varphi)\,\frac{e^{ikr}}{r}$ and second the formula (4.6) for $\psi_{l,m,k}(\vec{r})$ expressed in terms of phase shifts δ_l. If we can relate the two formulas, we will be able to express $f(\vartheta,\,\varphi)$ and therefore the differential cross section by phase shifts only.
To reach this goal, we have to express $e^{ik_0 z}$ in incoming spherical waves. Here we can use that $e^{ik_0 z}$ is a solution of the Schrödinger equation for $V = 0$. Therefore it can be written in the form

$$e^{ikz} = e^{ik\cos(\vartheta)} = \sum Y_l^m(\vartheta,\,\varphi)\, j_l(k\,r)\, a_{l\,m}$$

Our goal is to determine the (up to now) unkown parameters $a_{l\,m}$. As $e^{ik\cos(\vartheta)}$ depens only on ϑ but not on ϕ, only $m = 0$ contributes to the sum. We recall (from some other course which gave a more thorough introduction to spherical harmonics) that $Y_l^0(\vartheta,\,\varphi) = \sqrt{\frac{2l+1}{4\pi}}\,P_l(\cos(\vartheta))$, where P_l is a Legendre Polynomial defined by $P_l(x) = \frac{1}{2^l\,l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^2-1)^l$. Therefore we can write

$$e^{ikr\cos(\vartheta)} = \sum \alpha_l\, j_l(k\,r) P_l(\cos(\vartheta)) \tag{4.9}$$

The prefactors α_l can, e.g., be determined from a Taylor expansion

$$e^{ikr\cos(\vartheta)} = \sum_n \frac{(ikr\cos(\vartheta))^n}{n!} \tag{4.10}$$

If we use from Eq. (4.8) that $j_l(x) = \frac{x^l}{(2l+1)!!} + \mathcal{O}(x^{l-1})$ and that

$$P_l(x) = \frac{1}{2^l\,l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^{2l}+\ldots) = \frac{(2l)!}{l!\,l!\,2^l}\,x^l + \mathcal{O}(x^{l-1})$$

we find for the product of the two functions

$$j_l(k\,r)P_l(\cos(\vartheta)) = \frac{2l!}{(2l+1)!!\,2^l(l!)^2}\,(k\,r)^l(\cos(\vartheta))^l + \underbrace{\mathcal{O}((kr)^m\,(\cos(\vartheta))^n)}_{\text{with: } m\neq n}$$

Now we can compare the coefficients of the two expansions (4.9) and (4.10) by setting $n = l$ and find

$$\frac{i^n}{n!} = \alpha_n\,\frac{(2n)!}{(2n+1)!!\,(n!)^2} \quad \Rightarrow\; \alpha_n = \frac{i^n\,(2n+1)!!\,2^n n!}{(2n)!} == i^n\,(2n+1)$$

where we have used for the last equation $(2n+1)!!\,2^n\,n! = (2n+1)\cdot(2n-1)\cdot(2n-3)\cdot\ldots\cdot 2n(2(n-1))\cdot(2(n-2)) = (2n+1)!$. We therefore obtain

$$e^{ikr\cos(\vartheta)} = \sum_l i^l(2l+1)\,j_l(kr)P_l(\cos(\vartheta)) \tag{4.11}$$

We want to use this equation to rewrite

$$\psi(r\;\to\;\infty) = e^{ikr\cos(\vartheta))} + f(\vartheta)\,\frac{e^{ikr}}{r}$$

by using Eq. (4.11) and from Eq. (4.8) that $j_z(x\;\to\;\infty) = \frac{1}{x}\frac{1}{2i}\left(e^{i(kr-l\frac{\pi}{2})} - e^{-i(kr-l\frac{\pi}{2})}\right)$. Therefore,

$$\psi(r\;\to\;\infty) = \sum_l (-1)\,\underbrace{\frac{i^l(2l+1)}{2i}\left(\frac{e^{-ikr}\,e^{il\frac{\pi}{2}}}{kr}\right.}_{\text{incoming}} - \underbrace{\left.\frac{e^{ikr}\,e^{-il\frac{\pi}{2}}}{kr}\right)P_l(\cos(\vartheta)) + f(\vartheta)\frac{e^{ikr}}{r}}_{\text{outgoing}}$$

We use now that $\psi(r \to \infty)$ can be written as a linear combination of $\psi_{l,m,k}$ obtained from Eq. (4.6)

$$\psi(r \to \infty) = \sum_l \beta_l \, P_l(\cos(\vartheta)) \left(\underbrace{\frac{e^{-ikr} \, e^{il\frac{\pi}{2}}}{kr}}_{\text{incoming}} - \underbrace{\frac{e^{ikr} \, e^{-il\frac{\pi}{2}}}{kr} \left(1 + e^{2i\delta_l} - 1\right)}_{\text{outgoing}} \right)$$

Comparing the two equations, we find $\beta_l = (-1)^{\frac{i^l(2l+1)}{2i}}$ and

$$f(\vartheta) = \sum_l \left(\beta_l (e^{2i\delta_l} - 1) \, e^{-il\frac{\pi}{2}} \, P_l(\cos(\vartheta))(-1)\frac{1}{k} \right)$$

Using furthermore $e^{2i\delta_l} - 1 = e^{i\delta_l} \, \sin(\delta_l) \, 2i$ and $e^{-il\frac{\pi}{2}} = (-1)^l$ we obtain our final result

$$f(\vartheta) = \frac{1}{k} \sum_l (2l+1) \, e^{i\delta_l(k)} \sin(\delta_l(k)) \, P_l(\cos(\vartheta)) \tag{4.12}$$

valid for scattering from a rotationally invariant potential.
For the differential cross section we obtain immediately

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = |f(\vartheta, \, \varphi)|^2 = \frac{1}{k^2} \left| \sum_{l=0}^{\infty} (2l+1) \, e^{i\delta_l} \, \sin(\delta_l) \, P_l(\cos(\vartheta) \right|^2$$

To compute the total cross section $\sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \, \mathrm{d}\Omega$ we use that

$$\int P_l(\cos(\vartheta)) \, P_{l'}(\cos(\vartheta)) \, \mathrm{d}\Omega = \int (Y_l^0(\vartheta))^* \sqrt{\frac{4\pi}{(2l+1)}} \, Y_{l'}^0(\vartheta) \sqrt{\frac{4\pi}{(2l'+1)}} \, \mathrm{d}\Omega = \delta_{ll'} \frac{4\pi}{2l+1}$$

and finally obtain the simple formula

$$\sigma(k) = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l(k) \tag{4.13}$$

Note that the total cross section has the unit of an area (set by the wavelength of the incoming particles). We will discuss examples for the formula in the next chapter.

4.5 Scattering length, resonant scattering

In this section we will mainly discuss some examples for scattering and use this to introduce the concept of the scattering length and of resonant scattering.
First, we consider the quantum-mechanical scattering from a **hard sphere** of radius R. We therefore have to solve the radial Schrödinger equation

$$\left(-\frac{h^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l(l+1)}{2mr^2}\right)u_{kl}(r)=\frac{(\hbar k)^2}{2m}u_{kl}(r)$$

for $r>R$ with the boundary conditions $u_{kl}(R)=0$.
We already know that the solution of this equation are given by spherical Bessel functions, see Eq. (4.7), and therefore we just have to impose the boundary condition.

$$u_{kl}=2kr(\underbrace{\alpha j_l(kr)+\beta y_l(kr)}_{\text{spherical Bessel function}}) \quad \text{with: } u_{kl}(R)=0$$
$$\Rightarrow \quad u_{kl}(r)=2kr\left(j_l(kr)-\frac{j_l(kR)}{y_l(kR)}\,y_l(kr)\right)$$

To read off the phase shift, we have to analyze this result for $r\to\infty$. With $x=kr$, we use Eq. (4.8)

$$j_l(x\to\infty)=\frac{\sin(x-l\frac{\pi}{2})}{x}\,,\qquad y_l(x\to\infty)=-\frac{\cos(x-l\frac{\pi}{2})}{x}$$

Our goal is to write the result in the form given by (4.5)

$$\begin{aligned}u(x\to\infty)\propto\sin(x-l\frac{\pi}{2}+\delta_l)&=\sin(x-l\frac{\pi}{2})\cdot\cos\delta_l+\cos\left(x-l\frac{\pi}{2}\right)\sin\delta_l\\&=\cos\delta_l\left(\sin\Big(x-l\frac{\pi}{2}\Big)+\tan\delta_l\,\cos\Big(x-l\frac{\pi}{2}\Big)\right)\end{aligned}$$

Comparing the equations, we find

$$\tan\delta_l=\frac{j_l(kR)}{y_l(kR)} \tag{4.14}$$

which is the exact result for a hard sphere.
It is instructive to study the limit where the radius of the sphere is much smaller than the wavelength, $x=kR\ll 1$, using (4.8)

$$\frac{j_l(x)}{y_l(x)}=\frac{x^l}{(2l+1)!!}\left(-\frac{(2l+1)!!}{x^{l+1}}\right)^{-1}\quad\text{for } x\to 0$$

Therefore we obtain

$$\delta_l \approx -\frac{(kR)^{2l+1}}{(2l+1)!!\,(2l-1)!!} \propto k^{2l+1} \qquad \text{for } k \to 0 \tag{4.15}$$
$$\delta_0 \approx -kR \qquad \text{for } k \to 0$$

In this limit, scattering is dominated by **s-wave scattering**, $l = 0$, and we obtain from Eq. (4.13)

$$\sigma(k \to 0) \approx \frac{4\pi}{k^2} \sin^2 \delta_0 = 4\pi R^2$$

which is 4 times larger than classical value πR^2.
Motivated by the result for the hard sphere, we define the **scattering length**

$$a = -\lim_{k \to 0} \frac{\delta_{l=0}(k)}{k} \tag{4.16}$$

By construction, the scattering length of a hard sphere is given by its radius, $a = R$. While a is positive for repulsive potentials, it can also take negative values for attractive potentials. Below, we will see that for resonant scattering it can diverge.
Above, we have analyzed the limit that the radius of the hard sphere is small compared to the wavelength. It is also instructive to study the opposite limit, $kR \gg 1$. For short wave length, we expect to recover the classical result. Using again (4.14) and (4.8) we obtain

$$\tan \delta_l = -\frac{\sin\left(kR - l\frac{\pi}{2}\right)}{\cos\left(kR - l\frac{\pi}{2}\right)} \qquad \Rightarrow \; \delta_l = l\frac{\pi}{2} - kR \quad \text{for } l \lesssim l_{max}$$

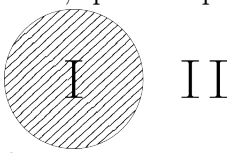
This result is valid up to a maximal angular momentum which we can obtain from the properties of the spherical Bessel functions. Instead of analyzing those, we estimate the maximal l from classical physics, which tells us that all incoming particles scatter which have a distance smaller than R from the origin. As the angular momentum of a particle passing at distance R is $\vec{L} = \vec{R} \times \vec{p}$, $L^2 = (\hbar k R)^2 \approx l_{max}(l_{max}+1)$ and therefore $l_{max} \approx kR$ for $kR \gg 1$.
For the cross section we find from Eq. (4.13)

$$\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l \approx \frac{4\pi}{k^2} \sum_{l < l_{\max}} (2l+1) \frac{1}{2} \left(1 - (-1)^l \cos(2kR)\right)$$
$$\approx \frac{4\pi}{k^2} \sum_{l < l_{\max}} (2l+1) \frac{1}{2} \approx \frac{4\pi}{k^2} \frac{1}{2} \int_0^{l_{\max}} 2l \, \mathrm{d}l \approx 2\frac{\pi}{k^2} l_{\max}^2 = 2\pi R^2 \quad \text{for } kR \gg 1$$

This is unexpected, as this is twice the classical result, πR^2. Usually, one has to obtain classical results when the wavelength of the particle gets shorter and shorter. Does this

imply that we have found a violation of classical physics in a regime where is has to be valid or do we have made a mistake in the calculation? Both is not the case. A more careful analysis shows that 50% of the scattering occurs in a tiny angle almost parallel to the incoming beam, $\theta \approx 0$. This angle vanishes for $k \to \infty$. An experiment which measures the total cross section is usually blind for very small angles as it should not count unscattered particles. Such an experiment will therefore always measure the classical cross section for $kR \gg 1$. In formulas, we can define a cross-section excluding very small angles, $\theta < \theta_0$, by $\sigma_{\theta_0} = \int_{\theta_0}^{\pi} \sin\theta \, d\theta \int_0^{2\pi} d\varphi \frac{d\sigma}{d\Omega}$. Then $\lim_{\theta_0 \to 0} \lim_{kR\to\infty} \sigma_{\theta_0} = \pi R^2$ is the classical result (easy to measure), while the other limit $\lim_{kR\to\infty} \lim_{\theta_0 \to 0} \sigma_{\theta_0} = 2\pi R^2$ gives the quantum result.
As a second example, we consider a spherical potential well, spherical potential well

$$V(r) = \begin{cases} V_0 & \text{for} \quad r < R \quad \text{(region I)} \\ 0 & \qquad\quad r > R \quad \text{(region II)} \end{cases}$$



We can use our previous results to solve first the problem in region I and II separately, gluing the solutions together in a second step. In region II, for $r > R_0$, we have

$$u_{kl}^{\mathrm{II}}(r) = 2kr(\alpha j_l(kr) + \beta y_l(kr)) \quad ; E = \frac{\hbar k^2}{2m}$$

In region I, $r < R_0$, the situation is simpler. As $y_l(kr)$ diverges for $r \to 0$ and $u_{kl}(r \to 0) = 0$, the solution is expressed in $j_l(\tilde{k}r)$ only, where $\tilde{k}$ has to be chosen to compensate for the constant potential V_0. We therefore find

$$u_{kl}^{\mathrm{I}}(r) = 2r\, j_l(\tilde{k}r), \qquad E - V_0 = \frac{(\hbar\tilde{k})^2}{2m}$$

To obtain also a solution of the radial Schrödinger equation for $r = R$, we have to fulfill the two boundary conditions

$$u_{kl}^{\mathrm{I}}(R) = u_{kl}^{\mathrm{II}}(R), \qquad \frac{\mathrm{d}}{\mathrm{d}R} u_{kl}^{\mathrm{I}}(R) = \frac{\mathrm{d}}{\mathrm{d}R} u_{kl}^{\mathrm{II}}(R)$$

From these two equations, we can determine the unknown coeffcients α and β as function of k and l.
We will focus on the limit of small k only, where only $l = 0$ contributes with $j_0(x) = \frac{\sin(x)}{x}$, $y_0(x) = \frac{-\cos(x)}{x}$. Therefore the boundary conditions can be written as

$$\begin{aligned} \sin(\tilde{k}R) &= \alpha \sin(kR) - \beta \cos(kR) = \alpha' \sin(kR + \delta_0) \\ \tilde{k} \cos(\tilde{k}R) &= \alpha' k \cos(kR + \delta_0) \end{aligned}$$

where we used trigonmetric formulas to rewrite $\alpha \sin(kR) - \beta \cos(kR)$ as $\alpha' \sin(kR + \delta_0)$ such that α' and δ_0 (the scattering phase shift) are now the constants to be determined.

After solving the first equation for α', we obtain from the second equation the condition

$$\tilde{k}\cos(\tilde{k}R) = \frac{\sin(\tilde{k}R)}{\sin(kR+\delta_0)}\, k\cos(kR+\delta_0)$$

or, equivalently,

$$\tan(kR+\delta_0) = \frac{k}{\tilde{k}}\tan(\tilde{k}R)$$

which is solved by

$$\delta_0(k) = \arctan\left(\frac{k}{\tilde{k}}\tan(\tilde{k}R)\right) - kR, \qquad \sigma = \frac{4\pi}{k^2}\sin^2\delta_0(k)$$

In the limit $k \to 0$ we have $\frac{(\hbar\tilde{k})2}{2m} = -V_0$ and therefore $\tilde{k} = \frac{1}{\hbar}\sqrt{-2mV_0}$. We can use the definition Eq. (4.16), to calculate the scattering length (i.e. the radius of a hard sphere which has the same cross section)

$$a = -\lim_{k\to 0}\frac{\delta_0(k)}{k} = R\left(1 - \frac{\tan(\tilde{k}R)}{\tilde{k}R}\right)$$

$$\frac{a}{R} = 1 - \frac{\tan\sqrt{-\alpha}}{\sqrt{-\alpha}} \quad , \; \alpha = \frac{V_0}{(\frac{\hbar}{R})^2\frac{1}{2m}} = (\tilde{k}R)^2$$

In Fig. 4.1, we plot $a/R = 1 - \frac{\tan(\sqrt{-\alpha})}{\sqrt{-\alpha}}$ as a function of $\alpha = -(\tilde{k}R)^2 = \frac{V_0}{(\frac{\hbar}{R})^2\frac{1}{2m}}$. For

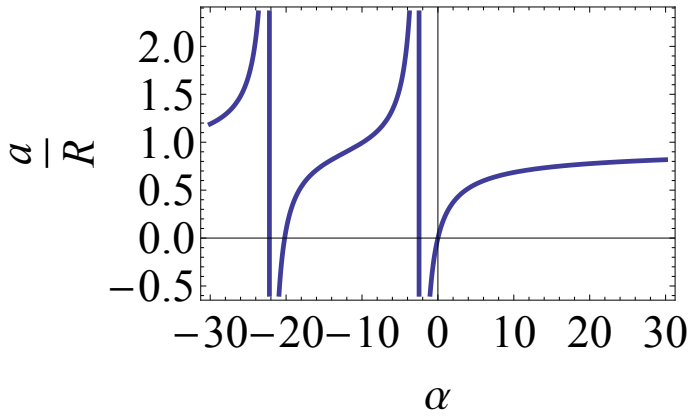


Figure 4.1: Scattering length as function of $\alpha = \frac{V_0}{(\frac{\hbar}{R})^2\frac{1}{2m}}$.

$V_0 > 0$, the scattering length is positive and approaches $a = R$ for $V_0 \to \infty$ as expected. a vanishes for $V_0 = 0$ and for small, negative V_0 one obtains a negative scattering length. Something dramatic happens, however, when for sufficiently negative V_0 we hit the pole of the tan function at $\sqrt{-\alpha} = \pi\,(n+\frac{1}{2})$. Let us analyze the proximity of this point by

setting $\sqrt{-\alpha} = \pi\ (n + \frac{1}{2}) + \Delta x$. For $\Delta x \to 0$ the scattering length diverges and changes its sign

$$a = R - \frac{1}{\tilde{k}} \frac{\sin\sqrt{-\alpha}}{\cos\sqrt{-\alpha}} \approx \frac{1}{\tilde{k}\Delta x}$$

What we observe here is **resonant scattering** : for sufficiently attractive potential one gets a bound state (see problem set, where we check this). The scattering length diverges and changes its sign exactly at the point where a new bound state forms at $E = 0$.
It is also instructive to calculate the total cross section directly at the resonance for small but finite $kR \ll 1$. We first consider the scattering phase shift

$$\delta_0(k) = \arctan\left(\frac{k}{\tilde{k}} \underbrace{\tan(\tilde{k}R)}_{\substack{\text{diverges at} \\ \text{resonance}}}\right) - kR = \pi\Big(\frac{1}{2} + n\Big) - \underbrace{kR}_{\ll 1} \approx \pi\Big(n + \frac{1}{2}\Big)$$

Therefore the total cross section is given by

$$\sigma = \frac{4\pi}{k^2} \sin^2\delta_0 \approx \frac{4\pi}{k^2} = \frac{1}{\pi}\lambda^2$$

Note that in our limit $\lambda = \frac{2\pi}{k} \gg R$ and therefore the cross section at the resonance is strongly enhanced. Directly at resonance it is given by the square of the wavelength.
The effect that the scattering length is strongly enhanced and can be changed easily when there is a resonant state, is frequently used to control the atom-atom scattering in experiments based on the manipulation of ultracold atom. One uses the above described effect to modify the atom-atom scattering using a so-called Feshbach resonance controlled by a small magnetic field. Here one uses that the number of bound states of a system of two atoms (i.e. the number of molecular states) can be changed by changing the magnetic field. In this case, the magnetic field plays exactly the same role as the depth of the potential V_0 (or, equivalently, the value of α) in the example above. Thus one can control the scattering length describing the atomic scattering with high precision. One can switch from repulsive ($a > 0$) to attractive interactions ($a < 0$) interactions, and one can strongly enhance the scattering of atoms. The use of Feshbach resonances is therefore a very important tool in a field which studies the collective states of ultracold atoms.

4.6 Lippmann-Schwinger equation and Green functions

The goal of this chapter will be to develop a new formulation of the Schrödinger equation, the Lippmann-Schwinger equation, which is especially useful to treat scattering problems. Importantly, we will use this approach to develop methods to calculate scattering rates and cross sections using perturbation theory.
Let us recall the general setup of a scattering problem. We want to solve the Schrödinger eqation, $H|\psi\rangle = E|\psi\rangle$, with the boundary condition of an incoming plane wave. The Hamiltonian is thereby separated into two parts,

$$H = H_0 + V$$

where H_0 is a part without the scattering center, in our case just, $H_0 = \frac{p^2}{2m}$, while V is the scattering potential. This general setup is flexible and can easily be generalized to complex many particle systems (e.g. electrons scattering from a defect in a solid).
The boundary condition is defined by an eigenstate of H_0

$$H_0|\phi_{\text{in}}\rangle = E|\phi_{\text{in}}\rangle$$

while the scattering state should fulfill

$$(H_0 + V)|\psi\rangle = E|\psi\rangle \quad \Leftrightarrow \quad (E - H_0)|\psi\rangle = V|\psi\rangle$$

It is not difficult to make a first guess, how a *formal* solution of this problem might look like

$$|\psi\rangle = (E - H_0)^{-1} V|\psi\rangle + |\phi_{\text{in}}\rangle$$

This equation obviously fulfills the Schrödinger equation (you can show this by multipliying it with $E - H_0$) and at least for $V = 0$ the boundary condition. While our final result will look very similar, it is important to note that this equation is *ill defined* (and therefore meaningless) due to the divergence of $(E - H_0)^{-1}$.
To find a solution to this problem, we consider a more well defined setup: Let us assume that initially (i.e., for $t \to -\infty$) the system was unperturbed, $V = 0$, with $|\psi(t \to -\infty)\rangle = |\phi_{\text{in}}\rangle$. Then, V is switched on very slowly ('adiabatically'), e.g. $V(t) = Ve^{-\epsilon|t|}$ for $t < 0$ and $V(t) = V$ for $t > 0$ with $\epsilon \to 0$. We expect to obtain by this construction an eigenstate $|\psi\rangle$ with energy E, $(H_0 + V)|\psi\rangle = E|\psi\rangle$, which does, however, still remember the initial value $|\phi_{\text{in}}\rangle$. We will not prove this, but the idea is that this setting (adiabatically switching-on of the perturbation), will give results which are equivalent to a setup where an incoming wave package is prepared in the far distance, then hits the obstacle, is scattered and finally detected again in the far distance from the scattering center.

Let us therefore consider the time dependent Schrödinger equation with

$$(i\hbar\partial_t - H_0)\,|\phi_{\text{in}}(t)\rangle = 0, \qquad (i\hbar\partial_t - H_0)\,|\psi(t)\rangle = V(t)\,|\psi(t)\rangle \tag{4.17}$$

To find a solution to this problem, let us pretend that we already know the right-hand side of the equation, $V(t)\,|\psi(t)\rangle$. Then a solution of the left-hand side with the right boundary condition can be found by introducing a **Green function** $G_0(t)$ with

$$(i\hbar\partial_t - H_0)\,G_0(t) = \delta(t)\cdot\mathbb{1} \tag{4.18}$$

with this definition (which we will have to refine soon), we can easily convince ourselves that

$$|\psi(t)\rangle = |\phi_{\text{in}}(t)\rangle + \int G_0(t-t')\,V(t')\,\big|\psi(t')\big\rangle\;\mathrm{d}t'$$

is a solution to the full time-dependent Schrödinger equation. Let us check this:

$$(i\hbar\partial_t - H_0)\,|\psi\rangle = 0 + \int \delta(t-t')\,\mathbb{1}\,V(t')\,\big|\psi(t')\big\rangle\;\mathrm{d}t' = V(t)\,|\psi(t)\rangle$$

Now comes the decisive step: to fulfill the correct boundary condition, we have to define $G_0(t)$ in such a way, that $|\psi(t)\rangle$ is only modified **after** the potential has changed (causality). The Green function which fulfills this condition is called **retarded Green function**, $G_0^+(t)$ with

$$G_0^+(t) = 0 \text{ for } t < 0$$

This condition and Eq. (4.18) is fulfilled by the retarded Green function

$$G_0^+(t) = \frac{1}{i\hbar}\Theta(t)\,e^{-iH_0t/\hbar} \tag{4.19}$$

Let us check this: $i\hbar\partial_t\,G_0^+ = H_0\,G_0^\dagger + \delta(t)\mathbb{1}$. Note that also a different solution of (4.18) exists, the **advanced Green function** (which we mention here only for completeness)

$$G_0^-(t) = -\frac{1}{i\hbar}\Theta(-t)\,e^{-iHt/\hbar}$$

fulfilling the boundary condition $G_0^-(t>0) = 0$. After having identified the Green function with the correct boundary condition, we obtain our central result, the **Lippmann-Schwinger equation** (here in the time domain)

$$|\psi(t)\rangle = |\phi_{\text{in}}(t)\rangle + \int \mathrm{d}t'\,G_0^+(t-t')\,V(t')\,\big|\psi(t')\big\rangle \tag{4.20}$$

This fulfills our boundary condition $|\psi(t\to-\infty)\rangle = |\phi_{\text{in}}(t)\rangle$ due to $G_0^+(t<0) = 0$ and the full time-dependent Schrödinger equation as we have already proven above. The Lippmann-Schwinger equation is fully equivalent to the time dependent Schrödinger with the added advantage that it explicitly includes the boundary condition at $t = -\infty$.

To obtain stationary states as function of the energy E we will need the Fourier transformation of $G_0^+(t)$

$$G_0^+(E) = \int_{-\infty}^{\infty} e^{-iEt/\hbar} G_0^+(t) \underbrace{e^{-\frac{\epsilon}{\hbar}t\,\mathrm{sgn}(t)}}_{\substack{\text{needed for convergence} \\ \text{at } t\to\pm\infty\,,\,\epsilon \text{ infinitesimal}}} \mathrm{d}t = \int_{-\infty}^{\infty} \frac{1}{i\hbar}\Theta(t)\, e^{i(E+i\epsilon-H_0)t/\hbar} = (E+i\epsilon-H_0)^{-1}$$

In the energy domain, we therefore find

$$\begin{aligned} &G_0^+(E) = \lim_{\epsilon\to 0^+} (E+i\epsilon-H_0)^{-1}, \qquad G_0^-(E) = \lim_{\epsilon\to 0^+} (E-i\epsilon-H_0)^{-1} \\ &\text{retarded Green function} \qquad\qquad \text{advanced Green function} \end{aligned} \tag{4.21}$$

The reader is strongly encouraged to check that the all-important ϵ factors guarantee that upon transforming the Green function back to the time domain, the proper $\theta(t)$ factors are recovered.

Defining the stationary wave functions $|\Psi\rangle$ and $|\Phi_{\text{in}}\rangle$ as usually from $|\psi(t)\rangle = e^{-iEt/\hbar}\,|\psi\rangle$ and $|\Phi_{\text{in}}(t)\rangle = e^{-iEt/\hbar}\,|\Phi_{\text{in}}\rangle$, we easily obtain for a time independet V by a Fourier transformation of Eq. (4.20) the stationary **Lippmann-Schwinger equation**

$$|\psi\rangle = |\phi_{\text{in}}\rangle + G_0^+(E)V\,|\psi\rangle \tag{4.22}$$

which is a reformation of the stationary Schrödinger equation appropriate for a scattering problem, which includes the boundary condition $|\phi_{\text{in}}\rangle$. We have been a bit sloppy in one step of the derivation of this stationary equation: we did not mention during the derivation that V is switched on adiabatically. It is, however, not difficult to convince oneself that this factor is precisely taken into account by the ϵ in the definition of $G_0^+(E)$.

Let us finally check the result

$$(E-H_0)\,|\psi\rangle = 0 + \lim_{\epsilon\to 0} \frac{E-H_0}{E+i\epsilon-H_0}\,V\,|\psi\rangle = V\,|\psi\rangle$$

By definition, $G_0^+(E)$ is an operator. For calculations it is necessary to write it in a suitable basis. We will therefore discuss its properties in momentum space and in real space. In momentum space we can write $G_0^+(E) = \sum_{k,k'} |k'\rangle\,\langle k'|\,G_0^+(E)\,|k\rangle\,\langle k|$. Therefore we define

$$\begin{aligned} &g_0^+(k',k) = \langle k'|G_0^+(E)|k\rangle = \delta_{k,k'}\, g_0^+(E,\vec{k}) \\ &g_0^+(E,\vec{k}) = \frac{1}{E+i\epsilon-\epsilon_k}, \qquad \epsilon_k = \frac{(\hbar k)^2}{2m} \end{aligned} \tag{4.23}$$

Similarly, we can find a representation in real space, which will be especially useful. In this case, the operator is written as $G_0^+(E) = \int \mathrm{d}^3r\,\mathrm{d}^3r'\,|r'\rangle\,\langle r'|\,G_0^+(E)\,|r\rangle\,\langle r|$ which can be

obtained from the momentum-space representation by a Fourier transformation as

$$g_0^+(E,r',r) = \langle r'|\, G_0^+(E)\,|r\rangle = \int \langle r'|\, k'\rangle \langle k'|\, G^+(E)\,|k\rangle \langle k|\, r\rangle \, \frac{\mathrm{d}^3k\,\mathrm{d}^3k'}{(2\pi)^6}$$
$$= \int \frac{\mathrm{d}^3k}{(2\pi)^3}\, e^{i\vec{k}(\vec{r}-\vec{r}')} \frac{1}{E+i\epsilon-\epsilon_k} = g_0^+(E,r'-r)$$

In spherical coordinates we obtain using $u = \cos\vartheta$

$$g_0^+(E,\vec{r}) = \frac{1}{(2\pi)^3} \int \mathrm{d}k\, k^2 \mathrm{d}\varphi \int_{-1}^{1} \mathrm{d}u\, e^{ikr\,u} \frac{1}{E+i\epsilon-\epsilon_k}$$
$$= \frac{2\pi}{(2\pi)^3} \int \mathrm{d}k\, k^2\, \frac{e^{ikr}-e^{-ikr}}{ikr} \frac{1}{E+i\epsilon-\epsilon_k}$$

We can use the residue theorem to evaluate this k integral using that $E + i\epsilon - \frac{(\hbar k)^2}{2m} = \frac{\hbar^2}{2m}\left((k_0+i\epsilon')-k\right)\left((k_0+i\epsilon')+k\right)$ where we define $E = \frac{(\hbar k_0)^2}{2m}$ with $k_0 > 0$. For the terms oscillating with e^{ikr} (with e^{-ikr}) we have to close the contour in the upper (lower) half of the complex plane and obtain a contribution from the pole at $k_0 + i\epsilon'$ (at $-(k_0+i\epsilon')$) as $r > 0$. Combining the two terms we get

$$g_0^+(E,r) = -\frac{m}{2\pi\hbar^2}\frac{e^{ik_0r}}{r} \quad , \; E = \frac{(\hbar k_0)^2}{2m} \; , \; k_0 > 0 \tag{4.24}$$

Note that $g_0^+(E,r)$ has the form of an *outgoing* spherical wave, a consequence of the $i\epsilon$ term characteristic for the retarded Green function. In contrast, the advanced Green function,

$$g_0^-(E,r) = -\frac{m}{2\pi\hbar^2}\frac{e^{-ik_0r}}{r}$$

is based on an *incoming* spherical wave.
It is worthwhile to check the important result (4.24):

$$(E-H_0)\, g^+(E,\vec{r}) = \left(E + \frac{\hbar^2}{2m}\nabla^2\right) g_0^+(E,r) \underbrace{=}_{\nabla^2\frac{1}{r}=-4\pi\delta(\vec{r})} \delta^3(r)$$

Using the real-space form of the Green function, we can also write the **Lippmann-Schwinger in real space** using $\langle r|\, \psi\rangle = \psi(r)$

$$\psi(r) = e^{i\vec{k}_0\vec{r}} + \int \mathrm{d}^3r'\, g_0^+(E,\vec{r}-\vec{r}')\, V(r')\, \psi(r') \tag{4.25}$$

Again, this is just a reformulation of the Schrödinger equation. Instead of a differential equation it is a linear integral equation. As we will see it is especially useful when calculation scattering problems in perturbation theory.

As a final check, we can convince ourself that $\Psi(r)$ from Eq. (4.25) indeed fulfills the usual Schrödinger equation

$$(E + \frac{\hbar^2}{2m}\nabla^2)\psi(r) = \int \mathrm{d}^3r'\, \delta(r - r')V(r')\psi(r') = V(r)\psi(r)$$

4.7 Born series and Born approximation

For small scattering potential, we can solve the Lippmann-Schwinger equation

$$|\psi\rangle = |\phi_{\text{in}}\rangle + G_0^+ V\,|\psi\rangle$$

iteratively, starting from the case $V = 0$:

$$\begin{aligned}
&\mathcal{O}(V^0):\ |\psi\rangle = |\phi_{\text{in}}\rangle \\
&\mathcal{O}(V^1):\ |\psi\rangle = |\phi_{\text{in}}\rangle + G_0^+ V\,|\phi_{\text{in}}\rangle \\
&\mathcal{O}(V^2):\ |\psi\rangle = |\phi_{\text{in}}\rangle + G_0^+ V\,|\phi_{\text{in}}\rangle + G_0^+ V G_0^+ V\,|\phi_{\text{in}}\rangle
\end{aligned}$$

Repeating this to infinite order, we obtain the **Born series**

$$|\psi\rangle = \sum_{n=0}^{\infty} \left(G_0^+(E)V\right)^n\,|\phi_{\text{in}}\rangle = \left(\mathbb{1} - G_0^+(E)V\right)^{-1}\,|\phi_{\text{in}}\rangle \tag{4.26}$$

We can rewrite the last expression

$$\begin{aligned}
\left(\mathbb{1} - G_0^+(E)V\right)^{-1}\,|\phi_{\text{in}}\rangle &= \left(G_0^+(E)\left(G_0^+(E)^{-1} - V\right)\right)^{-1}\,|\phi_{\text{in}}\rangle \\
&= \frac{1}{E + i\epsilon - H_0 - V}\,(E + i\epsilon - H_0)\,|\phi_{\text{in}}\rangle
\end{aligned}$$

which leads to the simple-looking but rather subtle equation for the scattering state

$$|\psi\rangle = \Omega^+\,|\Omega_{\text{in}}\rangle \qquad \text{with} \quad \Omega^+ = \frac{i\epsilon}{E + i\epsilon - H}\,|\phi_{\text{in}}\rangle = \lim_{t\to\infty} \underbrace{e^{-iHt/\hbar}}_{\substack{\text{time}\\ \text{evolution}}}\ \underbrace{e^{iH_0t/\hbar}}_{\substack{\text{removes trivial}\\ \text{time evolution}\\ \text{of } \Omega_{\text{in}}}}$$

where Ω^+ is called the Møeller operator. To show the last equality, we first note that $\lim\limits_{t\to\infty} f(t) = \delta \int\limits_0^\infty e^{-\delta t'}\, f(t')$ for $\delta \to 0$ if the limit exists. Therefore,

$$\begin{aligned}
\Omega^+\,|\phi_{\text{in}}\rangle \underbrace{=}_{\delta = \frac{\epsilon}{\hbar}} \frac{\epsilon}{\hbar}\int_0^\infty e^{-\epsilon t'/\hbar}\, e^{-iHt'/\hbar}\, e^{iH_0t'/\hbar}\,|\phi_{\text{in}}\rangle &= \frac{\epsilon}{\hbar}\int_0^\infty e^{-i(H-E+i\epsilon)t'/\hbar}\,|\phi_{\text{in}}\rangle \\
&= \frac{i\epsilon}{E + i\epsilon - H}\,|\phi_{\text{in}}\rangle
\end{aligned}$$

In the following we will introduce a few useful concepts for scattering theory. For the Lippmann-Schwinger equation the central element was the Green function $G_0^+(E) = (E - H_0 + i\epsilon)^{-1}$ defined with the help of the unperturbed Hamiltonian H_0. This is also sometimes called the 'bare' Green function distinguishing it from the 'full' Green function defined using H instead of H_0

$$G^+(E) = \frac{1}{E + i\epsilon - H} = \left(G_0^+(E)^{-1} + V\right)^{-1}$$

The Taylor series describing the perturbative expansion of $G^+(E)$ is given by

$$\begin{aligned} G^+(E) &= G_0^+(E) + G_0^+(E)VG_0^+(E) + G_0^+(E)VG_0^+(E)VG_0^+(E) + \dots \\ &= G_0^+(E) + G_0^+(E)T(E)G_0^+(E) \end{aligned}$$

where the last equation defines the so-called **T matrix**

$$T(E) = V + VG_0^+(E)V + VG_0^+(E)VG_0^+(E)V + \dots = V + VG^+(E)V$$

While we will not use the T matrix in the following, but we note that often the in practical calculation one often calculates first the T matrix and then expresses quantities like differential cross sections in terms of T.
Our next goal is the determine the scattering amplitudes $f(\vartheta, \varphi)$ starting from the Lippmann-Schwinger equation in real space, Eq. (4.25). As $f(\vartheta, \varphi)$ is defined, see Eq. (4.2), from the asymptotic behavior of the wave function, we have to determine $\Psi(r \to \infty)$. We have therefore to expand $g_0^+(r - r')$ for large r using that $|r - r'| = \sqrt{(\vec{r} - \vec{r}')^2} = \sqrt{r^2 - 2\vec{r}\vec{r}' + \dots} \approx r - \frac{\vec{r}\vec{r}'}{r}$. We find for $r \to \infty$

$$g_0^+(r - r') = -\frac{m}{2\pi\hbar^2}\frac{e^{ik_0|\vec{r}-\vec{r}'|}}{|r - r'|} \approx -\frac{m}{2\pi\hbar^2}\frac{e^{ik_0 r}}{r}\, e^{-ik_0\vec{r}'\,\hat{r}} + \mathcal{O}(\frac{1}{r^2})$$

where $\hat{r} = \frac{\vec{r}}{r}$. Therefore, we obtain

$$\psi(r \to \infty) \approx e^{i\vec{k}_0\vec{r}} - \frac{m}{2\pi\hbar^2}\frac{e^{ik_0 r}}{r}\int e^{-ik_0\vec{r}'\,\hat{r}} V(r')\Psi(r')\,\mathrm{d}^3r' \equiv e^{i\vec{k}_0\vec{r}} + \frac{e^{ik_0 r}}{r} f(\vartheta, \varphi)$$

This allows us to determine the scattering amplitude

$$f(\vartheta, \varphi) = f(\vec{k}_{\text{out}}, \vec{k}_0) = -\frac{m}{2\pi\hbar}\int e^{-i\vec{k}_{\text{out}}\vec{r}'} V(\vec{r}')\psi(r') \tag{4.27}$$

Here we have introduced a new notation, by writing $f(\vec{k}_{\text{out}}, \vec{k}_0)$ instead of $f(\vartheta, \varphi)$. We set

$$\vec{k}_{\text{out}} = k_0\hat{r}$$

This is the wave vector of the outgoing wave in the direction $\hat{r}$ where the detector sits. Instead of parameterizing the scattering amplitude by the angles ϑ and ϕ, we can use the

incoming momentum $\vec{k}_0$ and the **outgoing momentum** $\vec{k}_{\text{out}}$ instead with $|\vec{k}_{\text{out}}| = |\vec{k}_0|$ as we consider only energy-conserving elastic scattering from a potential.

In real space, the first few terms of the Born series, Eq. (4.26) are

$$\psi(R) = e^{i\vec{k}_0\vec{r}} + \int g_0^+(r-r')V(r')e^{ik_0r'}\,\mathrm{d}r' + \int g_0^+(r-r')V(r')g_0^+(r'-r'')V(r'')e^{ik_0r''}\,\mathrm{d}r'\mathrm{d}r'' + \ldots$$

This formula has a surprisingly simple (and instructive) interpretation: The first term describes the unperturbed wave, the second describes that when the wave hits the potential, each point becomes the source of a new spherical wave (reminiscent of Huygen's principle from optics). The third term encodes that the emitted spherical wave of the second term can again be scattered by the potential the due to the potential. The Born series is therefore just the sum of all scattering and re-scatteing events.
The lowest order approximation to the Born series, where one keeps only the first two terms is called **Born approximation** . This very useful approximation is therefore given by

$$\psi(r) \approx e^{i\vec{k}_0\vec{r}} + \int g_0^+(\vec{r}-\vec{r}')V(r')e^{i\vec{k}_0\vec{r}}\,\mathrm{d}^3r'$$

As Eq. (4.27) for the computation of the scattering amplitude already contains V, we just use $\psi(r) \approx e^{i\vec{k}_0\vec{r}}$ to obtain the scattering amplitude and therefore also the differential cross section in Born approximation

$$f(\vec{k}_{\text{out}}, \vec{k}_0) \approx -\frac{m}{2\pi\hbar^2}\int e^{-i(\vec{k}_{\text{out}}-\vec{k}_0)\vec{r}'}V(r')\,\mathrm{d}^3r' = -\frac{m}{2\pi\hbar^2}V_{\vec{k}_{\text{out}}-\vec{k}_0} \tag{4.28}$$

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \approx \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|V_{\vec{k}_{\text{out}}-\vec{k}_0}\right|^2 + \mathcal{O}(V^3) \tag{4.29}$$

The differential cross section is therefore up to a prefactor just the modulus square of the Fourier transformation of the potential, $V_{\vec{k}} = \int e^{-ikr}V(r)$, where $\vec{k}$ is identified with the transferred momentum, $\vec{k}_{\text{out}} - \vec{k}_0$.
As a first example, we consider the scattering from a purely local potential $V(\vec{r}) = U\delta(\vec{r})$. We directly obtain to $\mathcal{O}(U^2)$ the angle-independent result

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \left(\frac{mU}{2\pi\hbar^2}\right)^2$$

A very important example is the Rutherford scattering **Rutherford scattering**, i.e. the scattering from a a **Coulomb potential** $V(r) = \frac{e^2}{r}$. The Fourier transformation $V_k = \frac{4\pi e^2}{k^2}$ can be used directly in Eq. (4.29) to obtain the cross section. To express the differential cross section in terms of the angle ϑ and φ, we use that

$$k^2 = \left(\vec{k}_{\text{out}} - \vec{k}_0\right)^2 = k_{\text{out}}^2 + k_0^2 - 2k_{\text{out}}k_0\cos\vartheta = 2k_0^2(1-\cos\vartheta) = 2k_0^2\sin^2\frac{\vartheta}{2}$$

For the differential cross section, we for the Rutherford scattering the differential cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \approx \left(\frac{m}{2\pi\hbar}\right)^2 \left(\frac{4\pi e^2}{2k_0^2 \sin^2 \frac{\vartheta}{2}}\right)^2 = \left(\frac{e^2}{4E}\right)^2 \cdot \frac{1}{\sin^4\left(\frac{\vartheta}{2}\right)}$$

Due to the smallness of the finestructure constant α this perturbative result is a good approximation for electrons (or, for Rutherford's experiment, the α particle) with not too high energies.

4.8 Optical theorem

In this section we will derive a useful result. To obtain the total cross section, it is not necessary to integrate over all angles. Instead it is sufficient to study the scattering in the direction of the incoming beam.
The basic idea behind this result is almost trivial: due to probability conservation the total flux of incoming particles is either scattered or not scattered

$$I_{\text{in}} = I_{\text{scattered}} + I_{\text{not scattered}}$$

Therefore the total cross section can be obtained by computing how many particles are *not* scattered

$$\sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\,\mathrm{d}\Omega = \frac{I_{\text{scattered}}}{j_{\text{in}}} = \frac{I_{\text{in}} - I_{\text{not scattered}}}{j_{\text{in}}}$$

We start our analysis from the asymptotic expansion of the wave function, $\psi(r \to \infty) \approx \mathfrak{c}\left(e^{ik_0 r} + f(\vec{k},\vec{k}_0)\frac{e^{ik_0 r}}{r}\right)$ where $\vec{k} = |k_0| \cdot \hat{r}$ is the outgoing momentum. The corresponding probability current is given by

$$\vec{j} = \frac{1}{2m}\left(\psi^*(-i\hbar\vec{\nabla})\psi + \text{h.c.}\right) \approx |\mathfrak{c}|^2 \cdot \frac{\hbar k_0}{m}\Bigg(\underbrace{\hat{k}_0}_{\text{incoming current}} + |\underbrace{f(k,k_0)}_{\text{scattered}}|^2 \frac{\hat{r}}{r^2} + \frac{1}{2}\left(f(k,k_0)\frac{\hat{r}}{r}\,e^{i(k_0 r - \vec{k}_0\vec{r})} + f^*(k,k_0)\frac{\hat{r}}{r}\,e^{-i(k_0 r - \vec{k}_0\vec{r})} + \text{h.c.}\right)\Bigg) \tag{4.30}$$

where we used $\vec{\nabla}\frac{e^{ik_0 r}}{r} = ik_0\hat{r}\frac{e^{ik_0 r}}{r} + \mathcal{O}\left(\frac{1}{r^2}\right)$. We are mainly interested in the information encoded in the interference term given by the last line of Eq. (4.30). To determine the current of not-scattered particles, we have to ask what a detector would measure which is placed in 'forward' direction, measuring all not-scattered particles of the incoming beam. Let us assume that the detector has the opening angle ϑ_0 To add all the probability current

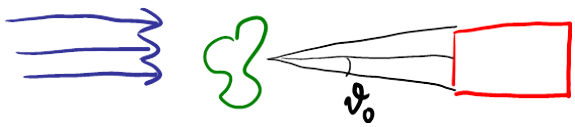


Figure 4.2: Sketch of a detector placed in forward direction with opening angle ϑ_0 measuring all particles which are not scattered.

into the detector arising from the interference term we need to calculate

$$\int\limits_{\vartheta<\vartheta_0} \frac{e^{\pm i(k_0 r - \vec{k}_0\vec{r})}}{r} r^2 \sin\vartheta\,\mathrm{d}\vartheta\mathrm{d}\varphi \approx \int_{\vartheta<\vartheta_0} \frac{e^{\pm ik_0 r\frac{\vartheta^2}{2}}}{r} r^2\,\mathrm{d}\varphi\,\vartheta\mathrm{d}\vartheta \approx 2\pi\int_0^\infty \frac{e^{\pm ik_0 r\frac{\vartheta^2}{2}}}{r} r^2\vartheta d\vartheta = \frac{2\pi}{\pm ik_0}$$

where we used that for small angles $k_0 r - \vec{k}_0\vec{r} = k_0 r\cdot(1-\cos\vartheta) \approx k_0 r\frac{\vartheta^2}{2}$. Furthermore, we used that for $r \to \infty$ only small angles, $\vartheta \lesssim \sqrt{k_0 r}$, contribute to the integral over $e^{\pm ik_0 r\frac{\vartheta^2}{2}}$.

Therefore one can extent the integral over ϑ to ∞.
The contribution from the last line of Eq. (4.30) gives precisely the change of the current in forward direction due to the impurity and therefore the difference of incoming and not-scattered current.

$$\sigma = \frac{I_{\text{in}} - I_{\text{not sca.}}}{j_{\text{in}}} = -\frac{2\pi}{ik_0}\left(f(\vec{k},\vec{k}_0) - f^*(\vec{k},\vec{k}_0)\right)\Big|_{k\to k_0}$$

From this, we obtain directly the **optical theorem**

$$\sigma = \int \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}\mathrm{d}\Omega = \int \left|f(\vec{k},\vec{k}_0)\right|^2 \mathrm{d}\Omega_k = \underbrace{\frac{4\pi}{k_0}\,\mathrm{Im}\Big(f(\vec{k}_0,\vec{k}_0)\Big)}_{\substack{\text{loss in forward}\\ \text{direction}}} \tag{4.31}$$

The total cross section can be computed from the imaginary part of the scattering amplitude in 'forward' direction, i.e. for $\vec{k} = \vec{k}_0$.

4.9 Inelastic many-particle scattering

Up to now, we have only considered scattering from a given potential. Due to energy conservation, the energy of the incoming and the outgoing particle were the same: the scattering was only elastic. In many situations, however, the energy of the scattered particle does change as, for example, some energy has been deposited in the scattering target. In this case, the scattering is called 'inelastic'.
We will not try to develop a complete theory of inelastic scattering here but focus on the limit of weak scattering where perturbation theory can be applied. This allows, for example, to understand what is measured in a neutron scattering experiment, one of the most important techniques to detect excitations in some material. As neutrons are interacting very weakly with matter, perturbation theory can be used reliably.

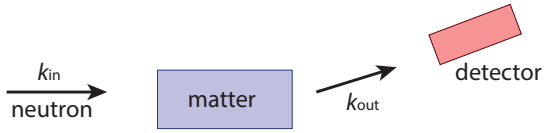


Figure 4.3: Sketch of a neutron scattering experiment. The kinetic energy of the neutron changes as some energy is deposited in the system.

We consider an (idealized) scattering experiment, where the incoming particle (e.g., a neutron) has the wavevector $\vec{k}_{\text{in}}$ and the associated energy $E^{\text{T}}_{\text{in}} = \frac{(\hbar k_{\text{in}})^2}{2m}$ where m is here the mass of the neutron ('T' refers to the 'testing' particle). Similiarly, the outgoing neutron has wavevector $\vec{k}_{\text{out}}$ and the energy $E^{T}_{\text{out}} = \frac{(\hbar k_{\text{out}})^2}{2m}$. The detector can measure the direction of the outgoing particle, $\hat{\Omega}$, and its energy E^{T}_{out}. From this one can compute the

the energy loss

$$E = E^T_{\text{out}} - E^T_{\text{in}}$$

.

In a typical scattering experiment, the detector will measure during the time Δt the number ΔN = number of arriving neutrons which have an energy in the energy interval $E^T_{\text{in}} + E \leq E^T_{\text{out}} \leq E^T_{\text{in}} + E + \Delta E$, where ΔE is the energy resolution of the detector. In analogy to the differntial cross section for elastic scattering, Eq. (4.1), one can compute a energy-resolved differential cross section

$$\frac{\mathrm{d}\sigma(E,\vartheta,\varphi)}{\mathrm{d}\Omega\,\mathrm{d}E} = \frac{\Delta N}{\Delta t\,\Delta E\,\Delta\Omega}\cdot\frac{1}{\text{incoming flux}}$$

which is a function of the transfered energy E. The total cross section is obtained by integrating over all angles and over the transferred energy,

$$\sigma = \int dE \int \sin\vartheta\, d\vartheta d\varphi \frac{\mathrm{d}\sigma(E,\vartheta,\varphi)}{\mathrm{d}\Omega\,\mathrm{d}E}$$

To describe the experiment, we consider the Hamiltonian

$$H = \underbrace{H^0_T}_{\substack{\text{testparticle}\\ \text{e.g. neutron}}} + \underbrace{H^0_S}_{\substack{\text{complex}\\ \text{system}}} + \underbrace{H_{\text{int}}}_{\substack{\text{interaction of test particle}\\ \text{with system}}}$$

Various interactions are possible. For neutrons, for example, the dominant interactions are with the nuclei in the system and also a dipole-dipole interaction of the electron spin with the spin of the neutron. For simplicity, we consider just a density-density interaction

$$H_{\text{int}} = \int \mathrm{d}^3r\mathrm{d}^3r' \underbrace{\rho_T(r)}_{\substack{\text{density of}\\ \text{test particle}}} V(r-r')\cdot \underbrace{\rho_S(r')}_{\substack{\text{density in}\\ \text{the system}}}$$

For neutrons, ρ_S could be the density of nuclei. In this case one can model the potental by a contact interaction, $V(r-r') = c\delta(\vec{r}-\vec{r}')$.

For neutrons, H_{int} is typically very small, and one can safely use perturbation theory, i.e., the generalization of Born's approximation for inelastic scattering. Equivalently, we can just use Fermi's golden rule, used previously by us in Sec. 2.3.2. According to Fermi's golden rule, the transition rate from the initial to the final state is given by

$$\Gamma_{\text{out, in}} \approx \frac{2\pi}{\hbar} \left|\langle \text{out}|\, H_{\text{int}}\, |\text{in}\rangle\right|^2 \delta(E_{\text{out}} - E_{\text{in}}) + \mathcal{O}(H^3_{\text{int}}) \tag{4.32}$$

where the initial state is given by

$$|\text{in}\rangle = \underbrace{|k\rangle}_{\text{test particle}} \underbrace{|n_s\rangle}_{\textit{system}}, \quad \text{energy} \quad E_{\text{in}} = \frac{(\hbar\, k)^2}{2m} + E^s_{n_s}$$

The total incoming energy is just the sum of the energy of the system, $E^s_{n_s}$, and the energy of the test particle. $|n_s\rangle$ is in general a very complicated quantum state describing all the particles in the system under investigation, with $H_s\,|n_s\rangle = E^s_{n_s}\,|n_s\rangle$. At a finite temperature T this state is occupied with the probability

$$P_{n_s} = \frac{e^{-E_{ns}/k_bT}}{Z} \quad ; \; Z = \sum_{n_s} e^{-E^s_{ns}/k_bT}$$

For the outgoing state we write

$$|\text{out}\rangle = \left|k'\right\rangle \left|n'_s\right\rangle, \quad E_{\text{out}} = \frac{(\hbar k')^2}{2m} + E^s_{n'_s}$$

where the quantum state $|n'_s\rangle$ of the system after scattering is in general not known (and not measured).
To obtain the scattering rate, we have to sum (4.32) over all incoming states with the weight P_{n_s} and also over all possible final states n'_s as each of them contributes to the probability to have a neutron scattered into the state k'.

$$\Gamma_{k,k'} = \frac{2\pi}{\hbar} \sum_{n_s,n'_s} P_{n_s} \left|\left\langle k'\right| \left\langle n'_s\right| H_{\text{int}} \left|n_s\right\rangle \left|k\right\rangle\right|^2 \delta(E_{n'_s} - E_{n_s} - E)$$

Here

$$E = \frac{(\hbar k)^2}{2m} - \frac{(\hbar k')^2}{2m}, \qquad \vec{q} = \vec{k}' - \vec{k}$$

are the energy loss and the transfered momentum, respectively. It is useful to rewrite the matrix element

$$\left\langle k'\right| \left\langle n'_s\right| H_{\text{int}} \left|n_s\right\rangle \left|k\right\rangle = \int \mathrm{d}^3r\, \mathrm{d}^3r' \left\langle k'\right| \rho_T(r) \left|k\right\rangle \, V(r-r') \cdot \left\langle n'_s\right| \rho_s(r') \left|n_s\right\rangle$$

In first quantized language, the density operator for our test particle (the neutron) is just given by $\rho_T(\vec{r}) = \delta(\vec{x} - \vec{r})$ and therefore $\langle k'|\,\rho_T(r)\,|k\rangle = \int e^{i(\vec{k}-\vec{k}')\vec{x}}\,\delta(\vec{x}-\vec{r}) = e^{i(\vec{k}-\vec{k}')\vec{r}} = e^{-i\vec{q}\vec{r}}$. Using the Fourier transformation of the scattering potential and the density of the measured particles, $V(r-r') = \int V_Q\, e^{i\vec{Q}(\vec{r}-\vec{r}')}\,\frac{\mathrm{d}^3Q}{(2\pi)^3}$ and $\rho_s(r') = \int e^{i\vec{Q}'\vec{r}'}\rho_s(Q')\,\frac{\mathrm{d}^3Q'}{(2\pi)^3}$ we obtain

$$\left\langle k'\right| \left\langle n'_s\right| H_{\text{int}} \left|n_s\right\rangle \left|k\right\rangle = V_{\vec{q}} \left\langle n'_s\right| \rho_s(\vec{q}) \left|n_s\right\rangle$$

To calculate finally $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega\,\mathrm{d}E}$, we need number of k' states flying into the detector for a given opening angle and given energy range, $[E^t_{\text{out}},\, E^t_{\text{out}} + \Delta E]$, Here we use that

$$\frac{\mathrm{d}^3k'}{(2\pi)^3} = \frac{1}{(2\pi)^3}\, k'^2\, \mathrm{d}k' \mathrm{d}\Omega_k = \frac{1}{(2\pi)^3}\, k'^2 \frac{\mathrm{d}k'}{\mathrm{d}E} \mathrm{d}E' \mathrm{d}\Omega_{k'} = \frac{1}{(2\pi)^3} k' \frac{m}{\hbar^2} \mathrm{d}E' \mathrm{d}\Omega$$

as $dE'/dk' = \hbar^2 k'/m$. Dividing further by the incoming flux and collecting all results, we

find

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega_k\,\mathrm{d}E} = \frac{1}{(2\pi)^3}k'\frac{m}{\hbar^2}\frac{1}{\frac{\hbar k}{m}}\frac{2\pi}{\hbar}\sum_{n_s n_s'} P_{n_s}\left|\langle n_s'|\, V_{\vec{q}}\,\rho^s(\vec{q})\,|n_s\rangle\right|^2\cdot\delta(E_{n_s}'-E_{n_s}-E)$$

or, equivalently,

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega_k\mathrm{d}E} = \frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2 S(\vec{q},E)$$
$$\text{with}\qquad \vec{q}=\vec{k}'-\vec{k}\quad;\; E=\frac{(\hbar k)^2}{2m}-\frac{(\hbar k')^2}{2m}$$

with the **correlation function**

$$S(\vec{q},E) = \sum_{n_s,n_s'} P_{n_s}\left|\langle n_s'|\, V_{\vec{q}}\,\rho^s(\vec{q})\,|n_s\rangle\right|^2\cdot\delta(E_{n_s}'-E_{n_s}-E) \tag{4.33}$$
$$= \int_{-\infty}^{\infty}\frac{dt}{\hbar}\; e^{iEt/\hbar}\;\left\langle\,\Phi_{-\vec{q}}(t)\,\Phi_q(0)\,\right\rangle \qquad \text{with}\;\; \Phi_{\vec{q}}=V_{\vec{q}}\,\rho^s(\vec{q}) \tag{4.34}$$

Before we derive the last line of this equation, let us interpret the result. The energy-resolved differential cross section measures directly the $\vec{q}$ and E dependence of the correlation function $S(\vec{q},E)$. Here $\vec{q}$ is the transferred momentum and E the transfered energy of the scattering test particle (the neutron), respectively. $S(\vec{q},E)$ gives rather direct informations about the excitation spectrum of the system which is investigated. A peak in $S(\vec{q},E)$ as function of E signalizes that there is an excitation in the system with energy E and momentum $\hbar\vec{q}$. That the excitation has the energy E, can directly be seen from the δ-function in Eq. (4.33). To show that the excitation has momentum $\hbar\vec{q}$, one uses that $|n_s\rangle$ and $|n_s'\rangle$ can (in a translationally invariant system) be chosen as (quasi-) momentum eigenstates. One can then show that the matrix element $\langle n_s'|\, V_{\vec{q}}\,\rho^s(\vec{q})\,|n_s\rangle$ is only finite if the (quasi-) momenta of $|n_s\rangle$ and $|n_s'\rangle$ differ by $\hbar q$. We conclude

From an inelastic scattering experiment one obtains the correlation function $S(\vec{q},E)$ which measures excitations with energy E and momentum $\hbar\vec{q}$ obtained from the energy- and momentum transfer of the scattering particle.

To derive Eq. (4.34), we first not that the time-dependent operator is defined using the Heisenberg picture, $\phi_{-q}(t) = e^{iHt/\hbar}\phi_{-q}e^{-iHt/\hbar}$. We use the definition of the expectation

value at finite temperature T

$$\begin{aligned}
\left\langle \phi_{-q}(t)\, \phi_q(0) \right\rangle &= \sum_n \frac{e^{-\frac{E_n}{k_B T}}}{Z} \left\langle n \right| \phi_{-q}(t) \phi_q(0) \left| n \right\rangle \\
&= \sum_{n,m} \frac{e^{-\frac{E_n}{k_B T}}}{Z} \left\langle n \right| e^{iHt/\hbar}\, \phi_{-q}\, e^{-iHt/\hbar} \left| m \right\rangle \left\langle m \right| \phi_q \left| n \right\rangle \\
&= \sum_{n,m} P_n e^{i(E_n - E_m)t/\hbar} \left\langle n \right| \phi_{-q} \left| m \right\rangle \left\langle m \right| \phi_q \left| n \right\rangle \\
&= \sum_{n,m} e^{i(E_n - E_m)t/\hbar}\, P_n \left| \left\langle m \right| \phi_q \left| n \right\rangle \right|^2
\end{aligned}$$

From a simple Fourier transformation one obtains Eq. (4.33).
Scattering techniques are very useful to obtain precise quantitative information on the excitation spectrum of a wide range systems, including nuclei, atoms, molecules or solids.

5 The Standard Model of Particle Physics

This chapter will give a brief introduction to the standard model of particle physics. It covers about 7 lectures, which are not enough to give a complete picture of all aspects of the standard model but can, hopefully, give an overview of its structure and of some of its most important properties.
The standard model is an extremely successful theory of – with the exception of gravity – all phenomena in the world around us. It is one of the most important intellectual achievements of physics. It show that it is possible to find an extremely compact description of nature based on a few symmetry principles. It has been tested in a large number of high-precision experiments. Nevertheless, the structure of the standard model also suggests that it is not the final answer to the question of how the world around us is build: like many other theories it is an approximation valid for only a certain range of energies.
While we will discuss in this chapter some of the most important building blocks of the standard model, we will not be able to discuss how one can actually calculate, e.g., scattering cross sections. For this further techniques have to be developed which are usually covered in courses on quantum field theory. The reader is encouraged to use this chapter also to recapitulate some basic notions of the previous chapters of this book, including topics like the quantization of light, relativistic quantum mechanics, or the principles of Gauge invariance. We denote such opportunities in the following by a box in the following way:

> **recapitulate:** ...

Some of the conventions used in the following are taken from the book by Peskin and Schröder, *An introduction to QFT*, which gives a much deeper coverage of the topic than we can present here. The book of Nachtmann, *Elementary Particle Physics*, is recommended as it gives a good non-technical overview over the standard model.

5.1 Lagrange formalism

When writing down the field theory describing the standard model, we will use in the following the Lagrange formalism. We assume that the reader is familiar with this approach from the theory lecture on analytical mechanics. We will, however, recapitulate the basic concepts in the following.

In classical physics, one can replace Newton's laws by a new postulate, **Hamilton's variation principle** .

> **recapitulate:** Lagrange formulation of classical mechanics

Here one investigates the properties of the action S which is defined as a functional of the path $x(t)$ of a particles, $S = S[x(t)]$. Hamilton's variational principle states, that along the physical trajectory the action is extremal (a miminum, a maximum or a saddle point), variations of S therefore vanish when the path is varied, $x(t) \to x(t) + \delta x(t)$ while the endpoints at $t = 0$ and $t = T$ are kept fixed

$$\delta S = S[x(t) + \delta x(t)] - S[x(t)] = 0 \quad \text{with } \delta x(0) = \delta x(T) = 0$$

An action can usually be written as an integral over a **Lagrange function** $L(x(t), \dot{x}(t), t)$, $S = \int_0^T dt L(x(t), \dot{x}(t), t)$. In this case the variation of the action is given by

$$\delta S = S[x(t) + \delta x(t)] - S[x(t)] = \int_0^T \mathrm{d}t \left(\frac{\partial L}{\partial x} \delta x + \underbrace{\frac{\partial L}{\partial \dot{x}} \delta \dot{x}}_{\substack{\text{integration} \\ \text{by parts}}} \right)$$

$$= \int_0^T \left(\frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{x}} \right) \delta x(t) + \underbrace{\frac{\partial L}{\partial \dot{x}} \delta x \Big|_0^T}_{\substack{=0 \text{ for} \\ \delta x(0) = \delta x(t) = 0}}$$

From the condition $\delta S = 0$ for arbitrary $\delta x(t)$ we therefore obtain the **Euler-Lagrange equation**

$$\frac{\mathrm{d}}{\mathrm{d}t} \frac{\partial L}{\partial \dot{x}_i} = \frac{\partial L}{\partial x_i}$$

written here for several components, $i = 1, .., N$.
For the Lagrange function $L = \frac{1}{2} m \dot{x}^2 - V(x)$, for example, the Euler-Lagrange equations give Newton's law,

$$\frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x}) = -\frac{\partial}{\partial x} V(x)$$

Newton's equation are differential equations. The same formalism can, however, also be applied for partial differential equations, i.e. for Schrödinger, Klein-Gordon, Maxwell, or Dirac equations. Why do we want to do this? For us, one main reason is that the Lagrange formalism provides a simple and compact way to write down theories and to identify their symmetries. The Lagrange formalism also has the advantage that it allows to choose suitable variables (important for the discussion of the Higgs mechanism). Furthermore, it is also a convenient starting point to formulate a theory in second quantization. Here one

can either use the Lagrange formalism to define momenta ($p_i = \partial L/\partial x_i$) and postulate canonical commutation relations ($[x_n, p_m] = i\delta_{nm}\hbar$). Alternatively, there exists also a formulation of quantum mechanics and quantum field theory based on actions S. This is discussed in courses on quantum field theory: it turns out that it is possible to obtain quantum mechanical amplitudes just by summing $e^{iS/\hbar}$ over all possible configurations.
To generalize Hamiltonian's principle to (classical) field theories, we have to consider actions which are functional of field configurations $\Phi_i(r,t)$, $i = 1, 2, ...N$. In one example, Φ_i may describe the displacement of a guitar string in another example it could be a wave function of a single particle. Assuming that the action is a local functional, it can be written as

$$\begin{aligned} S[\phi] &= \int \mathrm{d}^3 r \int_0^t \mathrm{d}t'\, L(\phi(\vec{r},t),\, \partial_{t'}\phi_i,\, \vec{\nabla}\phi_i(\vec{r},t')) \\ &= \int_c \mathrm{d}^4 x\, L(\phi_i,\, \partial_\mu \phi_i), \quad \mu = 0,1,2,3 \quad \text{with } \partial_\mu = \frac{\partial}{\partial x^\mu} \end{aligned}$$

Here L is the Lagrange density. As before, we study small variations of the field with fixed boundary conditions at the time $t = 0$ and $t = T$

$$\phi_i(r, t=0) = \phi_i^0(\vec{r}) \;,\; \phi_i(\vec{r}, T) = \phi_i^1(\vec{r}) \tag{5.1}$$

The boundary conditions in real space depend on the type of problem. For a guitar string one would, for example, consider fixed boundary conditions $\phi(r = 0) = \phi(r = L) = 0$. We will use infinite systems in the following thereby ignoring the boundary conditions.
To derive the Euler-Lagrange equations, we have to consider small variations of the field configuration by a small space- and time-dependent function $\delta\phi(r,t)$ which does vanish at the boundaries $t = 0$ and $t = T$.

$$\begin{aligned} \delta S = S[\phi_i + \delta\phi_i] - S[\phi_i] &= \int \mathrm{d}^4 x \left(\frac{\partial L}{\partial \phi_i}\delta\phi_i + \frac{\partial L}{\partial\, \partial_\mu \phi_i}\partial_\mu \delta\phi_i \right) \\ &= \int \mathrm{d}^4 x \left(\frac{\partial L}{\partial \phi_i} - \partial_\mu \frac{\partial L}{\partial\, \partial_\mu \phi_i} \right) \delta\phi_i + \text{surface terms} \end{aligned}$$

By demanding that δS vanishes for *arbitrary* $\delta\phi(r,t)$, we obtain the **Euler-Lagrange equations** for a field theory

$$\delta S = 0 \quad \forall\, \delta\phi_i \quad \Rightarrow \quad \partial_\mu \frac{\partial L}{\partial(\partial_\mu \phi_i)} = \frac{\partial L}{\partial \phi_i} \tag{5.2}$$

As a first example, we will consider the Lagrange density for a real field $\phi(\vec{r},t) = \phi(x) \in \mathbb{R}$. which has the property to be Lorentz invariant. As $d^4x = c\,dt\,d^3\vec{r}$ is Lorentz invariant, a Lorentz invariant Lagrange density implies a Lorentz invariant action S. Considering only

terms quadratic in ϕ, a natural candidate is

$$L = (\partial_\mu \phi)(\partial^\mu \phi) - c^2 m^2 \phi^2 = \frac{1}{c^2}(\partial_t \phi)^2 - \left(\vec{\nabla}\phi\right)^2 - c^2 m^2 \phi^2 \tag{5.3}$$

Using that $\partial_0 = \frac{1}{c}\frac{\partial}{\partial t}$ the Euler-Lagrange equations are given by

$$\begin{aligned}\frac{1}{c}\frac{\partial}{\partial t}\frac{\partial L}{\partial\, \partial_t\phi/c} + \vec{\nabla}\frac{\partial L}{\partial \vec{\nabla}\phi} &= \frac{1}{c}\frac{\partial}{\partial t}\left(2\frac{1}{c}\partial_t\phi\right) + \vec{\nabla}\left(-2\vec{\nabla}\phi\right) = 2\left(\frac{1}{c^2}\partial_t^2 - \vec{\nabla}^2\right)\phi \\ &= 2\partial_\mu\,\partial^\mu\,\phi \overset{!}{=} \frac{\partial L}{\partial \phi} = -2c^2m^2\phi\end{aligned}$$

We therefore obtain directly the **Klein-Gordon equation**

$$\left(\partial_\mu\partial^\mu + c^2m^2\right)\phi = 0$$

Similarly, one can find a Lagrange density describing the **Dirac equation** formulated for a spinor field, $\psi(r,t) \in \mathbb{C}^4$. For spinors, the following Lagrange density is Lorentz invariant

$$L = \overline{\psi}(i\partial\!\!\!/ - m)\psi \tag{5.4}$$

where $\partial\!\!\!/ = \gamma^\mu\partial_\mu$.

> **recapitulate:** Dirac equation and γ matrices

To calculate the corresponding Euler-Lagrange equation, one can express Ψ and $\bar{\Psi}$ in terms of 8 real fields $\mathrm{Re}(\psi)$ and $\mathrm{Im}\psi$. Much more convenient is, however, to remember that one can choose arbitrary coordinates when investigating the extrema of the action S. Therefore one can just consider the four component of ψ and the four components of $\bar{\psi}$ as 8 fields *independent* from each other. One obtains in total 8 Euler Lagrange equations, the first 4 from varying the action by changing $\bar{\Psi}_i$

$$\partial_\mu \underbrace{\frac{\partial L}{\partial\, \partial_\mu\overline{\psi}_i}}_{=0} = \frac{\partial L}{\partial \overline{\psi}_i} \quad \Rightarrow \quad 0 = \frac{\partial L}{\partial \bar{\psi}} = (i\partial\!\!\!/ - m)\psi$$

This already gives the Dirac equation in its usual form. 4 more equations are obtained from the variations with Ψ

$$\partial_\mu \frac{\partial L}{\partial\, \partial_\mu\psi} = \frac{\partial L}{\partial \overline{\psi}} \quad \Rightarrow \quad \partial_\mu(i\overline{\psi}\gamma^\mu) = -m\overline{\psi}$$

This equation looks less familiar but we can easily check that this is the Dirac equation for $\bar{\Psi} = \gamma^0\psi^*$. To check this, consider the Hermitian conjugate of the equation

$$\left(\partial_\mu\left(\overline{\psi}i\gamma^\mu\right)\right)^\dagger = -i\left(\gamma^\mu\right)^\dagger\left(\partial_\mu\overline{\psi}\right)^\dagger = -i\left(\gamma^\mu\right)^\dagger\gamma^0\,\partial_\mu\psi = -m\gamma^0\psi$$

Multiplying the equation from the left with γ^0 and using that $(\gamma^0)^2 = \mathbb{1}$ and $\gamma^0 (\gamma^\mu)^\dagger \gamma^0$ one obtains again the standard Dirac equation.

5.2 Lagrange function of electrodynamics

Before searching for a Lagrange function to describe quantum electrodynamics, QED, we recapitulate a few facts on Maxell's equations (see also chapter 2.1) using units where $c = 1$. As we have seen there, any quantum theory of electromagnetism builds on the concept of a vector potential. Originally this has been introduced so solve two of the four Maxwell's equations.

$$\begin{aligned} \text{I)} \quad & \vec{\nabla}\vec{B} = 0, \qquad & \vec{\nabla} \times \vec{E} + \partial_t \vec{B} = 0 \\ \text{II)} \quad & \vec{\nabla}\vec{E} = \rho, \qquad & \vec{\nabla} \times \vec{B} - \partial_t \vec{E} = \vec{j} \end{aligned}$$

The first two equations are solved by introducing the scalar potential ϕ and the vector potential $\vec{A}$ by

$$\vec{B} = \vec{\nabla} \times \vec{A}, \quad \vec{E} = -\vec{\nabla}\phi - \partial_t \vec{A}$$

Importantly, these potentials are not unique. All physical properties are invariant under a Gauge transformation

$$\phi \;\rightarrow\; \phi + \partial_t \Gamma(\vec{r}, t) \quad ; \; \vec{A} \;\rightarrow\; \vec{A} - \vec{\nabla}\Gamma(\vec{r}, t)$$

It is useful to rewrite these equations and also the current in terms of contravariant 4-vectors.

$$A^\mu = (\phi, \vec{A}), \qquad j^\mu = (\rho, \vec{j})$$

such that the Gauge transformation takes the form

$$A^\mu \rightarrow A^\mu + \partial^\mu \Gamma$$

with $\partial^\mu = \frac{\partial}{\partial x_\mu} = (\partial_t, -\vec{\nabla})$.

recapitulate: 4-vector notation, Lorentz transformations, chapter 3.1

The electric and magnetic fields are then described by the field strength tensor

$$F_{\mu\,\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu = \begin{pmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{pmatrix}$$

The field strength tensor has two important properties: First, it is manifestly gauge invariant as under a Gauge transformation

$$F_{\mu\nu} \to F_{\mu\nu} + \partial_\mu\partial_\nu\Gamma - \partial_\nu\partial_\mu\Gamma = F_{\mu\nu}.$$

Second, it transforms as a tensor under Lorentz-transformation

$$\begin{aligned} F &\to F' = \Lambda^T F\,\Lambda \\ F_{\mu\,\nu} &\to F_{\mu\,\nu} = \Lambda_\mu^{\ \mu'}\, F_{\mu'\,\nu'}\, \Lambda^{\nu'}_{\ \nu} \end{aligned}$$

We will not try to find an action S as a functional of $\vec{A}^\mu$ build such that its Euler-Lagrange equations reproduce Maxwells equations. More precisely, we will pretend that we do not know Maxwell's equation. We will instead try to **guess** the correct action S (and therefore Maxwell's theory) guided by symmetries. We demand

1. Lorentz invariance of S
2. gauge invariance
3. simplicity (low powers of the fields)

The field strength tensor is Gauge invariant, a natural way to build something Lorentz invariant from it, is to consider $F_{\mu\,\nu}\,F^{\mu\,\nu}$. If we want to include the electric current j^μ in the action, we have to multiply it by another 4-vector to obtain something Lorentz invariant: therefore one naturally considers the combination $j_\mu A^\mu$. We can therefore expect that the action should have the form

$$S[A] = \int \mathrm{d}^4x\, c_1\,(F_{\mu\,\nu}\,F^{\mu\,\nu}) + c_2 A_\mu j^\mu \tag{5.5}$$

where c_1 and c_2 are unknown constants. To confirm Lorentz invariance, note that d^4x has this property as $\left|\dfrac{\partial x'_\mu}{\partial x_\nu}\right| = \det\Lambda = 1$. We should also check Gauge invariance

$$S[A^\mu + \partial^\mu\,\Gamma] - S[A^\mu] = \int \mathrm{d}^4x\, c_2\,(\partial_\mu\Gamma) j^\mu = \int \mathrm{d}^4x c_2\Gamma \underbrace{\partial_\mu j^\mu}_{=0} + \text{surface terms}$$

where we used a partial integration for the last equality. Using charge conservation, $\partial_\mu j^\mu = 0$ we see that at least up to surface terms everything is Gauge invariant.

The Euler-Lagrange equations are given by

$$\partial_\mu \frac{\partial L}{\partial\, \partial_\mu A_\mu} = \frac{\partial L}{\partial A_\mu} \quad \Rightarrow\ 4\, c_1\, \partial^\nu F_{\nu\,\mu} = c_2\, j_\mu$$

Looking at these equations, we see that only the ratio of the two constants, c_2/c_1, enters. Fixing this ratio is, however, only a convention (it can be reabsorbed into a redefinition of the charge). One uses $c_2 = 4c_1$ as a convention. An overall prefactor of the action obviously cannot be obtained by just considering the Euler Lagrange equations. We choose it in such a way that when switching from the Lagrange- to the Hamilton formalism, the Hamiltonfunction can be identified with the energy. From this condition, one finds $c_2 = -1$ and therefore

$$L = -\frac{1}{4} F_{\mu\,\nu} F^{\mu\,\nu} - A_\mu j^\mu \tag{5.6}$$

Amazingly, just from a few simple arguments based on gauge invariance and symmetries, we were able to derive an action describing all aspects of Maxwell's equation. Postulating Gauge invariance also for the Dirac equation and the associated action, we will even be able to get QED, quantum electrodynamics.

5.3 U(1) gauge invariance and Quantum Electrodynamics (QED)

> **recapitulate:** Gauge invariance, Sec. 3.4

As discussed in Sec. 3.4, the coupling of matter to electromagnetism follows from one powerful postulate, the invariance under **local** phase transformations of the quantum fields describing charged particles. As we will see later, a very similar principle can be used to describe also the strong and weak interactions. Therefore we repeat the essential argument here as it allows us to construct the action describing QED. Related concepts are also used in general relativity – from this field the expression 'Gauge invariance' (in German: Eichinvarianz) arises (the invariance under changing, e.g., the way how length is measured). The basic idea of Gauge invariance is to postulate of a invariance of fields under the U(1) transformation $\Psi(r,t) \to e^{i\phi(r,t)}\Psi(r,t)$. This can, however, be only be achieved, if one considers simultaneously a the transformation of the vector potential

Gauge invariance:
All physical observables are invariant under the gauge transformation

$$\Phi(x) \to \exp\Big(i\frac{q}{\hbar c}\varphi(x)\Big)\ \Phi(x) \quad ,\ A^\mu(x) \to A^\mu(x) - \partial^\mu\varphi(x) \tag{5.7}$$

In this case, the combination of derivative and vector potential ('minimal coupling') becomes Gauge invariant

$$D^\mu = \partial^\mu + \frac{iq}{\hbar c} A^\mu \tag{5.8}$$

as we have shown in chapter 3.4. Here q is the elementary charge, i.e. the electron charge for cases when Ψ describes electrons.
To obtain the Lagrange density of QED, we just have to combine the Lagrange density of the electromagnetic fields, Eq. (5.6), with the Lagrange density corresponding to the Dirac equation, Eq. (5.4) replacing $\not{\partial} = \gamma^\mu \partial_\mu$ by $\not{D} = \gamma^\mu D_\mu$ using Eq. (5.8).

$$\mathcal{L}_{\text{QED}} = \overline{\psi}(i\not{D} - m)\psi - \frac{1}{4}\left(F^{\mu\,\nu} F_{\mu\,\nu}\right) \tag{5.9}$$

This simple Lagrange density (together with the appropriate quantization rules) encodes all of QED and therefore most of the physics in the world around us. From this one can derive Maxwell's equations, the Dirac equation, the Schrödinger equation and describe – at least in principle – everything from a piece of metal to the laser.[1]

> **recapitulate:** Quantization of the electromagnetic field, chapter 2.1

By comparing Eq. (5.9) to Eq. (5.6), one can obtain directly a formula for the current

$$j^\mu = -\frac{d}{dA_\mu}(\overline{\psi}(i\not{D} - m)\psi) = \frac{q}{\hbar c}\,\overline{\psi}\gamma^\mu\psi$$

where q can be identified with the electron charge e. This is up to a prefactor consistent with Eq. 3.21.

5.4 Regularization and renormalization of QED

It turns out, that the Lagrange density (5.9) of QED (together with the corresponding quantization rules) is not sufficient to define properly the theory of quantum electrodynamics. This can be seen when trying to calculate physical quantities using perturbation theory: typical calculations give divergent results. Therefore one also need a way to treat these divergencies. The reader should study chapter 3.11 where this problem is discussed.

> **recapitulate:** Renormalization and regularization, chapter 3.11

[1] In the Quantum Field Theory course you will discuss that the fermionic field ψ in the Lagrange density (5.8) is not a complex field but a different mathematical object (a Grassmann field) taking into account that it describes anticommuting fermions rather than commuting bosons. This does, however, not have any direct consequences for the arguments we want to make in this lecture.

Two main results of chapter 3.11 are important for our discussion. First, QED (and the whole standard model) is only well defined when one defines a cutoff Λ, i.e., a maximally allowed energy or momentum (this step is called regularization). For finite Λ (and finite energy) one obtains finite results from perturbation theory, which do, however, diverge for $\Lambda \to \infty$. Second, by expressing the results of the calculation in terms of the **measured** electron mass and the **measured** fine structure constants one obtains results for all physical observables which are finite and **independent** of Λ for $\Lambda \to \infty$ (see chapter 3.11). This property is called renormalizability and is a feature of all Gauge theories of the standard model.

While the standard model is renormalizable, this is not true for many other competing theories. For example, a local interaction of Fermions described by a term $\int (\Psi^\dagger(x)\Psi(x))^2$ in the Lagrange function (or the Hamilton operator in second quantization language) turns out to be **not** renormalizable, implying that in general (unknown) details of the physics at some high-energy scale influence the physics at low energies, which drastically reduces the predictive power of a theory. In high-energy physics such non-renormalizable theories have therefore been viewed as less suitable theories to describe nature.

It is the general believe that the standard model in its present form is only a low-energy approximation to some other, presently unknown theory. The fact that the standard model is renormalizable means that one can nevertheless predict all experiments with high precision without any knowledge of the high-energy theory. While this helps a lot to understand the laws of nature around us, it also implies that it is very difficult to access the physics beyond the standard model in present-day experiment. From this point of view, the success of the standard model is actually the main obstacle to understand what it behind the standard model.

5.5 Strong interactions: quarks and gluons

5.5.1 Quarks

Protons and neutrons are not elementary particles. High-energy scattering experiment have revealed that they are actually made of so-called **quarks**. Quarks are fermionic spin 1/2 particles described by a Dirac equation (see below).

> Bound states of 3 quarks are called **baryons** – the most important examples are the proton and the neutron – while **meson** is the name for bound states of a quark and an antiquark.

A pion is, for example, a meson. A single free quark has never been observed and – as we will discuss in Sec. 5.5.3 – cannot even exist at low energies: only certain types of bound states are allowed. As quarks are fermions, this implies that baryons are fermions while pions act as bosons.

There are, in total, 6 different types of quarks:

u: up	c: charm	t: top
d: down	s: strange	b: bottom

One speaks of 6 different **flavors** of quarks. As we will see later when discussing electroweak interactions, the u/d, the c/s and the t/b quarks each form a pair. The quantum numbers of the quarks, e.g. their charge, will be discussed later in Sec.5.8, after we have worked out the electroweak theory.

The quarks have all different masses[2]. With the two lightest types of quarks, the up and the down quark, one can form a stable bound states of 3 quarks which cannot decay (at least not within the standard model) as one cannot form states with lower energy starting from 3 quarks. This lowest-energy state is the proton.

The **proton** is made from two up and one down quark (uud). The antiproton is therefore build from two three antiquarks ($\bar{u}\bar{u}\bar{d}$, denoting here anti-particles by a bar). The **neutron**, in contrast, is made from two down and one up quark (udd).

As a single particle in vacuum, the neutron decays after about 15 min (see Sec. 5.6) but it is stable when it is part of a non-radioactive nucleus. Also an anti-neutron (made from $\bar{u}\bar{d}\bar{d}$) exist. All other bound states of three quarks decay much faster.

The quark picture was developed in the early 80th by people like Murray Gell-Mann which tried to understand a large zoo of different baryons and mesons by assuming that they are bound states of some unknown elementary particles. It was realized early that just two quarks (the u and d) are not sufficient but that at least a third one was needed. Indeed the c, t and b quarks are much heavier than the u, d and s quarks and therefore all 'lighter' baryons and mesons are made from the latter three. Ignoring all of the heavier quarks, one can as a first crude approximation consider the mass of the three remaining lighter quarks u, d and s as being approximately equal (or even zero). Considering only the strong interactions, u, d and s also feel the same forces. Therefore an *approximate* SU(3) symmetry exist: just changing the u, d and s wave function by an SU(3) matrix, $(u, d, s) \to U(u, d, s)$ with $U \in SU(3)$ should not strongly affect the mass of a bound state.[3] This approximate symmetry is called the SU(3)-flavor symmetry, which should **not** be confused with the SU(3) gauge symmetry (acting on the color instead of flavor) discussed in Sec. 5.5.2.

A discussion of the SU(3)-flavor symmetry is not part of this lecture and the remarks below are therefore perhaps a bit too short but have been added as this approximate symmetry was historically very important to obtain an understanding how quarks form bound states. The usefulness of the SU(3)-flavor symmetry relies on the fact that it allows to classify, sort and even predict the zoo of barionic and mesonic states by using the theory of representations of SU(3).

[2] As no free single quarks exist, the precise definition of the mass of a quark is a tricky business. Note that the mass of the proton is not just the sum of the masses of the quarks it is made from as according to $E = mc^2$ also the binding energy contributes to the mass.

[3] SU(3) the is the group of all unitary 3×3 matrices U with $\det U = 1$.

We will not explain the representation theory of SU(3) or how it is precisely related to the baryons and mesons but just remind the reader that one can classify for example atoms by the total angular moment $\vec{J} = \vec{S} + \vec{L}$. While a singlet state, $j = 0$, is unique, one obtains two degenerate states for $j = 1/2$, three states for $j = 1$ and so on. Each $j = 0, 1/2, 1, 3/2, ...$ labels one representation of SU(2) and gives rise to a $2j + 1$-fold degenerate state.

> **recapitulate:** total angular moment (Sec. 3.6), spin-orbit coupling (Sec. 3.10)

Similarly, SU(3) has various representations and one expects that the bound states of quarks can be labeled by these. The approximate SU(3)-flavor symmetry and the group theory for SU(3) therefore predicts that there is a group of 8 light mesons (the origin of the number 8 will become clear in Sec. 5.5.2) of similar mass (3 pions, 4 K-mesons and 1 eta meson) and, similarly, that is a group of 8 light baryons (an octet) to which the neutron and proton and 6 more baryons belong. Another group of 10 baryons (a decuplet) can also be viewed as belonging to one representation of the approximate SU(3) flavor symmetry. Long before the strong interactions had been understood and long before any bound states of quarks could be calculated (and before even quarks have been introduced), it was therefore possible to understand the basic structure of baryons and mesons based on the quark model and some symmetry considerations. This approach was coined the 'eightfold way' by Murray Gell-Mann (refering to the 'Noble Eightfold Path' of Buddhism).

5.5.2 Color and SU(3) gauge theory

Quarks have an important extra quantum number, their so-called **color**. Each quark comes in three different colors, often referred to a red, green and blue. We will also label them by $i = 1, 2, 3$. To describe all 6 flavors of quarks we need $72 = 6 \times 3 \times 4$ quantum fields as each quark (for example a red up-quark) is described by a 4-component Dirac spinor: the 4 spinor components describe the spin-up and spin-down states of the quark and its antiparticle. The 12 up-quark fields, for example, we will write in the form

$$u_i(x) = \begin{pmatrix} u_{i1} \\ u_{i2} \\ u_{i3} \\ u_{i4} \end{pmatrix} \qquad i = 1, 2, 3$$

where $i = 1, 2, 3$ describes the color and the second index of $u_{i\alpha}$ is the spinor index. The Lagrange density of the up-quarks is given for vanishing quark mass by the usual Dirac equation.

$$L_0 = \sum_{i=1}^{3} \bar{u}_i \, i\partial\!\!\!/ \, u_i$$

recapitulate: Dirac equation and its interpretation, Sec. 3.5

To discuss that color index we group the three colors in a 3-component vector $\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}$, where $q = u, d, s, c, t, b$ for each of the 6 quarks and each q_i stands for a 4-component spinor as discussed above for $q = u$.

Let us recall that the basic idea behind the theory of electromagnetism is the U(1) gauge invariance: physical laws and observables do not change under a transformation $\Psi \to e^{i\varphi(t,\vec{r})}\Psi$. The basic idea behind the strong interaction is exactly the same: here one postulates that the physical laws do not change under an arbitrary local renaming of the three color states.

$$\vec{q}(x) = \begin{pmatrix} q_1(x) \\ q_2(x) \\ q_3(x) \end{pmatrix} \to \vec{q'}(x) = \begin{pmatrix} q'_1(x) \\ q'_2(x) \\ q'_3(x) \end{pmatrix} = U(x) \begin{pmatrix} q_1(x) \\ q_2(x) \\ q_3(x) \end{pmatrix} \quad , U(x) \in SU(3)$$

where $x = (t, \vec{r})$ and $U(x)$ as an element of $SU(3)$ is an arbitary unitary 3×3 matrix with $\det U = 1$. The SU(3) Gauge theory of the color-index is called **quantum chromodynamics**, or shorter, **QCD**.

Before learning how to cope with such a situation, we have to study a few basic properties of $SU(3)$. We start by counting the number of independent real parameters needed to describe a SU(3) matrix. A complex 3×3 matrix is described by 18 real fields but the 9 equations $U^\dagger U = \mathbb{1}$ and the extra equation $\det U = 1$ reduce the number of independent components to $8 = 18 - 9 - 1$. We need a convenient way to parametrize the matrices with 8 real fields. Before doing so, let us recall how this is accomplished in the $SU(2)$ case which probably more familiar to the reader. An arbitrary SU(2) matrix can be written as $e^{i\sum_{i=1}^{3}\phi_i\sigma_i/2}$ where ϕ_i are three angles parametrizing the matrix and σ_i are the three Pauli matrices which form a basis of the hermitian, traceless 2×2 matrices with $\mathrm{tr}\,\sigma_i\sigma_j = 2\delta_{ij}$. Similarily, a SU(3) matrix can be written as

$$U(x) = e^{i\sum_{\alpha=1}^{8}\varphi_\alpha(x)\frac{\lambda_\alpha}{2}} \tag{5.10}$$

The eight functions $\varphi_\alpha(x)$ parametrize $U(x)$ and the eight 3×3 matrices λ_α are the natural generalizations of the Pauli matrices to SU(3). They are a basis of all traceless, hermitian

3×3 matrices normalized to $\mathrm{tr}\,\lambda_i\lambda_j = 2\delta_{ij}$. A possible parametrization is, for example,

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix},\ \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},\ \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}$$

$$\lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},\ \lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},\ \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}$$

The λ_i are the 8 generators of SU(3). Similar to QED, we face the problem that when computing the derivative $\partial_\mu(U(x)\vec{q}) = \partial_\mu(e^{i\sum_{\alpha=1}^{8}\varphi_\alpha(x)\frac{\lambda_\alpha}{2}}\vec{q})$ eight terms $U(x)\partial_\mu\varphi_\alpha\frac{\lambda_\alpha}{2}$ are generated. For QED the solution of this problem was to introduce a vector potential to cancel the corresponding term. This is precisely what we are forced to do also in the SU(3) case. Local SU(3) invariance is only possible if for each φ_α we also introduce a corresponding vector potential.

Eight vector potentials, $G_\mu^\alpha(x)$, $\alpha = 1, ..., 8$, $\mu = 0, 1, 2, 3$ are needed to ensure SU(3)-gauge invariance

The quantized vector potential A_μ describes photons.

> **recapitulate:** Quantization of the electromagnetic field, Sec. 2.1

Siimilarly, in quantized form the fields $G_\mu^\alpha(x)$ describe eight bosonic particles, the **gluons**. While electromagnetic forces are described by the photon field A_μ, the gluons are the particles responsible for the strong forces. They glue the quarks together in each baryon or meson.

It is useful to combine the 8 gluon fields in one Hermitian and traceless 3×3 matrix G_μ using the definition

$$G_\mu(x) = \sum_{\alpha=1}^{8} G_\mu^\alpha(x)\frac{\lambda^\alpha}{2}$$

The formulas for non-abelian gauge groups like SU(3) or SU(2) are slighty more complicated than for the abelian U(1) gauge group. Gauge invariance is achieved by the following *combined* transformation of quark fields and gluon fields

$$\begin{pmatrix} q_1(x) \\ q_2(x) \\ q_3(x) \end{pmatrix} \to U(x) \begin{pmatrix} q_1(x) \\ q_2(x) \\ q_3(x) \end{pmatrix}, \quad U(x) \in SU(3)$$

$$G_\mu(x) \to U(x)\, G_\mu(x)\, U(x)^\dagger - \frac{i}{g_s} U(x) \partial_\mu U^\dagger(x) \tag{5.11}$$

The equations above have been constructed such that the combination

$$D_\mu = \partial_\mu + i g_s G_\mu \tag{5.12}$$

is allows to formulate a SU(3) gauge invariant Lagrange density $L = i\,\bar{\vec{q}}\, D_\mu \gamma^\mu\, \vec{q}$. Let us check this claim by studying the Gauge transformation of $D_\mu \vec{q}$

$$\begin{aligned} (\partial_\mu + i g_s G_\mu) \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} &\to \left(\partial_\mu + i g_s U G_\mu U^\dagger + U(\partial_\mu U^\dagger) \right) U \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} \\ &= U \left(\partial_\mu + i g_s G_\mu + \underbrace{U^\dagger(\partial_\mu U) + U^\dagger U (\partial_\mu U^\dagger) U}_{=0} \right) \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} = U D_\mu \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} \end{aligned} \tag{5.13}$$

where we used that $U(\partial_\mu U^\dagger) = -(\partial_\mu U) U^\dagger$ as $0 = \partial_\mu \mathbb{1} = \partial_\mu (U U^\dagger) = (\partial_\mu U) U^\dagger + U(\partial_\mu U^\dagger)$. From Eq. 5.13 it follows directly that the Lagrange density

$$L = i\,\bar{\vec{q}}\, D_\mu \gamma^\mu\, \vec{q} \tag{5.14}$$

does not change under an SU(3) gauge transformation.

Note that in the $U(1)$ case where $U(x) = e^{i g_s \varphi(x)}$ the complicated looking formulas (5.11) reduce to the simpler formulas (5.7) when identifying $g_s = q/\hbar c$ as, for example, $-\frac{i}{g_s} U \partial_\mu U^\dagger = -\partial_\mu \varphi$ in this case.

After we have found that the postulate of Gauge invariance enforces the existence of gluons and fixes the form of their coupling to the quarks, we still have to find the SU(3) generalization of the electric and magnetic fields and of the Maxwell equations. To solve this question, we have to repeat just the arguments of Sec. 5.2, where we constructed the action underlying Maxwell's equations. We first need the the tensor describing the SU(3) version of electric and magnetic fields. It is defined by

$$\begin{aligned} G_{\lambda\rho} &= \frac{1}{i g_s} [D_\lambda, D_\rho] \\ &= \partial_\lambda G_\rho - \partial_\rho G_\lambda + \underbrace{i g_s [G_\lambda, G_\rho]}_{\text{non-linearity}} \end{aligned} \tag{5.15}$$

where we used that the commutator of ∂_λ with an arbitrary function $f(x)$ is given by $\partial_\lambda f(x)$ as $[\partial_\lambda, f]g = \partial_\lambda(fg) - f\partial_\lambda g = (\partial_\lambda f)g$ for arbitrary $f(x)$ and $g(x)$. Note that each $G_{\lambda\rho}$ is a 3×3 matrix in color space.
We have to check how $G_{\lambda\rho}$ transforms under a SU(3) Gauge transformation. We can use that we have shown above, that $D_\lambda \vec{q} \to U D_\lambda \vec{q} = U D_\lambda U^\dagger U \vec{q}$. Therefore,

$$D_\lambda \to U D_\lambda U^\dagger, \qquad G_{\lambda\rho} \to \frac{1}{g_s}[U D_\lambda U^\dagger, U D_\lambda U^\dagger]) = U G_{\lambda\rho} U^\dagger \tag{5.16}$$

This implies directly that the combination $\mathrm{tr}\left[G_{\lambda\rho} G^{\lambda\rho}\right]$ is both invariant under a gauge transformation and a Lorentz transformation (the trace runs over the color indices while the summation over λ and ρ is part of the usual Einstein convention). $\mathrm{tr}\left[G_{\lambda\rho} G^{\lambda\rho}\right]$ is therefore the natural candidate to describe in the Lagrange density the gluon analog of Maxwell's equations.[4] Combining this insight with the the action (5.14), we conclude that Lagrange density of QCD which describes the strong interactions is given by

$$\mathcal{L}_{\mathrm{QCD}} = -\frac{1}{2}\mathrm{tr}\left[G_{\lambda\rho} G^{\lambda\rho}\right] + \sum_{j=1}^{6} i\, \bar{\vec{q}}^{\,j}\, \gamma^\mu (\partial_\mu + i g_s G_\mu)\, \vec{q}^{\,j} \tag{5.17}$$

Here the index j runs over the 6 quark flavors, with $q^{1,\dots,6} = u, d, s, t, b, c$. Each of these fields has two indices, $q^j_{\nu,i}$, where $\nu = 1, 2, 3, 4$ is the spinor index while $i = 1, 2, 3$ is the color index. The 4×4 Dirac matrices γ^μ act on the spinor index while the 3×3 matrices G_μ act on the color index. The factor $1/2$ in front of the first term is just a convention (it can be absorbed in a redefinition of the fields and g_s. Therefore the only free parameter of this theory (as long as we neglect the masses of the quarks as above) is the coupling constant of the strong interaction, g_s.
$\mathcal{L}_{\mathrm{QCD}}$ describes all aspectes of the strong interaction, the force which holds, for example, the quarks in the nucleus together. It is parametrized by one coupling constant g_s, which takes over the r
The most important qualitative aspect which distinguishes $\mathcal{L}_{\mathrm{QCD}}$ from QED arises from the last term in Eq. (5.15) which is quadratic, not linear in the fields G^α_μ. Therefore the first term in $\mathcal{L}_{\mathrm{QCD}}$ has contributions of the form $\mathrm{tr}((\partial_\lambda G_\rho)[G_\lambda, G_\rho])$ and $\mathrm{tr}([G_\lambda, G_\rho] \cdot [G^\lambda, G^\rho])$. G^α_μ. These terms describe interactions of gluons.

Gluons interact with each other, as described by terms cubic and quartic in the gluon fields G^α_μ. The coupling constant is given by g_s.

While photons do not interact with each other directly, gluons have strong interactions. The consequences of this are discussed in Sec. 5.5.3.

[4] It is possible to add another term, the so-called θ term which does, however, violate time-reversal symmetry. According to experiment this term is either absent or has an extremly small prefactor.

5.5.3 Confinement and asymptotic freedom

A single free gluon or a single free quark has never been observed. Quarks and gluons occur only in bound states involving either three (baryons) or two (mesons) quarks. Also some other state might exist like bound states of gluons alone (gluonballs) or bound states of 4 quarks.

This is a consequence of a phenomenon called **confinement** which states that it costs an infinite amount of energy to create any object which has a color quantum number. This implies that only "colorless" bound states exist at low energies. More precisely, only states exist which are color-singlets whose wave function does not change under any (global) SU(3) rotation. Here color plays the same role as charge in QED. A charge-neutral object (e.g. an atom) does not couple to and does not create electromagnetic fields at large distances. Any object with a net charge, in contrast, creates an electric field $E \propto 1/r^2$ at large distances. In this case the contribution of this electric field to the energy of the charged object is finite. Similarly, a colorless bound state does not create any gluon fields at large distances, but the energy contribution of the gluon fields of an object with color (a free quark or gluon) would be infinite.

Three quarks can bind to a colorless object by forming a bound state of a red, a green and a blue quark, symbolically written as $|rgb\rangle = q_r^\dagger q_g^\dagger q_b^\dagger |0\rangle$. One can check that this state does not change under an SU(3) transformation $\begin{pmatrix} q_r \\ q_g \\ q_b \end{pmatrix} \to U \begin{pmatrix} q_r \\ q_g \\ q_b \end{pmatrix}$. Such states are baryons.

Also the combination of a quark and an antiquark (a meson) can be colorless, for example by combing a red quarks and a red antiquark.

What is the origin of the this confinement? The most important aspect is that gluons interact with each other. This does effectively change how the strong interactions change with distance (or, equivalently, with momentum).

Let us first discuss the more familiar case of electrodynamics. Photons do not interact with each other but the Coulomb field of, for example, an electric charge is influenced by the fact that virtually electron-positron pairs can be created in the vacuum. They **screen** the Coulomb interaction and weaken it for large distances. Effectively, this can be described by a momentum dependence of the fine-structure constant for large momenta compared to the electron mass m

$$\alpha_{\mathrm{QED}}(q) \approx \frac{\alpha}{1 - \frac{2}{3}\frac{\alpha}{\pi}\ln|\frac{q}{mc}|} \quad \text{for } qc \gg m \tag{5.18}$$

For large momenta, α_{QED} grows while it shrinks for small momenta (or large distances).

For the strong interaction the creation of quark-antiquark pairs also leads to screening as for QED. The interaction of gluons gives, however, a contribution with opposite sign: the gluon interaction gives rise to **antiscreening**. For the corresponding strong coupling

constant one obtains from perturbative calculations

$$\alpha_{\rm s}(q) = \frac{g_s^2}{4\pi} \approx \frac{\alpha_s}{1 + (11 - \frac{2}{3}f)\frac{\alpha_s}{2\pi}\ln|\frac{q}{cM}|} \approx \frac{2\pi}{(11 - \frac{2}{3}f)\ln|\frac{q}{\Lambda}|} \tag{5.19}$$

Here M is an arbitrary mass scale and α_s is defined correspondingly in such a way that $\alpha_s(q = Mc) = \alpha_s$. f is the number of quark species with a mass smaller than q/c, for high energies $f = 6$. The constant Λ of the last equality is defined such that $1 = \frac{\alpha_s}{2\pi}(11 - \frac{2}{3}f)\ln(M/\Lambda)$. As $11 - \frac{2}{3}6 = 7 > 0$ the effective strength of the strong interactions **grows** for smaller momenta (i.e., larger distances).

Strong interactions become therefore stronger and stronger at large distances and the perturbative formula (5.19) is not valid any more. The regime where α_s effectively becomes of order 1 is very difficult to calculate analytically but both numerical approaches and analytical arguments suggest that the interactions indeed become so strong that they lead ultimately to the confinement scenario discussed above: only colorless bound states can exist.

Note that the same arguments imply that the strong interactions become less and less important at **high energies**. This phenomenon is called **asymptotic freedom** and it implies that in experiments which probe quarks at very high energies (like the LHC at CERN) the strong interactions become weaker and weaker and can be well described by perturbation theory.

A major success of numerical approaches to QCD (so-called "lattice QCD") was the calculation of the proton mass with the precision of a few percent from direct simulations of $\mathcal{L}_{\rm QCD}$. Despite an enormous recent progress in such numerical approaches, it is still not possible to reach the level of accuracy of QCD predictions which can by achieved for QED from perturbative calculations.

5.6 Electroweak interaction (Glashow-Weinberg-Salam model)

While the SU(3) gauge theory describes the binding of quarks to bound states, it fails to describe another important nuclear reaction, the

β decay of a neutron into a proton, an electron and an antineutrino

$$n \to p + e^- + \bar{\nu}_e$$

Despite this decay channel, the neutron in vacuum has a very long lifetime (compared to nuclear energy scales) of about 15 min. The new particle, the **neutrino**, showing in the equation above, is very difficult to detect directly. Originally, its existence and basic properties have only be revealed by measuring the energies, momenta and spin-orientation of the proton and the electron. Comparing the energy of the initial state to the total energy of proton and electron reveals that one more particle has transported away the energy. Analyzing also the momentum shows that the mass of this particle is very small.

The neutrino is a very light (much lighter than the electron) spin-1/2 particle, which couples neither to the electromagnetic fields nor to the strong forces.
A major surprise was revealed from the analysis of the spin-orientation of the neutrino which can be reconstructed from the conservation of the total angular momentum $\vec{J} = \vec{L} + \vec{S}$. In the β decay and similar nuclear reactions

only **left-handed** neutrinos are produced, with a spin orientation **antiparallel** to the momentum.

This is a very surprising result, especially when one takes into account that under inversion, $\vec{r} \to -\vec{r}$, a left-handed particle is mapped to a right-handed particle. This implies that the laws of nature are **not inversion symmetric**: left and right are **not** equivalent. In particle-physics context, the inversion symmetry is called parity, P. As we will see, P is completely broken by the weak interaction responsible for the β decay.
To understand the math behind the weak interactions, we first analyze the Dirac equation for $m = 0$, given by $i\partial\!\!\!/\Psi = 0$. According to Eq. (3.26) the solutions of the Dirac equations are simply given by

$$\Psi_i^+ = \frac{1}{\sqrt{2|p|}} e^{-ip_\mu x^\mu} \begin{pmatrix} \chi_i \\ \vec{\sigma}\cdot\hat{p}\,\chi_i \end{pmatrix}, \qquad \Psi_i^- = \frac{1}{\sqrt{2|p|}} e^{ip_\mu x^\mu} \begin{pmatrix} \vec{\sigma}\cdot\hat{p}\,\chi_i \\ \chi_i \end{pmatrix} \tag{5.20}$$

It is therefore convenient to choose the spin-quantization axis always parallel to the direction of the momentum $\hat{p}$ such that $\sigma\cdot\hat{p} = \sigma_z$ in this basis. Then, the 4 solutions have the following simple spinor structure

$$\underbrace{\Psi_\uparrow^+ \sim \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}}_{\text{right-handed}}, \quad \underbrace{\Psi_\downarrow^+ \sim \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix}}_{\text{left-handed}}, \quad \underbrace{\Psi_\uparrow^- \sim \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}}_{\text{right-handed}}, \quad \underbrace{\Psi_\downarrow^- \sim \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}}_{\text{left-handed}}, \tag{5.21}$$

The $+$ fields describe particles with spin orientation parallel or antiparallel to the momentum, the $-$ fields the corresponding anti-particles. They are all eigenstates of $\gamma^5 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}$. We can now rewrite the spinor field Ψ in terms of such eigenfunctions of γ^5 using the definition

$$\Psi = \Psi_R + \Psi_L = \frac{1}{\sqrt{2}} \left(\Psi_R^1 \begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix} + \Psi_R^2 \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} + \Psi_L^1 \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} + \Psi_L^2 \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} \right) \tag{5.22}$$

with $\Psi_{R/L} = \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi^1_{R/L} \\ \Psi^2_{R/L} \\ \pm\Psi^1_{R/L} \\ \pm\Psi^2_{R/L} \end{pmatrix}$. With this definition, $\Psi_{R/L}\gamma^5 = \pm\Psi_{R/L}$. This equation is invariant under Lorentz transformations.

We can now rewrite the Lagrange function (5.4) in these new fields. For example the term $\bar{\Psi}\Psi$ can be written as $\Psi^\dagger\gamma^0\Psi = (\Psi^\dagger_R + \Psi^\dagger_L)\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}(\Psi_R + \Psi_L) = \Psi^\dagger_R\Psi_L + \Psi^\dagger_L\Psi_R$.

In the new variable the Lagrange function of the Dirac equation therefore has the form

$$L = \underbrace{\bar{\Psi}_R i\partial\!\!\!/\Psi_R + \bar{\Psi}_L i\partial\!\!\!/\Psi_L}_{\text{conserves chirality}} - m\underbrace{(\Psi^\dagger_R\Psi_L + \Psi^\dagger_L\Psi_R)}_{\text{mixes chirality}} \tag{5.23}$$

After the success of Gauge theories for QED and QCD, we will now try to describe also the weak interaction responsible for the β decay with a gauge theory. The structure of the Gauge theory has to reflect that only left-handed neutrinos are produced in a β decay. In the following we will denote the spinor describing electrons by $e = e_L + e_R$ and the spinor of the electron neutrino by $\nu_e = \nu_{eL} + \nu_{eR}$, each splitted up in the left and right component as defined above.

To obtain a Gauge theory able to describe β-decay, we start from an idea which – at first glance – seems to contradict all experiments drastically. We claim that it is a symmetry operation to "relabel" a left-handed neutrino and a left-handed electron at each point in space time by an SU(2) transformation $U(x)$ according to

$$\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} \to U(x)\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}, \quad e_R \to e_R, \quad \nu_{eR} \to \nu_{eR}, \quad U(x) \in SU(2) \tag{5.24}$$

Note that this symmetry contradicts the obvious experimental fact that an electron and a neutrino have completely different properties – a fact which we will ignore for the moment and explain later when we discuss the Higgs mechanism.

We will now follow precisely the program described in the previous chapter on QCD. The postulate of the Gauge invariance enforces the introduction of corresponding Gauge fields. As a general SU(2) matrix is described by three angles,

$$U(x) = e^{i\sum_{\alpha=1}^{3}\phi_\alpha(x)\tau_i/2}$$

where τ_i are the standard Pauli matrices which act on $\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$. We follow directly the procedure used in the SU(3) case: The postulate of SU(2) gauge invariance enforces the existence of 3 vector potentials, W^α_μ, $\alpha = 1, 2, 3$, $\mu = 0, 1, 2, 3$, one for each SU(2) angle.

We define

$$W_\mu = \sum_{\alpha=1}^{3} W_\mu^\alpha \frac{\tau_\alpha}{2}$$

and the SU(2) field strength tensor

$$W_{\mu\nu} = \partial_\mu W_\nu - \partial_\nu W_\mu + ig[W_\mu, W_\nu]$$

where g is a new coupling constant. Copying Eq. (5.11) and Eq. (5.16), a simultaneous gauge transformation of fields and SU(2) vector potentials leads to

$$\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} \to U(x) \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}, \quad e_R \to e_R, \quad \nu_{eR} \to \nu_{eR}, \quad U(x) \in SU(2)$$

$$W_\mu(x) \to U(x)\, W_\mu(x)\, U(x)^\dagger - \frac{i}{g} U(x) \partial_\mu U^\dagger(x) \tag{5.25}$$

$$D_\mu = \partial_\mu + igW_\mu \to U(x) D_\mu U(x)^\dagger, \qquad W_{\mu\nu} \to U(x) W_{\mu\nu} U(x)^\dagger \tag{5.26}$$

We can also add to this theory an extra U(1) gauge symmetry so that the total gauge symmetry is $SU(2) \times U(1)$. This new U(1) gauge symmetry will *not* be the same gauge symmetry as we discussed for QED but instead we will argue later that QED is a certain subgroup $SU(2) \times U(1)$. To obtain an $SU(2) \times U(1)$ gauge symmetry we have to introduce the new symmetry in such a way that the SU(2) gauge symmetry is not affected. This means that the left-handed doublet $\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$ has to be multiplied with one phase while we can use a different phase factor for the right-handed component. We therefore postulate the Gauge invariance

$$e_R \to e^{i\varphi(x) y_R} e_R, \qquad \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} \to e^{i\varphi(x) y_L} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} \tag{5.27}$$

where y_R and y_L are two constants called *hypercharge*. At the moment y_L and y_R are unknown. We are allowed to fix e.g. y_L by convention but then the hypercharges of all other particles are fixed. Later we will show that $y_L = -\frac{1}{2}$ and $y_R = -1$.
We will name the corresponding vector potential B_μ and the corresponding field strength tensor is by definition

$$B_{\mu\nu} = \partial_\mu B_\nu - \partial_\nu B_\mu$$

The U(1) gauge transformation of the vector potential corresponding to Eq. (5.27) reads

$$B_\mu \to B_\mu - \frac{1}{g'} \partial_\mu \varphi, \qquad B_{\mu\nu} \to B_{\mu\nu}$$

with a new coupling constant g'.

As we now have to cope with two gauge symmetries simultaneously, it is useful to introduce for the gauge-invariant derivative the following notation

$$D_\mu = \partial_\mu + igW_\mu^\alpha T_\alpha + ig' B_\mu Y \tag{5.28}$$

where we define two new operators, Y and T_α by the way they act on the various fields

$$\begin{aligned} Y \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} &= y_L \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}, \qquad Y e_R = y_R e_R, \qquad Y \nu_{eR} = 0 \\ T_\alpha \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} &= \frac{\tau_\alpha}{2} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}, \qquad T_\alpha e_R = T_\alpha \nu_{eR} = 0 \end{aligned} \tag{5.29}$$

All fields are eigenstates of these operators, their only job is to multiply each field with the correct prefactor. Note that we have set the hypercharge of the left-handed electron neutrino, ν_{eR}, to zero (taking the experimental information into account that it interacts with nothing).
We can now write down the full $U(1) \times SU(2)$ gauge theory for the electron, $e = e_L + e_R$, and the electron-neutrino, $\nu_e = \nu_{eL} + \nu_{eR}$,

$$\begin{aligned} \mathcal{L}_{U(1)\times SU(2)} = &-\frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{2} \mathrm{tr}[W_{\mu\nu} W^{\mu\nu}] \\ &+ (\bar{\nu}_{eL}, \bar{e}_L) i\gamma^\mu D_\mu \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} + \bar{e}_R \, i\gamma^\mu D_\mu \, e_R + \bar{\nu}_{eR} \, i\gamma^\mu D_\mu \, \nu_{eR} \end{aligned} \tag{5.30}$$

Whether one adds the right-handed electron neutrino at this stage or not is a question of taste as it couples to nothing and therefore has no experimentally observable effect.
Eq. (5.30) defines a very nice gauge theory. It has only one drawback: it is apparently completely wrong as its prediction contradict completely the properties of nature around us. First of all, the electron and neutrino have very different properties and are definitely not the same: this is obviously not consistent with the SU(2) invariance. The electron also has a mass, described by the term $m\bar{e}_R e_L$ (see Eq. (5.23)) which clearly violates SU(2) invariance as defined above. Furthermore, the theory predicts that there are 4 types of photons – observed is only 1 – and long ranged electroweak interactions with $1/r$ potentials – observed are only short-ranged interactions (we can't use confinement as an excuse here as free electron do exist). It is therefore very obvious that the SU(2) gauge symmetry is not present in nature. Surprisingly, this is not the end of the story: when we add only one more element to the theory, the Higgs mechanism, all these problems will be resolved.

5.7 Higgs mechanism

5.7.1 Spontaneous symmetry breaking and Higgs condensate

As discussed above, the nature around us, definitely does not have a $U(1) \times SU(2)$ symmetry. Here a concept originally coming from solid state physics, **spontaneous symmetry breaking**, turns out to be very useful: The symmetries of a given state of matter do **not** have to be the same as the symmetries of the laws of nature.[5] A magnet, for example, where the magnetization points in a certain direction is not rotationally invariant. Any crystal breaks translational symmetry. This occurs despite the fact that the laws of nature responsible for forming the magnet or the crystal do have rotation and translation symmetry. Similarly, it can happen that our theory (i.e., the Lagrange function) has a SU(2) symmetry but the vacuum, describing the world around us, does **not** have this symmetry. To capture this effect, a new field has to be introduced: the Higgs field.
The Higgs field is a two-component complex field

$$\Phi = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}$$

Under the previously discussed SU(2) and U(1) gauge transformations (Φ has no color and does not transform under SU(3)) it transforms as

$$\begin{aligned} &\Phi \to U(x)\Phi, \qquad U(x) = e^{i\sum_{\alpha=1}^{3}\phi_\alpha(x)\tau_\alpha} \in SU(2) \\ &\Phi \to e^{i\varphi(x)y_H}\Phi, \qquad e^{i\varphi(x)y_H} \in U(1) \end{aligned} \tag{5.31}$$

where the hypercharge of the Higgs field, y_H with $Y\Phi = y_H\Phi$, will be determined below. The Lagrange density describing the Higgs field is given by

$$\mathcal{L}_H = (D_\lambda \Phi^\dagger)(D^\lambda \Phi) - V(\Phi^\dagger\Phi) \tag{5.32}$$

$$V(\Phi^\dagger\Phi) = -\frac{1}{2}\mu\Phi^\dagger\Phi + \frac{1}{4}\lambda(\Phi^\dagger\Phi)^2 \tag{5.33}$$

where D_λ is usual gauge-invariant derivative. The first part of the action is well-known from the Klein-Gordon equation, see Eq. (5.3). The **Higgs potential** V is, however, a new element. It is chosen in such a way, that it enforces spontaneous symmetry breaking. As shown in Fig. 5.1, its minimum is **not** at $\Phi = (0, 0)$ but for $\mu > 0$ it is located at

$$\Phi^\dagger\Phi = \frac{\mu}{\lambda}.$$

[5] A bit of care has to be used when describing the spontaneous symmetry breaking of Gauge theories as Gauge degrees of freedom are in principle unobservable. This is, however, at the end only a minor technical issue of no relevance for our discussion.

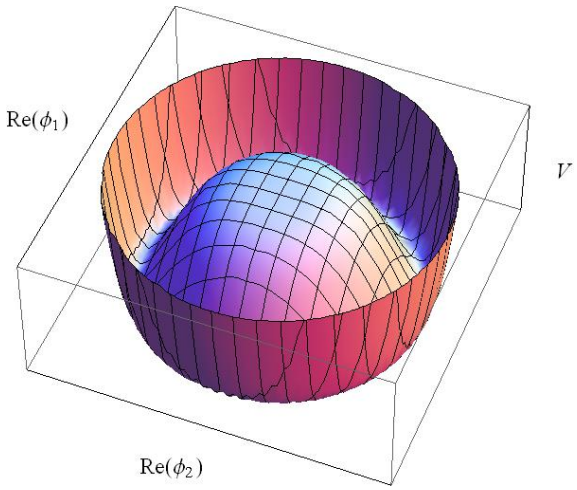


Figure 5.1: The Higgs potential plotted as the function of ReΦ_1 and ReΦ_2 (for ImΦ_1 = Im $\Phi_2 = 0$. Note that the minimum is at a finite field thus breading the U(1) $\times$ SU(2) symmetry partially. The potential is sometimes described as a Mexican-hat potential.

A given minimum configuration of the field selects a state which does not have the full U(1) $\times$ SU(2) symmetry.

We will dicuss the consequences later, we first complete the discussion of the Lagrange function: the **Yukawa coupling** describing how the Higgs field interacts with the electron and neutrino. The corresponding Lagrange function has to fulfill three requirements: it has to obey tbe U(1) $\times$ SU(2) gauge symmetry, has to be Lorentz invariant and has to contain an even number of fermionic fields as the Lagrange density is just a number while fermions anticommute. The simples term which obeys all these conditions is given by

$$\mathcal{L}_{\text{Yuk}} = -c_e\, \bar{e}_R \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}^{\dagger} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} + h.c. \tag{5.34}$$

where c_e is just a numerical coupling constant. Let us check the invariance of this term. First, it is obviously SU(2) invariant as it couples $\Phi^{\dagger}$ to the SU(2) doublet $\begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$. Second, it is Lorentz invariant as it couples the spinor index of ν_{eL} and of e_L to the spinor index of $\bar{e}_R$ and we already know that such a combination is Lorentz invariant. It also contains an even number of fermionic fields. We have, however, still to check the U(1) symmetry related to the hypercharge. Under such a transformation

$$\mathcal{L}_{\text{Yuk}} \rightarrow \mathcal{L}_{\text{Yuk}} e^{i\varphi(y_L - y_R - y_H)}$$

If we want that such a term is present (later we will show that it gives rise to the mass of the electron), we therefore conclude that

$$y_H = y_L - y_R \tag{5.35}$$

Using the values $y_L = -1/2$ and $y_R = -1$, determined below, we obtain $y_H = \frac{1}{2}$. Combining all terms, we obtain the U(1) × SU(2) **Higgs model**.

$$\mathcal{L} = \mathcal{L}_{U(1)\times SU(2)} + \mathcal{L}_{\text{Yuk}} + \mathcal{L}_H \tag{5.36}$$

What are the consequences of the fact that the Higgs potential has a minimum at a finite value of the field? It implies that the expectation value of the Higgs field $\langle\Phi\rangle = \langle 0|\Phi|0\rangle$ is finite even for the groundstate of the field theory which is the vacuum $|0\rangle$ of our universe. We can parametrize the field configurations at the minimum by

$$\langle\Phi\rangle = e^{i\varphi_0(x)} U_0(x) \begin{pmatrix} 0 \\ \rho_0/\sqrt{2} \end{pmatrix}, \qquad e^{i\varphi_0(x)} \in U(1), U(x) \in SU(2)$$

where ϕ_0 and U_0 are arbitrary. Ignoring quantum fluctuations, by minimizing the Higgs potential (5.33), we have $\rho_0/\sqrt{2} = \frac{\mu}{\lambda}$ for $\mu > 0$ (the $\sqrt{2}$ factor is just a convention). At this point it is convenient to fix that gauge and choose one where

$$\langle\Phi\rangle = \begin{pmatrix} 0 \\ \rho_0/\sqrt{2} \end{pmatrix} = const. \tag{5.37}$$

One can compare this to a magnet, where $\langle\vec{M}\rangle$ is finite in the ground state. Fixing the direction of $\langle\vec{M}\rangle$ means that for this specific groundstate, the system does not have the full symmetry any more. We have given more careful discussion of spontaneous symmetry breaking and why it is a useful concept in the chapter on Bose-Einstein condensation: we encourage the reader to study again the arguments given there. In analogy to the Bose Einstein condensation one calls $\langle\Phi\rangle$ **Higgs condensate**.

> **recapitulate:** Spontaneous symmetry breaking, BEC, chapter 1.5.1

Before proceeding, it is useful to analyze the symmetries of the theory for fixed $\Phi \propto (0, 1)$. Obviously, part of the $U(1) \times SU(2)$ symmetry is gone, but a subgroup survives. The transformation

$$\begin{pmatrix} 0 \\ \frac{\rho_0}{\sqrt{2}} \end{pmatrix} \to \begin{pmatrix} e^{i\varphi(x)} & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ \frac{\rho_0}{\sqrt{2}} \end{pmatrix} = \exp\left[i\varphi(x) \left(\frac{\tau_z}{2} + \frac{1}{2y_H} Y \mathbb{1} \right) \right] \begin{pmatrix} 0 \\ \frac{\rho_0}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{\rho_0}{\sqrt{2}} \end{pmatrix}$$

does not affect the Higgs condensate.
This implies that despite the spontaneous symmetry breaking a certain U(1) subgroup of U(1) × SU(2) is still intact.

The U(1) subgroup of gauge transformations of the form $e^{i\varphi(x)Q}$ with $Q = T_z + \frac{1}{2y_H}Y$ is unaffected by the condensation of the Higgs field. This U(1) gauge symmetry gives rise to electromagnetism and Q is the electromagnetic charge.

We will work this out in more detail below, but as a first check we investigate how the new operator $Q = T_z + \frac{1}{2y_H}Y$ affects the electron using the definitions in Eq. (5.29):

$$Qe_R = (0 + \frac{y_R}{2y_H})e_R, \quad Qe_L = (-\frac{1}{2} + \frac{y_L}{2y_H})e_L, \quad Q\nu_{eL} = (+\frac{1}{2} + \frac{y_L}{2y_H})\nu_{eL}$$

Using that $y_H = y_L - y_R$, Eq. (5.35), we now use the experimental result that the neutrino does **not** have a charge, therefore $\frac{1}{2} + \frac{y_L}{2(y_L - y_R)} = 0$ equivalent to $y_L = \frac{y_R}{2}$. Therefore $y_H = \frac{y_R}{2} - y_R = -\frac{y_R}{2}$. As mentioned above, we are free to choose an arbitrary value for y_R, e.g., $y_R = -\frac{1}{2}$. We conclude that

$$Q = T_z + Y, \qquad Qe_R = -e_R, \quad Qe_L = -e_L, \quad Q\nu_{eL/R} = 0 \tag{5.38}$$

The charge of the electron with respect to the remaining U(1) symmetry is therefore -1 in our units, while the neutrino does not have a charge.

5.7.2 Massive gauge fields, electron mass and Higgs particle

It is not difficult to derive the effective action in the presence of the Higgs condensate. Technically, one can just do a straightforward Taylor expansion of all fields taking the Higgs condensate as the leading term. We will not follow this brute force strategy but instead take a look at the most important terms.

First, an obvious first task is to identify the electromagnetic fields and the corresponding vector potential. As $Q = T_z + Y$, we expect that the vector potential is a linear combination of W^3_μ and B_μ responsible for the Gauge transformations generated by T_z and Y, respectively. We introduce two orthogonal linear contributions

$$A_\mu = \cos\theta_W B_\mu + \sin\theta_W W_\mu, \qquad Z_\mu = -\sin\theta_W B_\mu + \cos\theta_W W_\mu \tag{5.39}$$

where the **Weinberg angle**, θ_W, is determined by rewriting D_μ in the new fields.

$$D_\mu = \partial_\mu + igW^a_\mu T_a + ig'B_\mu Y = \partial_\mu + iA_\mu(g\sin\theta_W T_z + g'\cos\theta_W Y) + \cdots \equiv \partial_\mu + iA_\mu q_e Q + \ldots$$

where $-q_e$ is the electron charge. The last equality hold only for $g\sin\theta_W = g'\cos\theta_W = q_e$, equivalent to

$$\tan\theta_W = \frac{g'}{g}, \qquad q_e = \frac{gg'}{\sqrt{g^2 + g'^2}}$$

The combination Z_μ in Eq. (5.39) defines the **Z boson**. The action for the photon, $\mathcal{L}_{\text{photon}} = -\frac{1}{4}F_{\mu\nu}F^{\mu\nu}$ can easily be extracted by rewriting $\mathcal{L}_{U(1)\times SU(2)}$ in the new fields.
Second, we investigate the consequence of the term $D_\lambda\Phi^\dagger D^\lambda\Phi$ in Eq. (5.32) evaluated by replacing the Higgs field by its condensate, $\langle\Phi\rangle = \begin{pmatrix} 0 \\ \rho_0/\sqrt{2} \end{pmatrix}$.

$$D_\lambda\langle\Phi^\dagger\rangle D^\lambda\langle\Phi\rangle = \frac{1}{4}g^2\rho_0^2\left(W_\lambda^1 W^{1\lambda} + W_\lambda^2 W^{2\lambda}\right) + \frac{g^2+g'^2}{8}\rho_0 Z_\lambda Z^\lambda$$

Instead of discussing the two real fields W^1 and W^2, one often introduces the complex fields $W^{+/-} = W^1 \pm iW^2$.
The physical consequences of these terms can be seen by realizing that the new terms have just the form of a mass term in the Klein-Gordon Lagrange function, Eq. (5.3).

The W bosons and the Z bosons become massive particles

$$m_W^2 = \frac{g^2}{4}\rho_0^2, \qquad m_Z^2 = \frac{g^2+g'^2}{4}\rho_0^2, \tag{5.40}$$

while the photon field A_λ remains massless.

An important prediction of the Higgs mechanism is that the ratio of the masses of the Z boson and the W bosons is given by

$$\frac{m_W}{m_Z} \approx \cos\theta_W$$

To understand better the effect of the mass terms, we can consider how a mass term modifies the equation for a potential Φ (to be identified, for example, with Z_0) in the presence of a static point charge at the origin

$$(-\nabla^2 + m^2)\Phi = 4\pi\delta^3(\vec{r}) \quad \Rightarrow \quad \Phi(r) = \frac{1}{r}e^{-mr}$$

which can be, for example, be derived by Fourier transformation. We conclude

Interactions mediated by the $W^\pm$ and Z bosons are short ranged and decay on the length scale $\hbar/(m_W c)$ and $\hbar/(m_Z c)$. Only the Coulomb interaction mediated by the photon is long ranged.

The mass of the Z and W bosons are approximately 91 GeV and 80 GeV, respectively, almost 100 times more heavy than a proton. Correspondingly, the length scale of weak interactions is extremely short, of the order of about 10^{-18} m, much shorter than, e.g., the radius of a proton.
Next, we analyze the Yukawa coupling, Eq. (5.34) by replacing again Φ by its expectation value $\begin{pmatrix} 0 \\ \rho_0/\sqrt{2} \end{pmatrix}$. We obtain directly

$$\mathcal{L}_{\text{Yuk}} \approx -\frac{c_e \rho_0}{\sqrt{2}} \left(\bar{e}_R\, e_L + \bar{e}_L\, e_R\right)$$

The electron obtains a mass term proportional to the Higgs condensate and the Yukawa coupling c_e

as can be seen by comparing this term to Eq. (5.23).

Due to the spontaneous symmetry breaking the electron and neutrino have very different properties. Most importantly,

only the electron interacts with the electromagnetic field ($Q\nu_e = 0$) and only the electron obtains a mass from the Yukawa coupling c_e

One can ask what would have happened if we had chosen a different value for the condensate of the Higgs, e.g. $\frac{\rho_0}{\sqrt{2}} \begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix}$ with arbitrary α. Due to the SU(2) invariance, this has to give the same physics: in this case the field of the physical left-handed electron would be given by $\begin{pmatrix} \cos\alpha \\ \sin\alpha \end{pmatrix} \cdot \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$ instead of e_L.

The last step of our analysis is to investigate excitations of the Higgs field itsself which is described by fluctuations of the Higgs field around its minimum. Here it is convenient to choose a gauge in such a way that

$$\vec{\Phi}(x) = \begin{pmatrix} 0 \\ \frac{\rho_0 + \tilde{\rho}(x)}{\sqrt{2}} \end{pmatrix}$$

with a field $\tilde{\rho}(x)$ which is purely real for the chosen gauge. In its quantized form, this field will describe the **Higgs particle**. In Fig. 5.1 the Higgs particle corresponds to a fluctuation perpendicular to the minimum of the potential.

To proceed, one just has to expand the Lagrange density (5.36) in $\tilde{\rho}(x)$. Collecting all terms quadratic in $\tilde{\rho}$ we obtain

$$\mathcal{L}_{\text{Higgs-particle}} = \frac{1}{2} D_\mu \tilde{\rho}\; D^\mu \tilde{\rho} - \frac{1}{2} m_H^2\; \tilde{\rho}^2, \qquad m_H^2 = 2\lambda\rho_0^2 \tag{5.41}$$

which is the field theory for a massive bosonic particle with the mass m_H. The Higgs mass is determined by the curvature of the Higgs potential at its minimum, see Fig. 5.1. This is the celebrated Higgs particle. It interacts with the electron (and other fermions) through the Yukawa coupling (5.34).

Written in the new fields, our original U(1)× SU(2) gauge theory with Higgs field has in the symmetry-broken phase the form

$$\mathcal{L} = \mathcal{L}_{\text{photon}} + \mathcal{L}_{W^\pm,Z} + \mathcal{L}_{e,\nu} + \mathcal{L}_{\text{Higgs-particle}} + \mathcal{L}_{\text{couplings}}$$

describing the (massless) photon, the massive $W^\pm$ and Z bosons, a massive electron and a neutrino (massless in the present approximation) and a Higgs particle plus their coupling

which includes scattering processes of Higgs particles and of Higgs particles with electrons and neutrinos.
We will add all the other fields from a standard model in the next chapter. Before doing so, it is useful to make a count of the *bosonic* degrees of freedom in the system (here we consider the electroweak theory only, omitting QCD):
If there were no symmetry breaking (a negative parameter μ in Eq. (5.33)), we can count: $1 + 3$ Gauge fields, each contribution 2 phonon-like degrees of freedom (there are two polarizations of light), two complex Higgs fields corresponding to 4 real degrees of freedom gives in total $(1 + 3) \cdot 2 + 2 \cdot 2 = 12$ bosonic degrees of freedom to which the massless fermions have to be added. In the symmetry broken phase in contrast, the massive $W^{\pm}$ and Z bosons contribute with three degrees of freedom each (they are spin-1 particles, and all Gauge freedom is gone after we fixed the Gauge for the Higgs particle). The photon has still two polarization directions and we have now one Higgs particle. We therefore count again $3 \cdot 3 + 2 + 1 = 12$ bosons plus the fermions.

5.8 The standard model

5.8.1 Leptons, gauge fields and Higgs field

In the previous chapters, we have discussed the Higgs mechanism, the electroweak interaction with electron and neutrino and the strong interactions with the quarks. The only step left is to combine all aspects of the theory adding a few missing particles (the muon, the tau and the corresponding neutrinos).
The main defining element of the standard model are the

$$\text{Gauge symmetries: } U(1) \times SU(2) \times SU(3)$$

These gauge symmetries enforce the existence of gauge fields, one for angle ϕ parametrizing elements of the group.

$$\text{1+3+8 gauge fields:} \qquad B_\mu, \qquad W_\mu^\alpha,\ \alpha = 1, 2, 3, \qquad G_\mu^\alpha,\ \alpha = 1, \ldots, 8$$

where $\mu = 0, 1, 2, 3$ is a Lorentz index. The G fields describes 8 types of gluons while a combination of the B and W fields encodes the photon, the $W^{\pm}$ and Z bosons.
For the Gauge fields, one defines the **field strength tensors**

$$\begin{aligned}
B_{\mu\nu} &= \partial_\mu B_\nu - \partial_\nu B_\mu \\
W_{\mu\nu} &= \partial_\mu W_\nu - \partial_\nu W_\mu + ig[W_\mu, W_\nu], \qquad W_\mu = \sum_{\alpha=1}^{3} W_\mu^\alpha \frac{\tau_\alpha}{2} \\
G_{\mu\nu} &= \partial_\mu G_\nu - \partial_\nu G_\mu + ig_s[W_\mu, W_\nu], \qquad G_\mu = \sum_{\alpha=1}^{8} W_\mu^\alpha \frac{\lambda_\alpha}{2}
\end{aligned}$$

Here τ_α are the 3 Pauli matrices generating SU(2) while λ_α are the corresponding matrices generating SU(3) (see chapter 5.5.2). For each gauge symmetry, there is one coupling constant

coupling constants: g' of U(1), g of SU(2), g_s of SU(3).

The **gauge invariant derivative** D_μ will be written in the form

$$D_\mu = \partial_\mu + ig'\, B_\mu\, Y + ig \sum_{\alpha=1}^{3} W_\mu^\alpha\, T^\alpha + ig_s \sum_{\alpha=1}^{8} G_\mu^\alpha\, F^\alpha$$

where we introduced charge operators Y, T^α and G^α. The operator F^α is given by $\frac{\lambda_\alpha}{2}$ whenever it acts on a quark field and is zero otherwise. How the hypercharge operator Y acts on various fields is described below. The operator T^α acting on all doublets (defined below) of fields as $\frac{\tau_\alpha}{2}$ and gives zero otherwise.

All fermions of the standard model are spin-$\frac{1}{2}$ particles described by 4 component spinors which are each split into a left-handed and a right-handed component. They are called **leptons** and can be grouped into **three families** (or three **generations**): for unknown reason nature has provided three versions of all fermionic fields with identical quantum numbers but vastly different masses. Each family consists of two types of quarks (each coming in three colors, two spin directions and as particle and antiparticle), and two fermions, one electron-like particle and one neutrino (each again with two spin-direction, particle and antiparticle). The left-handed fields are always grouped in doublets which couple to the SU(2) gauge transformation and right-handed singlets not affected by SU(2). They can be ordered in a table:

The three lepton families (also called generations):

			T^3	Y	$Q = T^3 + Y$
$\begin{pmatrix}\nu_{eL}\\ e_L\end{pmatrix}$	$\begin{pmatrix}\nu_{\mu L}\\ \mu_L\end{pmatrix}$	$\begin{pmatrix}\nu_{\tau L}\\ \tau_L\end{pmatrix}$	$1/2$ $-1/2$	$-\frac{1}{2}$	0 -1
e_R	μ_R	τ_R	0	-1	-1
ν_{eR}	$\nu_{\mu R}$	$\mu_{\tau R}$	0	0	0
$\begin{pmatrix}u_L\\ d_L\end{pmatrix}$	$\begin{pmatrix}c_L\\ s_L\end{pmatrix}$	$\begin{pmatrix}t_L\\ b_L\end{pmatrix}$	$1/2$ $-1/2$	$\frac{1}{6}$	$2/3$ $-1/3$
u_R	c_R	t_R	0	$2/3$	$2/3$
d_R	s_R	b_R	0	$-1/3$	$-1/3$
electron e-neutrino up-quark down-quark	muon μ μ-neutrino charm-quark strange-quark	tau τ τ-neutrino top-quark bottom-quark			

The muon and tau are heavier copies of the electron and are accompanied each by an extra neutrino. The last three columns show how the SU(2) generator T^3 and the hypercharge

operator Y acts on the fields. The electromagnetic charge is given by $Q = T^3 + Y$ and is shown in the last column. While all neutrinos have charge 0 and the electron-like particles have charge -1, the quarks have either charge $2/3$ or charge $-1/3$. This guarantees that bound states of three quarks always have integer charges, as observed experimentally. Antiparticle have always the opposite charge of the particle. Therefore all quark-antiquark pairs have either charge 0 or charge ± 1 as $\frac{2}{3} - \left(-\frac{1}{3}\right) = 1$.

A special role is played by the **Higgs field** $\Phi = \begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}$, a doublet of complex fields which also couples to the SU(2) gauge transformations with the quantum numbers given by the table

		T_3	Y	$Q = T_3 + Y$
Higgs field	$\begin{pmatrix} \Phi_1 \\ \Phi_2 \end{pmatrix}$	$1/2$	$\frac{1}{2}$	1
		$-1/2$		0

When we identified the particles and their charges in the two tables given above, we implicitly assumed that we use a gauge where the Higgs condensate, the expecation value of the Higgs field in the vacuum has the form $\langle \Phi \rangle = \begin{pmatrix} 0 \\ \rho_0/\sqrt{2} \end{pmatrix}$. With this convention the Higgs particle is an excitation of the lower component and therefore carries the electric charge 0. The Higgs is the only bosonic degree of freedom in the standard model besides the Gauge bosons.

To write down the Lagrange function of the standard model, it is convenient to group all fermionic fields (i.e., all leptons) into one big field

$$\Psi = (\nu_{eL}, e_L, e_R, \nu_{eR}, u_L^1, u_L^2, u_L^3, d_L^1, d_L^2, d_L^3, \dots)$$

In total, these are

$$(2 \cdot 2 + 2 \cdot 2 + 3 \cdot 2 \cdot 2 \cdot 2) \cdot 3 = 96 \text{ lepton fields}$$

and therefore types of particles (each lepton comes with two spin-orientations, all quarks carry three colors).

We can finally (rolling drums) write down the Lagrange density which defines the **standard model** of particle physics in its full glory

$$\begin{aligned} \mathcal{L}_{\text{SM}} = & -\frac{1}{4} B_{\mu\nu} B^{\mu\nu} - \frac{1}{2} \text{tr}[W_{\mu\nu} W^{\mu\nu}] - \frac{1}{2} \text{tr}[G_{\mu\nu} G^{\mu\nu}] \\ & + \bar{\Psi}\, i\gamma^\mu D_\mu\, \Psi + (D_\mu \Phi)(D^\mu \Phi) - V(\Phi^\dagger \Phi) + \mathcal{L}_{\text{Yuk}} \end{aligned} \tag{5.42}$$

with the Higgs potential $V = -\frac{1}{2}\mu \Phi^\dagger \Phi^\dagger + \frac{1}{4}\lambda (\Phi^\dagger \Phi)^2$. The first line gives the Lagrange density of all gauge fields (i.e., the generalized Maxwell's equations). The coupling of the gauge fields to the other fields is fixed by the principles of gauge invariance. With the

exception of the Yukawa couplings just 5 numbers $(g, g', g_S, \mu, \lambda)$ determine all interactions and the properties of the strong and electroweak interactions.

5.8.2 Yukawa coupling

Unfortunately, the last missing part, the Yukawa coupling, $\mathcal{L}_{\text{Yuk}}$, is less universal and a bit more complicated. It describes the coupling of the leptons to the Higgs field and is responsible for the mass of the leptons. It is obtained by writing down all cubic coupling terms allowed by the gauge symmetries.

$$\begin{aligned}\mathcal{L}_{\text{Yuk}} = &- (\bar{e}_R, \bar{\mu}_R, \bar{\tau}_R)\, \mathbf{C_e} \begin{pmatrix} \Phi^\dagger \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} \\ \Phi^\dagger \begin{pmatrix} \nu_{\mu L} \\ \mu_L \end{pmatrix} \\ \Phi^\dagger \begin{pmatrix} \nu_{\tau L} \\ \tau_L \end{pmatrix} \end{pmatrix} + (\bar{\nu}_{eR}, \bar{\nu}_{\mu R}, \bar{\nu}_{\tau R})\, \mathbf{C'_e} \begin{pmatrix} \Phi^T \boldsymbol{\epsilon} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} \\ \Phi^T \boldsymbol{\epsilon} \begin{pmatrix} \nu_{\mu L} \\ \mu_L \end{pmatrix} \\ \Phi^T \boldsymbol{\epsilon} \begin{pmatrix} \nu_{\tau L} \\ \tau_L \end{pmatrix} \end{pmatrix} \\ &- (\bar{d}_R, \bar{s}_R, \bar{b}_R)\, \mathbf{C_q} \begin{pmatrix} \Phi^\dagger \begin{pmatrix} u_L \\ d_L \end{pmatrix} \\ \Phi^\dagger \begin{pmatrix} c_L \\ s_L \end{pmatrix} \\ \Phi^\dagger \begin{pmatrix} t_L \\ b_L \end{pmatrix} \end{pmatrix} + (\bar{u}_R, \bar{c}_R, \bar{t}_R)\, \mathbf{C'_q} \begin{pmatrix} \Phi^T \boldsymbol{\epsilon} \begin{pmatrix} u_L \\ d_L \end{pmatrix} \\ \Phi^T \boldsymbol{\epsilon} \begin{pmatrix} c_L \\ s_L \end{pmatrix} \\ \Phi^T \boldsymbol{\epsilon} \begin{pmatrix} t_L \\ b_L \end{pmatrix} \end{pmatrix} + h.c.\end{aligned} \tag{5.43}$$

The Yukawa coupling mixes the fields from the three families. This mixing is described by the four 3×3 matrices $\mathbf{C_e}$, $\mathbf{C'_e}$, $\mathbf{C_q}$ and $\mathbf{C'_q}$ (we will discuss below, that there is some freedom in choosing those matrices). The $\boldsymbol{\epsilon}$ in $\mathcal{L}_{\text{Yuk}}$ is the two-component ϵ-tensor with $\boldsymbol{\epsilon} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$. For example, $\Phi^T \boldsymbol{\epsilon} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} = (\Phi_1, \Phi_2) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} = \Phi_1 e_L - \Phi_2 \nu_{eL}$. We should check whether all terms in $\mathcal{L}_{\text{Yuk}}$ are gauge invariant. First, they are invariant under SU(3) as all quark fields only occur in combinations like $\bar{q}_i q_j = \sum_{\alpha=1}^{3} \bar{q}_i^\alpha q_j^\alpha$ where α is the color index. Second, all terms are invariant under SU(2). This is obvious for the combinations like $\Phi^\dagger \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$ which transforms under a SU(2) gauge transformation to $\Phi^\dagger U(x)^\dagger U(x) \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix} = \Phi^\dagger \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$. But also the combination $\Phi^T \boldsymbol{\epsilon} \Phi^\dagger \begin{pmatrix} \nu_{eL} \\ e_L \end{pmatrix}$ is gauge invariant as $U(x)^T \boldsymbol{\epsilon}\, U(x) = \boldsymbol{\epsilon} \det U(x) = \boldsymbol{\epsilon}$. Finally, we have to check the invariance under U(1) hypercharge transformations $e^{i\varphi Y}$. The first term in $\mathcal{L}_{\text{Yuk}}$ transforms as $\exp[i\varphi(-(-1) - \frac{1}{2} - \frac{1}{2})] = 1$ and also the other terms are invariant under this $U(1)$ transformations ($0 + \frac{1}{2} - \frac{1}{2} = 0$, $\frac{1}{3} - \frac{1}{2} + \frac{1}{6} = 0$, $-\frac{2}{3} + \frac{1}{2} + \frac{1}{6} = 0$). Moreover, it is not possible

to invent other products of three fields which are also gauge invariant. Therefore $\mathcal{L}_{\text{Yuk}}$ is the most general Yukawa coupling which one can write down.
An important element of the standard model is, see Sec. 5.7, the

$$\text{spontaneous symmetry breaking: } \langle\Phi\rangle = \begin{pmatrix} 0 \\ \rho_0/\sqrt{2} \end{pmatrix}$$

Instead of the full symmetry of the gauge group $U(1) \times SU(2) \times SU(3)$ only a symmetry of the form $U(1) \times SU(3)$ survives. As discussed in Sec. 5.7, this induces a mass for three of the Gauge bosons (the $W^{\pm}$ and the Z) and is responsible, e.g., only the electron has an electromagnetic charge but not the neutrino and also for the fact that left-handed up- and down quarks have different properties. It also gives rise to the mass of the leptons, as we can see when replacing Φ by $\langle\Phi\rangle$. We obtain

$$\begin{aligned}\mathcal{L}_{\text{Yuk}} \approx &- (\bar{e}_R, \bar{\mu}_R, \bar{\tau}_R) \frac{\rho_0}{\sqrt{2}} \mathbf{C_e} \begin{pmatrix} e_L \\ \mu_L \\ \tau_L \end{pmatrix} - (\bar{\nu}_{eR}, \bar{\nu}_{\mu R}, \bar{\nu}_{\tau R}) \frac{\rho_0}{\sqrt{2}} \mathbf{C'_e} \begin{pmatrix} \nu_{eL} \\ \nu_{\mu L} \\ \nu_{\tau L} \end{pmatrix} \\ &- (\bar{d}_R, \bar{s}_R, \bar{b}_R) \frac{\rho_0}{\sqrt{2}} \mathbf{C_q} \begin{pmatrix} d_L \\ s_L \\ b_L \end{pmatrix} - (\bar{u}_R, \bar{c}_R, \bar{t}_R) \frac{\rho_0}{\sqrt{2}} \mathbf{C'_q} \begin{pmatrix} u_L \\ c_L \\ t_L \end{pmatrix} + h.c. \quad (5.44)\end{aligned}$$

The four terms give the mass for the electron-like particles, e, μ, τ, the corresponding neutrinos, the d, s, b quarks with electric charge $-1/3$ and for the remaining u, c, t quarks with charge $2/3$.
When interpreting $\mathcal{L}_{\text{SM}}$ and the matrices $\mathbf{C_e}, \mathbf{C'_e}, \mathbf{C_q}, \mathbf{C'_q}$, we have to realize that up to now, we have not yet properly defined the fields of the standard model! We can, for example, rename fields and introduce new variables, for example, by a unitary transformation affecting the three families $\begin{pmatrix} e_L \\ \mu_L \\ \tau_L \end{pmatrix} \to U_0 \begin{pmatrix} e_L \\ \mu_L \\ \tau_L \end{pmatrix}$, $U_0 \in SU(3)$. This is **not** a gauge transformation, U_0 is just a constant matrix. **If** we simultaneously transform also the left-handed neutrinos with the same matrix U_0, the transformation will not affect any of the terms of the standard model besides the Yukawa coupling. We can use this freedom, to diagonalize, e.g., the matrix $\mathbf{C_e}$. Indeed the electron, muon and tau are **defined** to be the eigenstate of $\mathbf{C_e}$ with the smallest, the second largest and the largest eigenvalue. Without any loss of generality, we can therefore **choose the matrices $\mathbf{C_e}$ and $\mathbf{C_q}$ to be diagonal**.
The remaining two matrices, $\mathbf{C'_e}$ and $\mathbf{C'_q}$, **cannot** be diagonalized without affecting other terms of $\mathcal{L}_{\text{SM}}$. If one, for example, diagonalizes $\mathbf{C'_q}$ (i.e, if one uses mass eigenstates for the quarks), one has to pay the prize, that now the coupling of quarks by the $W^{\pm}$ bosons is described by a 3×3 matrix (the Cabibbo-Kobayashi-Maskawa or, short, CKM matrix).
We briefly discuss two important consequences of the mass matrices. In the most important nuclear process in the sun, four protons effectively merge into on α-particle (a ^{4}He nucleus)

made from two protons and two neutrons. Two neutrinos are generated in this process. As one knows the amount of energy generated by the sun, one can reliably calculate how many neutrinos should arrive here on earth coming from the sun. Surprisingly, only 50% of those are measured. The explanation for this striking result is not difficult: the matrix $\mathbf{C'_q}$ mixes left-handed and right-handed neutrinos: a left-handed neutrino generated in the sun oscillates back and forth between a right-handed and left-handed version. On average, 50% of the neutrinos arrive the neutrino detectors in their right-handed version which cannot trigger any electroweak scattering event and therefore remain undetected. In older versions of the standard model, the matrix C'_e was omitted because at that time experiments were compatible with a vanishing mass of the neutrinos. Even today, often the neutrino masses and oscillations are considered as being "beyond the standard model". We follow, however, the philosophy that the matrix $\mathbf{C'_e}$ is naturally part of the standard model.
Another remarkable aspect is that the Yukawa coupling matrices $\mathbf{C'_e}$ and $\mathbf{C'_q}$ can have – and actually do have – entries which are complex and one cannot remove the imaginary part of $\mathcal{L}_{\rm SM}$ by any basis transformation. This can only occur if there are three or more lepton families. A consequence of this imaginary entries is that

the standard model is **not** invariant under time reversal, T.

Surprisingly, the microscopic time reversal symmetry which we know well from most laws of physics (Schrödinger, Dirac, Maxwell, ... equations) is apparently only an approximation. The violation of T is only an extremely tiny effect at low energies as it only occurs in processes where the third and heaviest lepton family is involved.

recapitulate: Lorentz group, chapter 3.2, and symmetries of Dirac equation, chapter 3.6.

It is worthwhile to study three discreet symmetries: time reversal symmetry T, the inversion of space P and a transformation of particles to antiparticles, C (see chapter 3.6). We have seen that P is maximally broken by weak processes like the β decay, which are, however, symmetric under the product CP. The so-called **CPT theorem** going back to Wolfgang Pauli states that any causal, local, Lorentz invariant quantum field theory has to be symmetric under the product CPT: the laws of nature do not change when one simultaneously reverses the arrow of time, replaces particles by antiparticles and does an inversion of space such that left-handed particles become right-handed particles. As CPT is a symmetry of $\mathcal{L}_{\rm SM}$ and T is not a symmetry, also the CP symmetry is absent when considering the mixing of the three quark families.

5.9 Outlook and concluding remarks

In 2012 the Higgs particle was discovered at CERN in Geneva and in 2013 the theoreticians Englert and Higgs have been awarded the Nobel prize *"for the theoretical discovery*

of a mechanism that contributes to our understanding of the origin of mass of subatomic particles, and which recently was confirmed through the discovery of the predicted fundamental particle, by the ATLAS and CMS experiments at CERN's Large Hadron Collider".
Remarkably, the Higgs particle has all the properties expected from the standard model, and thus its discovery is a spectacular success of the standard model. Here it is useful to make a careful distinction between the Higgs mechanism (spontaneous symmetry breaking, mass generation for gauge fields) and the existence of the Higgs particle. While the Higgs mechanism was well established before the 2012 discoveries, it was much less clear whether the mechanism for symmetry breaking has anything to do with something like a Higgs field and whether something like a Higgs particle does indeed exist. Here it is worthwhile to compare the situation to superconductors: it turns out that superconductivity is a realization of the Higgs mechanism (spontaneous symmetry breaking giving rise to a mass of the photon) but in most superconductors an analog of the Higgs particle does not exist.
The success of the standard model is really impressive: with the exception of phenomena related to gravity it is believed to explain each and every experiment ever done on earth. Beautifully, its structure is to a large extent fixed by simple symmetry principles (Lorentz invariance and the gauge symmetries $U(1)\times SU(2)\times SU(3)$). Nevertheless, some aspects of it are less satisfying. There are 25 free parameters (20 thereof arising from the Yukawa coupling) which appear to be completely arbitary.[6] What determines their values? Why are electrons a million times heavier than neutrinos? Why is the top quark 100.000 times larger than the mass of an up quark? Why are all these energy scales a factor 10^{16} smaller than the Planck energy, the energy scale believed to govern quantum gravity? Equivalently, why is the weak force a factor 10^{32} larger than gravitational forces? Such questions are referred to as the hierarchy problem. Looking at the world around us, it is difficult to reconcile the standard model with the fact that around us there is almost only matter but no antimatter. Where does this come from? Furthermore, it seems that the cosmos around us is best explained by assuming that it consists of about 70% dark energy, 25% so-called dark matter, but only 5% is given by the stuff described by the standard model. This clearly shows that the standard model is not the ultimate answer for everything.
From a modern point of view, the standard model is an effective theory which is very successful in describing processes up to a certain energy scale. Whether it will ever be possible to derive the standard model and all its parameters from some other, more general theory is far from clear at the moment. One can, however, expect surprises in the endeavor to test its limits experimentally and to find theories beyond the standard model.

[6] We have not discussed one more free parameter of the standard model, the vacuum angle, θ_{QCD}, related to the generalized Maxwell equations describing QCD. Experimentally, θ_{QCD} is either zero or extremely small.

Index