Quantum Field Theory I

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This is a script to Prof. Wetterich's QFT I lecture at the university of Heidelberg in the winter semester 2005/06. The latest version can be found at the course homepage `http://www.thphys.uni-heidelberg.de/~cosmo/view/Main/QFTWetterich`.

If you find an error, please check whether you have the newest version (see date above), and if so report it to `thequantumfive@gmx.net`. Also if you find something confusing and think it should be explained in more detail or more clearly, please let us know. Your feedback will be the main force to improve the script.

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1.1 Introduction

Quantum field theory (QFT) is a theory that is useful not only for elementary particle physics, but also for understanding certain aspects of e.g. atoms, gases or solids. One can say that

> QFT is quantum mechanics (QM) for systems with many (sometimes infinitely many) degrees of freedom.

QFT is conceptually <u>not</u> beyond QM. But the large number of degrees of freedom create qualitatively new effects. The relationship between QFT and QM is similar to the relationship between statistical mechanics and mechanics.

> The basic problem of QFT is how to treat these infinitely many degrees of freedom.

A good theory should be independent of how exactly this limit process is done.

One topic in QFT is the *renormalization group*. It is concerned with the question of how to translate microscopic, short distance laws to larger systems. Only part of the information is appearing on larger scales.

The key method to make QFT simple is *functional integrals*. We will however start with the more familiar *creation/annihilation operators* in this chapter and then move on to functional integrals in chapter 2.

1.2 Units

We use units in which

$$\hbar = c = 1. \tag{1.1}$$

From $c = 1$ it follows that $1\,\mathrm{s} = 299792458\,\mathrm{m}$ and that mass and energy have the same units ($E = mc^2$). We measure mass and energy in eV. The mass of an electron is therefore $m_e = 510\,998.902(12)\,\mathrm{eV} \approx 9.1 \cdot 10^{-31}\,\mathrm{kg}$. Obviously, velocities are dimensionless. Momentum is therefore also measured in eV.

¿From $\hbar = 1$ it follows that the unit of length is the inverse of the unit of energy. Knowing that $\hbar c \approx 197\,\mathrm{GeV\,m}$ in the SI system we can easily convert between units, for example:

$$\begin{aligned} 1\,\mathrm{fm} &= 10^{-15}\,\mathrm{m} = \frac{1}{197\,\mathrm{MeV}} \approx 5\,\mathrm{GeV}^{-1} \\ 1\,\mathrm{Hz} &= 1\,\mathrm{s}^{-1} = 6.66 \cdot 10^{-16}\,\mathrm{eV} \end{aligned} \tag{1.2}$$

As an example of how our new units make life simple consider the commutator relation between the position operator Q and the momentum operator P, which used to be $[Q, P] = i\hbar$ and now simply is $[Q, P] = i$, i.e. QP is dimensionless.

Exercise: Express the Bohr radius $a_0 \approx 0.5 \cdot 10^{-10}\,\mathrm{m}$ in eV^{-1}.

1.3 Non-Relativistic Many-Body Systems 1: Phonons

We will treat these systems now with the so called *operator formalism*, which is also called *canonical quantization*, because students already know this method from QM. In chapter 2 we will do the same problem again with a new, better method called *functional formalism*.

1.3.1 One Dimensional Crystal

The reason why we start with this system is that all the basic concepts of QFT are already present here. Doing it in three dimensions would only increase the number of indices and give nothing conceptually new.

We consider a one dimensional lattice with $\mathcal{N}$ lattice sites ($\mathcal{N}$ even) and one atom at every lattice site j. For simplicity we connect the lattice to a torus and identify $\mathcal{N}/2$ with $-\mathcal{N}/2$. For large $\mathcal{N}$ that is physically the same as the linear lattice, but is mathematically more simple because there are no boundaries.

Let Q_j be the displacement from the equilibrium position and P_j the momentum of the atom at lattice site j. Then we have the following commutator relations:

$$\begin{aligned} [Q_i, P_j] &= i\delta_{ij}, \\ [Q_i, Q_j] &= 0, \\ [P_i, P_j] &= 0. \end{aligned} \tag{1.3}$$

They express that different atoms are completely independent, but position and momentum of one particle are related.

As a first dynamical model for our crystal we treat the atoms as independent harmonic oscillators. This is described by the simple Hamiltonian

$$H_0 = \sum_j \left(\frac{D}{2} Q_j Q_j + \frac{1}{2M} P_j P_j \right) \tag{1.4}$$

which has $\mathcal{N}$ degrees of freedom and no interaction between lattice sites. To solve this problem we define for each lattice site j two operators which are linear combinations of the position and the momentum operator of that site:

$$\begin{aligned} \text{annihilation operator}: \ a_j &= \frac{1}{\sqrt{2}} \left((DM)^{\frac{1}{4}} Q_j + i (DM)^{-\frac{1}{4}} P_j \right), \\ \text{creation operator}: \ a_j^\dagger &= \frac{1}{\sqrt{2}} \left((DM)^{\frac{1}{4}} Q_j - i (DM)^{-\frac{1}{4}} P_j \right). \end{aligned} \tag{1.5}$$

The fact that $a_j^\dagger$ is the adjoint of a_j, i.e. that $a_j^\dagger = (a_j)^\dagger$, justifies the notation $a_j^\dagger$. These operators satisfy the following relations:

$$\begin{aligned} [a_i, a_j^\dagger] &= \delta_{ij}, \\ [a_i, a_j] &= 0, \\ [a_i^\dagger, a_j^\dagger] &= 0. \end{aligned} \tag{1.6}$$

We can express the Hamiltonian in terms of the annihilation and creation operators:

$$\begin{gathered} H_0 = \omega_0 \sum_j (a_j^\dagger a_j + \frac{1}{2}) = \omega_0 \sum_j a_j^\dagger a_j + \frac{\mathcal{N}}{2}\omega_0, \\ \text{where } \omega_0 := \sqrt{D/M}. \end{gathered} \tag{1.7}$$

For $\mathcal{N} \to \infty$, the second term in the Hamiltonian goes to infinity. However, this divergence is not problematic, since we measure only differences in energy and the point of zero energy is a matter of definition. We simply subtract the term to get the right result. But this is a phenomenon we will encounter quite often in QFT and we always have to make sure that the divergent terms are not connected to observable quantities, otherwise we will be in trouble.

Occupation Number Representation

A basis vector in the *occupation number representation* contains for each possible state of a system the number of particles that occupy it. We can describe the state $|\Psi\rangle$ in the occupation number basis by

$$|\Psi\rangle = |n_{-\frac{\mathcal{N}}{2}}, \ldots, n_{-1}, n_0, n_1, \ldots, n_{\frac{\mathcal{N}}{2}-1}\rangle. \tag{1.8}$$

The particle number operator for the lattice site j can be expressed as

$$\hat{n}_j = a_j^\dagger a_j. \tag{1.9}$$

It counts the number of phonons at lattice side j

$$\hat{n}_j | \ldots, n_j, \ldots \rangle = n_j | \ldots, n_j, \ldots \rangle. \tag{1.10}$$

The total occupation number operator is given by

$$\hat{N} = \sum_j \hat{n}_j. \tag{1.11}$$

Note the different meaning of $\mathcal{N}$ and N:

$\mathcal{N} =$ number of *degrees of freedom* of the system (here the number of lattice sites)

$N =$ total number of *excitations* in the system (here the number of phonons)

QFT deals with large $\mathcal{N}$, not necessarily with large N. For example QFT can describe phonon-phonon scattering in a crystal. There you have $\mathcal{N} \approx 10^{23}$ and $N = 2$. The situation is similar for processes like electron-photon or electron-electron scattering. They involve only $N = 2$ particles (particles are described as excitations of the vacuum), but $\mathcal{N} = \infty$ degrees of freedom, namely the possible momenta of the outgoing particles. Even the ground state $|0\rangle$, where $N = 0$, is often a very complicated object in QFT!

N can be large too in QFT, e.g. if you want to describe a cold atom gas you can easily have $N \approx 10^5$. But the important characteristic of all systems studied in QFT is that they have very many degrees of freedom.

Basic Concepts of QFT

By now we have already met all the basic concepts of QFT:

vacuum = ground state: We call the ground state of our world the vacuum. The vacuum state $|0\rangle = |0, 0, 0, \ldots, 0, \ldots, 0\rangle$ is a normalized state in Hilbert space. It is the state of lowest energy, not necessarily zero energy. $|0\rangle \neq 0$, the vacuum is not empty, it can be very complicated.

particles = excitations of ground state: The excitations of the ground state are the particles. Particle properties depend on the ground state. For a solid that is obvious, the phonons depend on D and M. But for any system they depend on the Hamiltonian.

- $\langle \hat{n}_j \rangle = 0.3$ says that the expectation value of finding a phonon at site j is 0.3
- If a state has a sharp number of n_j phonons at site j then the equation $\hat{n}_j|\Psi\rangle = n_j|\Psi\rangle$ says that $|\Psi\rangle$ is a superposition of states $|\ldots, n_j, \ldots\rangle$ which all have n_j atoms at site j.

operator fields: We have a field of operators $a_j \equiv a(j) \equiv a(x)$ with $x = j \cdot a$ (a denotes the distance between adjacent lattice sites). That is a new concept, e.g. in electrodynamics of quantum mechanics we just dealt with scalar of vector fields. You can't measure these operators because they are not Hermitian, but Hermitian fields are easily constructed from $a(x)$ and $a^\dagger(x)$:

$$q(x) = \frac{1}{\sqrt{2}}\left(a(x) + a^\dagger(x)\right) = (DM)^{\frac{1}{4}} Q(x),$$
$$p(x) = -\frac{i}{\sqrt{2}}\left(a(x) - a^\dagger(x)\right) = (DM)^{-\frac{1}{4}} P(x) \tag{1.12}$$

are observables with real expectation values and $[q_i, p_j] = i\delta_{ij}$.

QFT is conceptually very simple, but it is technically difficult because the Hamiltonians describing real physical systems are complicated.

1.3.2 Propagating Phonons

So far our "phonons" are quite boring: Eigenstates of H_0 are confined to a given lattice site. Each lattice site can be treated independently of other sites. It is only a collection of one particle systems, we need interaction between lattice sites for propagation. Therefore we introduce next neighbor interaction into our Hamiltonian.

$$
\begin{aligned}
H &= H_0 + H_{nn}, \\
H_{nn} &= -\frac{B}{2}\sum_j Q_{j+1}Q_j = -\frac{B}{4}\sum_j (Q_{j+1}Q_j + Q_{j-1}Q_j)
\end{aligned} \tag{1.13}
$$

Now we have coupled oscillators! We consider $B > 0$ so the "alignment" of Q_j is favored because it needs less energy. The solution is still simple because this is a linear system. The diagonalization of H is possible.

Classical System

We will setup and solve the equations of motion for the classical system. The equations are

$$
\begin{aligned}
\dot{Q}_j &= \frac{1}{M}P_j, \\
\dot{P}_j &= -\frac{\partial H}{\partial Q_j}.
\end{aligned} \tag{1.14}
$$

The equation of motion is given by

$$
M\ddot{Q}_j = -DQ_j + \frac{B}{2}(Q_{j+1} + Q_{j-1}) \tag{1.15}
$$

and the Fourier transform of Q_j is

$$
F_q = \sum_j e^{-iqaj} Q_j. \tag{1.16}
$$

Here we used the same definitions as already introduced in chapter 1.3.1. a is the periodicity constant of our lattice such that $a \cdot j = x$ is the continuous spacial variable. The classical momentum is q. Inserting the Fourier transform into the equation of motion gives

$$
\begin{aligned}
M\ddot{F}_q &= \sum_j e^{-iqaj}(-DQ_j + \frac{B}{2}(Q_{j+1} + Q_{j-1})) \\
&= -\{D\sum_j e^{-iaqj}Q_j - \frac{B}{2}\sum_j e^{-iqa(j-1)}Q_j - \frac{B}{2}\sum_j e^{-iqa(j+1)}Q_j\} \\
&= -\sum_j e^{-iqaj}Q_j\{D - \frac{B}{2}(e^{iqa} + e^{-iqa})\} = -F_q \cdot (D - B\cos qa).
\end{aligned} \tag{1.17}
$$

This equation is solvable with the ansatz

$$
F_q(t) = e^{i\omega_q t}F_{q1} + e^{-i\omega_q t}F_{q2}, \text{ where } \omega_q^2 = \frac{D - B\cos qa}{M} \text{ and } |B| \le D. \tag{1.18}
$$

Quantum System

For the quantum system, we need to make a finite Fourier transform. This gives us the creation and annihilation operator of a wave mode (phonon) with momentum q:

$$\begin{aligned} a_q &= \frac{1}{\sqrt{\mathcal{N}}} \sum_j e^{-iqaj} a_j, \\ a_q^\dagger &= \frac{1}{\sqrt{\mathcal{N}}} \sum_j e^{iqaj} a_j^\dagger. \end{aligned} \tag{1.19}$$

Note that this isn't the Fourier transform of the momenta P_j and the space variables Q_j. We are interested in the momentum properties of a discrete torus lattice. The circumference is $L = a\mathcal{N}$, the longest wavelength possible is $L/2$ and the shortest is $2a$. Thus the momenta are $q = 2\pi\frac{k}{L}$, where all integers $k =, 0, \pm 1, \pm 2, \pm 3, \ldots, \pm\frac{\mathcal{N}}{2}$ are possible. One finds the periodicity in j

$$e^{-iqa(j+\mathcal{N})} = e^{-iqaj} \tag{1.20}$$

and the periodicity in q

$$q' = q + \frac{2\pi}{a} \rightarrow a_{q'} = a_q \rightarrow \text{ identify } q \text{ and } q + \frac{2\pi}{a}k. \tag{1.21}$$

Let's calculate the commutator of $a_q^\dagger$ and $a_{q'}$:

$$\begin{aligned} a_q^\dagger a_{q'} &= \frac{1}{\mathcal{N}} \sum_j \sum_{j'} e^{ia(qj-q'j')} a_j^\dagger a_{j'} \\ a_{q'} a_q^\dagger &= \frac{1}{\mathcal{N}} \sum_j \sum_{j'} e^{ia(qj-q'j')} a_{j'} a_j^\dagger, \\ [a_{q'}, a_q^\dagger] &= \frac{1}{\mathcal{N}} \sum_{jj'} e^{ia(qj-q'j')} [a_{j'}, a_j^\dagger] \end{aligned} \tag{1.22}$$

We know that $[a_{j'}, a_j^\dagger] = \delta_{j'j}$ and thus we have (m integer)

$$[a_{q'}, a_q^\dagger] = \frac{1}{\mathcal{N}} \sum_j e^{iaj(q-q')} = \widetilde{\delta}(q-q') = \begin{cases} 1 \text{ for } q' = q + 2mq_{max} \text{ where } q_{max} = \frac{\pi}{a} \\ 0 \text{ otherwise.} \end{cases} \tag{1.23}$$

<u>Proof:</u> A useful identity is $\frac{1}{\mathcal{N}} \sum_j e^{\frac{2\pi i}{\mathcal{N}} kj} = \widetilde{\delta}_{k,0}$ for: j, k integer, $|j| \le \frac{\mathcal{N}}{2}$, $j = \pm\frac{\mathcal{N}}{2}$ identified, $\mathcal{N}$ even, $\widetilde{\delta}_{k,0} = 1$ for $k = 0 \; mod\mathcal{N}, 0$ otherwise.

The number operator for a phonon in q-mode is given by $\widehat{n}_q = a_q^\dagger a_q$, with the conditions $-\frac{\pi}{a} \le q \le \frac{\pi}{a}$, with $-\frac{\pi}{a}$ and $\frac{\pi}{a}$ identified (momenta on torus!). It follows that $[a_q, a_q^\dagger] = 1$ and that all other commutators vanish.

The inverse finite Fourier transformation is given by

$$a_j = \frac{1}{\sqrt{\mathcal{N}}} \sum_q e^{iaqj} a_q \qquad \left(\text{with } \sum_q = \sum_{|q| \le \frac{\pi}{a}} = \sum_{|k| \le k_{max}} = \sum_{|k| \le \frac{\mathcal{N}}{2}} \right) \tag{1.24}$$

Proof: Insert the definition of a_q.

We now want to express H_{nn} in terms of a_q and $a_q^\dagger$:

$$\begin{aligned} H_{nn} &= -\frac{B}{2} \sum_j Q_{j+1} Q_j, \\ Q_j &= \frac{1}{\sqrt{2}} (DM)^{-\frac{1}{4}} (a_j + a_j^\dagger), \\ \Rightarrow \quad H_{nn} &= -\frac{B}{2} \frac{(DM)^{-1/2}}{2} \sum_j (a_{j+1} + a_{j+1}^\dagger)(a_j + a_j^\dagger). \end{aligned} \tag{1.25}$$

Setting $\beta = \frac{B(DM)^{-1/2}}{4}$ gives

$$H_{nn} = -\sum_j \sum_{qq'} \frac{\beta}{\mathcal{N}} (e^{iaq(j+1)} a_q + e^{-iaq(j+1)} a_q^\dagger)(e^{iaq'j} a_{q'} + e^{-iaq'j} a_{q'}^\dagger) \tag{1.26}$$

replace q by $-q$ for $a^\dagger$, this is just rearranging the sums

$$\begin{aligned} H_{nn} &= -\frac{\beta}{\mathcal{N}} \sum_{qq'} \sum_j e^{ia(q(j+1)+q'j)} (a_q + a_{-q}^\dagger)(a_{q'} + a_{-q'}^\dagger) \\ &= -\frac{\beta}{\mathcal{N}} \sum_{qq'} e^{iaq} \sum_j e^{ia(q+q')j} (a_q + a_{-q}^\dagger)(a_{q'} + a_{-q'}^\dagger). \end{aligned} \tag{1.27}$$

Using formula (1.23) $\sum_j e^{ia(q+q')j} = \mathcal{N} \delta_{q,-q'}$ we get

$$H_{nn} = -\beta \sum_q e^{iaq} (a_q + a_{-q}^\dagger)(a_{-q} + a_q^\dagger) \tag{1.28}$$

With $a_q, a_{q'}^\dagger = a_{q'}^\dagger a_q + \delta_{q,q'}$ one finds

$$H_{nn} = -\beta \sum_q e^{iaq} (a_{-q}^\dagger a_{-q} + a_q^\dagger a_q + 1 + a_q a_{-q} + a_q^\dagger a_{-q}^\dagger). \tag{1.29}$$

With $\sum_q e^{iaq} = 0$ follows

$$\begin{aligned}
H_{nn} &= -\beta \sum_q (e^{iaq} + e^{-iaq})\{a_q^\dagger a_q + \frac{1}{2}(a_q a_{-q} + a_q^\dagger a_{-q}^\dagger)\}, \\
&= -\frac{B(DM)^{-1/2}}{2} \sum_q \cos aq \{a_q^\dagger a_q + \frac{1}{2}(a_q a_{-q} + a_q^\dagger a_{-q}^\dagger)\}, \qquad (1.30) \\
H_0 &= \sqrt{\frac{D}{M}} \sum_j a_j^\dagger a_j = \sqrt{\frac{D}{M}} \sum_q a_q^\dagger a_q. \qquad (1.31)
\end{aligned}$$

Proof: The reader should verify this!

The general Hamiltonian H is then given by

$$\begin{aligned}
H &= H_0 + H_{nn} = \sqrt{\frac{D}{M}} \sum_q h_q, \\
h_q &= (1 - \frac{B}{2D} \cos aq) a_q^\dagger a_q - \frac{B}{4D} \cos aq (a_q a_{-q} + a_q^\dagger a_{-q}^\dagger). \qquad (1.32)
\end{aligned}$$

As we now see, H separates into contributions from individual $|q|$ modes, but it still mixes between a_q and $a_{-q}^\dagger$!

1.3.3 Block Diagonalization

Until now, we have been able to decompose all modes of H, with different $|q|$. To decompose the terms with q and $-q$, we introduce new operators A_q and A_{-q} for $\alpha, \beta \in \mathbb{R}$ via

$$\begin{aligned}
a_q &= \alpha A_q + \beta A_{-q}^\dagger, & a_q^\dagger &= \alpha A_q^\dagger + \beta A_{-q}, \\
a_{-q} &= \alpha A_{-q} + \beta A_q^\dagger, & a_{-q}^\dagger &= \alpha A_{-q}^\dagger + \beta A_q. \qquad (1.33)
\end{aligned}$$

At first glance, one assumes, that this is an orthogonal transformation, but we'll see it's NOT. The reason is, that we would like the algebra (commutator relation) to be preserved, this means: $[a_q, a_q^\dagger] = [A_q, A_q^\dagger] = 1$. Let's compute $[a_q, a_q^\dagger]$:

$$\begin{aligned}
a_q^\dagger a_q &= \alpha^2 A_q^\dagger A_q + \alpha\beta(A_q A_{-q} + A_q^\dagger A_{-q}^\dagger) + \beta^2 A_{-q} A_{-q}^\dagger \\
&= \alpha^2 A_q^\dagger A_q + \alpha\beta(A_q A_{-q} + A_q^\dagger A_{-q}^\dagger) + \beta^2 (A_{-q}^\dagger A_{-q} + 1) \\
a_q a_q^\dagger &= \alpha^2 A_q A_q^\dagger + \alpha\beta(A_q A_{-q} + A_q^\dagger A_{-q}^\dagger) + \beta^2 A_{-q}^\dagger A_{-q} \\
&= \alpha^2 (A_q^\dagger A_q + 1) + \alpha\beta(A_q A_{-q} + A_q^\dagger A_{-q}^\dagger) + \beta^2 A_{-q}^\dagger A_{-q} \\
\Rightarrow \quad [a_q, a_q^\dagger] &= \alpha^2 - \beta^2 = 1 \qquad (1.34)
\end{aligned}$$

Obviously, this transformation isn't orthogonal ($\alpha^2 + \beta^2 \neq 1$). The transformation group with this property is called the *symplectic group*. We'll discuss it later on.

We can now express H in terms of A_q and $A_q^\dagger$. We define $\widetilde{H}$ by

$$
\begin{aligned}
h_q &= \frac{1}{2}\left(1 - \frac{B}{2D}\cos(qa)\right)\widetilde{H} \qquad\qquad \text{(see (1.32))} \\
\Rightarrow \quad \widetilde{H} &= a_q^\dagger a_q + a_{-q}^\dagger a_{-q} + c(a_q a_{-q} + a_q^\dagger a_{-q}^\dagger) \qquad (1.35)
\end{aligned}
$$

We compute all the terms using the commutator relations for $A_q^\dagger$ and A_q,

$$
\begin{aligned}
a_q^\dagger a_q + a_{-q}^\dagger a_{-q} &= (\alpha^2+\beta^2)(A_q^\dagger A_q + A_{-q}^\dagger A_{-q}) + 2\alpha\beta(A_q A_{-q} + A_q^\dagger A_{-q}^\dagger) + \alpha^2 + \beta^2, \\
a_q a_{-q} &= \alpha^2 A_q A_{-q} + \beta^2 A_{-q}^\dagger A_q^\dagger + \alpha\beta(A_q A_q^\dagger + A_{-q}^\dagger A_{-q}), \\
a_q^\dagger a_{-q}^\dagger &= \alpha^2 A_q^\dagger A_{-q}^\dagger + \beta^2 A_{-q} A_q + \alpha\beta(A_q^\dagger A_q + A_{-q} A_{-q}^\dagger). \qquad (1.36)
\end{aligned}
$$

Since we don't want any 'mixed terms' $(A_q A_{-q})$ in H, the following equation must be true:

$$2\alpha\beta + c(\alpha^2+\beta^2) = 0. \tag{1.37}$$

Using $\beta^2 = \alpha^2 - 1$, we solve for α^2:

$$\alpha^2 = \frac{1}{2} \pm \frac{1}{2\sqrt{1-c^2}} \tag{1.38}$$

Only '+' is possible, since $\alpha^2 \geq 0$. Taking $\alpha \geq 0$, we finally get the result

$$\widetilde{H} = \sqrt{1-c^2}(A_q^\dagger A_q + A_{-q}^\dagger A_{-q}) \tag{1.39}$$

with

$$
\begin{aligned}
A_q &= \alpha a_q - \beta a_{-q}^\dagger, \quad & A_{-q} &= \alpha a_{-q} - \beta a_q^\dagger, \\
A_q^\dagger &= \alpha a_q^\dagger - \beta a_{-q}, \quad & A_{-q}^\dagger &= \alpha a_{-q}^\dagger - \beta a_q. \qquad (1.40)
\end{aligned}
$$

1.3.4 One Dimensional Phonons

Now we assume a one dimensional lattice. We write down the full Hamiltonian

$$H = \sum_q \sqrt{\frac{D}{M}}(\frac{1}{2} - \frac{B}{4D}\cos aq)\widetilde{H}, \tag{1.41}$$

$$c = -\frac{B}{4D}\cos aq(\frac{1}{2} - \frac{B}{4D}\cos aq)^{-1}. \tag{1.42}$$

Writing

$$H = \sum_q \omega_q A_q^\dagger A_q \tag{1.43}$$

we find the expression

$$\omega_q^2 = \frac{D}{M}(1 - \frac{B}{D}\cos aq) \tag{1.44}$$

This is exactly the expression one gets in the classical limit, see (1.18).

1.3.5 Summary

- Now we have entirely diagonalized H into phonon modes with momenta q. The eigenstates $|n\rangle$ of H are also eigenstates of $A_q^\dagger A_q$. Because of the commutator relation, $A_q^\dagger A_q$ is an occupation number operator (its eigenvalue is the number of phonons with mode q. Remember: its possible to have more phonons with the same momentum q. In this picture the phonons are the particles!).

- The transformation we applied is not orthogonal. The underlying group is called the symplectic group. It has the property of preserving the commutator.

- We have $\omega_q = \omega(q)$. This is called the *dispersion relation*. It embodies all micro-physics.

  For example we can calculate the energy of the system:
  The canonical sum is given by

  $$Z_c = Tr(e^{-\beta H}) = \sum_{n_q} \langle n_q | e^{-\beta \sum_q \omega_q A_q^\dagger A_q} | n_q \rangle. \tag{1.45}$$

  Here $\sum_{n_q}$ means $\sum_{n_1} \sum_{n_2} \ldots$. We normally would have the restriction $\sum_q n_q = N$ (N = number of phonons). But since N is not constant, we can omit this restriction! We assume

  $$A_q^\dagger A_q | n_q \rangle = n_q | n_q \rangle \tag{1.46}$$

  and can now calculate Z_c:

  $$Z_c = \sum_{\{n_q\}} e^{-\beta \sum_q \omega_q n_q} = \sum_{n_{q1}} \sum_{n_{q2}} \ldots e^{-\beta \sum_q \omega_q n_q} = \prod_q \frac{1}{1 - e^{-\beta \omega_q}}. \tag{1.47}$$

  In the last step we used the geometric series. So the energy of the system is

  $$E = \frac{1}{Z_c}(-\partial_\beta Z_c) = \sum_q \frac{\omega_q}{e^{-\beta \omega_q} - 1}. \tag{1.48}$$

  Here we can see that the macroscopic quantity energy is entirely determined by the ω_q's!

1.3.6 The Symplectic Group Sp(V)

The symplectic group $\mathbf{Sp}(V)$ is the group of transformations, which preserve any non-degenerate, skew symmetric form $\omega : V \times V \rightarrow \mathbf{K}$.

$$\omega(\mathbf{M}u, \mathbf{M}v) = \omega(u, v) \tag{1.49}$$

with $u, v \in V$ and $\mathbf{M} \in \mathbf{Sp}$. If we express ω within a certain basis by a skew symmetric matrix $\mathbf{J}$, the elements $\mathbf{M} \in \mathbf{Sp}$ must then fulfill the following condition:

$$\mathbf{M}^T \mathbf{J} \mathbf{M} = \mathbf{J} \tag{1.50}$$

Another property of $\mathbf{Sp}(V)$ is that its elements also preserve so called volume forms $\widetilde{v} = v_{ijk}\ e_i \wedge e_j \wedge e_k$. It follows that the *orientation* of the given vector space is also preserved.

1.3.7 Further Discussion of Phonons

Now, that we have diagonalized the Hamiltonian of the one dimensional solid and that we have found the dispersion relation (1.44) for the phonons, we want to discuss these quasi-particles a little bit more, although they are not one of our major interests in this lecture on QFT.

Real Phonons in a Cubic Lattice

To come to the "real world", we have to consider a 3D lattice. This is a little bit more complicated, as we may have several sorts of phonons with different dispersion relations $\omega_\alpha(q)$. But if we restrict ourselves to cubic lattices and consider only longitudinal waves, the planes of lattice sites (atoms) oscillate as a whole, so our problem becomes one-dimensional, just as we discussed it on the previous pages.

Let us consider the dispersion relation a little bit more in detail: What does it look like in the following cases:

$$D = B, \quad D = B + \Delta > B, \quad D < B. \tag{1.51}$$

A) Remember our original Hamiltonian,

$$H = \sum_j \left\{ \frac{D}{2} Q_j Q_j - \frac{B}{2} Q_{j+1} Q_j + \frac{1}{2M} P_j P_j \right\}. \tag{1.52}$$

Setting $B = D$ gives

$$\begin{aligned}
H &= \sum_j \left\{ \frac{B}{2} Q_j^2 - \frac{B}{2} Q_{j+1} Q_j + \frac{P_j^2}{2M} \right\} \\
&= \sum_j \left\{ \frac{B}{4} Q_j^2 + \frac{B}{4} Q_{j+1}^2 - \frac{B}{2} Q_{j+1} Q_j + \frac{P_j^2}{2M} \right\} \\
&= \sum_j \left\{ \frac{B}{4} (Q_{j+1} - Q_j)^2 + \frac{P_j^2}{2M} \right\}
\end{aligned} \tag{1.53}$$

In equation (**??**) we observe that this Hamiltonian corresponds to a potential energy that is only dependent on the distance between two next neighbors (atoms in 1D, planes of atoms in 3D).

The dispersion relation is now

$$\omega_q = \sqrt{\frac{B}{M}} \sqrt{1 - \cos(aq)}. \tag{1.54}$$

For small values of q we use the Taylor expansion of the cosine and find

$$\omega_q = \sqrt{\frac{B}{2M}}\, a|q|. \tag{1.55}$$

The group velocity of longitudinal waves (sound velocity in solids) can also be calculated

$$v_g = \frac{\partial \omega_q}{\partial q} = \operatorname{sgn}(q) \cdot a\sqrt{\frac{B}{2M}}. \tag{1.56}$$

So we found the result, that the sound velocity is constant for small $|q|$. Remember that we only considered longitudinal and no transversal waves, which usually have higher sound velocities. Dealing with transversal waves we would be confronted with the problem, that we do no longer have oscillating planes of atoms - and with this, we can no longer say that our problem is one dimensional.

B) Let us come to the second case, $D = B + \Delta$ with a positive Δ. In this case we have the Hamiltonian

$$\begin{aligned} H &= \sum_j \left\{ \frac{B+\Delta}{2} Q_j^2 - \frac{B}{2} Q_{j+1} Q_j + \frac{P_j^2}{2M} \right\} \\ &= \sum_j \left\{ \frac{\Delta}{2} Q_j^2 + \frac{B}{4} (Q_{j+1} - Q_j)^2 + \frac{P_j^2}{2M} \right\}. \end{aligned} \tag{1.57}$$

The additional term is looking like the harmonic oscillator potential, and its effect is to “remind” every oscillator of its equilibrium position. An example would be a lattice with two different atoms in the fundamental cell, a very heavy and a relatively light one. The heavier atoms then may have fixed positions while only the light ones are oscillating. Due to a coupling between the two atoms in the fundamental cell, the light atoms are always “feeling” a reacting force towards the equilibrium position.

What about the dispersion relation? Well, this time we have

$$\begin{aligned} \omega_q &= \sqrt{\frac{B+\Delta}{M}} \sqrt{1 - \frac{B}{B+\Delta} \cos(aq)} \\ &\overset{\text{Taylor}}{\approx} \sqrt{\frac{B+\Delta}{M}} \sqrt{1 - \frac{B}{B+\Delta} + \frac{B}{B+\Delta} \frac{a^2 q^2}{2}} \\ &= \sqrt{\frac{1}{M}} \sqrt{\Delta + B \frac{a^2 q^2}{2}}. \end{aligned} \tag{1.58}$$

So even for $q = 0$ we get a finite frequency ω_q (“gap”).

For $\Delta \to 0, D \to B$ we get the same result as we had in case A).

C) For $D < B$ or $D = B - \Delta$, we use the result (1.57) from case B), and just switch the sign of Δ. We find

$$H = \sum_j \left\{ -\frac{\Delta}{2} Q_j^2 + \frac{B}{4}(Q_{j+1} - Q_j)^2 + \frac{P_j^2}{2M} \right\}. \tag{1.59}$$

Notice that this time we have an additional, quadratic potential energy with negative sign. At this point we get into trouble, because this means that our ground state is unstable.

Actually, this is not just a mathematical problem: For example phonon-phonon interaction is described by a negative, linear quadratic term, but also with an additional term $\propto \lambda Q_j^4$. Transforming this into creation and annihilation operators we get

$$H_W \propto \lambda a_q a_q a_q^\dagger a_q^\dagger. \tag{1.60}$$

This is not a linear system anymore! It causes very difficult problems to find the ground state and to classify, what an excitation is. A possibility is to do small λ perturbation theory, but even this method fails for $B \approx D$.

For the moment, this is too complicated for us. We will come back to this point later, when we have learned the method of path integrals.

Real Phonons, Arbitrary Lattices

So far we have only considered the cubic lattice. We transformed our Hamiltonian to

$$H = \sum_{\mathbf{q}} \omega(\mathbf{q}) A^\dagger(\mathbf{q}) A_(\mathbf{q}) \tag{1.61}$$

and realized, that all details of the lattice and interactions are reflected in the dispersion relation $\omega(\mathbf{q})$. It depends strongly on the relation between B and D.

Now, in the more general case, we may have several “branches” $H = \sum_\alpha H_\alpha$ with different dispersion relations ω_α.

Application: For many purposes it is convenient to treat a solid as a phonon gas. This is similar to the photon gas, but with a different dispersion relation: Photons have $\omega(\mathbf{q}) = |q|$, and our phonons usually (for $D > B$) have $\omega(\mathbf{q}) \propto |q|^2$.

Real Phonons in Position Space

What happens if we are going back to position space? Let us transform our annihilation operator $A(\mathbf{q})$:

$$A(\mathbf{q}) = \frac{1}{\sqrt{\mathcal{N}}} \sum_j e^{-ia\mathbf{q}\mathbf{j}} A_{\mathbf{j}}. \tag{1.62}$$

Please keep in mind that we do not really know what our A_j operators are, especially not their relation to our original operators a_j and $a_j^\dagger$. We just *define* them to be the Fourier coefficients of the Fourier series in (1.62). However, one thing we *know* is their commutation relation, because we know those for the $A_{\mathbf{q}}$ and already proved that Fourier transformations do not change them:

$$[A_{\mathbf{j}}, A_{\mathbf{k}}^\dagger] = \delta(\mathbf{j}-\mathbf{k}) = \delta_{j_1 k_1}\delta_{j_2 k_2}\delta_{j_3 k_3}. \tag{1.63}$$

This allows to write the Hamiltonian as

$$H = \sum_{\mathbf{j}\mathbf{j}'} T(\mathbf{j},\mathbf{j}') A_{\mathbf{j}}^\dagger A_{\mathbf{j}'}, \tag{1.64}$$

with a function T that is *uniquely fixed* by $\omega(\mathbf{q})$ (and vice versa) which can be seen by Fourier transformation. An example would be the next neighbor interaction:

$$T(\mathbf{j},\mathbf{j}') \propto \delta(\mathbf{j}-\mathbf{j}'-1). \tag{1.65}$$

IMPORTANT NOTE ON NOTATION: Because we don't need our "old" $a_{\mathbf{q}}$ and $a_{\mathbf{q}}^\dagger$ operators anymore, we will change our notation:

$$A_{\mathbf{q}} \to a_{\mathbf{q}} \tag{1.66}$$

(and the same for creation operators).

Quasi-Momentum of Phonon States in one Dimension

In our new notation the Hamiltonian is

$$H = \sum_q \omega(q) a_q^\dagger a_q \tag{1.67}$$

with the operators a_q and $a_q^\dagger$ that annihilate or create phonons of a "quasi-momentum" q. But what is the meaning of this "quasi-momentum"? To answer this question, let us first define the total quasi momentum of a system,

$$\widehat{q} = \sum_q q a_q^\dagger a_q. \tag{1.68}$$

This is obviously a reasonable definition, because $a_q^\dagger a_q$ gives us the number of phonons with quasi-momentum q, so $q a_q^\dagger a_q$ will be the quasi-momentum of all phonons having q. The sum over all q should then give us the total quasi-momentum of all quasi-particles.

Well, somehow we used the word "quasi" very often in the last sentences. The reason is that $\widehat{q}$ has obviously *nothing* to do with the *physical* momentum $\widehat{P}_{total} = \sum_j \widehat{P}_j$. Imagine, for instance, a solid that is fixed in space. In this case, we have surely no total momentum $\widehat{P}_{total} = \sum_j \widehat{P}_j$ (or, to be more precise, the eigenvalue of $\widehat{P}_{total}$ will be zero: $\widehat{P}_{total}|\psi\rangle = 0|\psi\rangle$).

Nevertheless, the atoms of the solid may oscillate, so the momenta of the individual atoms are non-zero. This is where we originally had started: We defined our operators $a_j^\dagger$ and a_j, transformed them to $a_q^\dagger$ and a_q, then transformed them to $A_q^\dagger$ and A_q (which we now again write as $a_q^\dagger$ and a_q). So the number operators $a_q^\dagger a_q$ will be non-zero for at least some q, which gives us a non-zero eigenvalue for $\widehat{q}$: $\widehat{q}|\psi\rangle \neq 0|\psi\rangle$.

The commutation relation of $\widehat{q}$ with the Hamiltonian is

$$[\widehat{q}, H] = 0, \tag{1.69}$$

which is true because $\widehat{q}$ is a conserved quantity (remember that operators of conserved quantities commute with the Hamiltonian).

Interpretation: One-Phonon State with Quasi-Momentum q

We have already learned a lot about phonons so far, but still we do not have a very clear idea of these quasi-particles. In order to change this, let's consider a very simple system: A solid where we have just one single phonon with momentum q:

$$|q\rangle = a_q^\dagger|0\rangle. \tag{1.70}$$

The eigenvalue of the total quasi-momentum operator $\widehat{q}$ is q:

$$\widehat{q}|q\rangle = q|q\rangle. \tag{1.71}$$

And the eigenvalue equation of H is

$$H|q\rangle = \sum_q \omega_q a_q^\dagger a_q|q\rangle = \omega_q|q\rangle. \tag{1.72}$$

In the occupation number basis the system is obviously very simple, but it can be quite complicated when we try to express it in terms of the (time dependent) positions of every single atom in the lattice.

Nevertheless, this is exactly what we want to do now, because we want to get a better idea of phonons. But to make the calculation as simple as possible, we will make one further simplification: We set $B = 0$, which means that we are going back to uncoupled lattice sites. With this, we also have $A_q = a_q$.

The time-dependent Schrödinger equation looks like

$$i\frac{\partial}{\partial t}|q\rangle = \omega_q|q\rangle, \tag{1.73}$$

and the solution is

$$|q\rangle(t) = e^{-i\omega_q t}|q\rangle_{t=0} = e^{-i\omega_q t}a_q^\dagger|0\rangle, \tag{1.74}$$

where we have chosen the phase to be 1 at $t = 0$.

Now we express the operator $a_q^\dagger$ in terms of the a_j and $a_j^\dagger$ similar to equations (1.19). This leads to

$$|q\rangle = \frac{1}{\sqrt{\mathcal{N}}} \sum_j e^{i(qx-\omega_q t)} a_j^\dagger |0\rangle, \text{ where } x = aj. \tag{1.75}$$

Because we have an uncoupled system, the ground state wave function is a product of the wave functions of the single lattice sites,

$$|0\rangle = \prod_j |0\rangle_j = \prod_j \psi_{j,0}(y_j). \tag{1.76}$$

In the last step, we've been a little bit sloppy with our notation, because now we have a ket vector on the left-hand side and a function of spatial coordinates on the right-hand side. To be more precise, we should have written $\langle x|0\rangle$ or something like that. Anyway, don't worry when we continue with this notation down below. Just keep in mind that we identify our ket vectors with the spatial representation of the wave function.

The argument y_j needs as well a little bit of explanation. With this, we mean the deviations of the position of a lattice site x_j to its equilibrium position $x_{j,eq.}$,

$$y_j = x_j - x_{j,eq}. \tag{1.77}$$

Fortunately, we know the $\psi_{j,0}(y_j)$ from quantum mechanical harmonic oscillator:

$$\psi_{j,0}(y_j) = C e^{-\kappa y_j^2}. \tag{1.78}$$

The operator Q_j acts like

$$Q_j \psi_{j,0}(y_j) = y_j \psi_{j,0}(y_j). \tag{1.79}$$

According to equation (1.75), we need to know how $a_j^\dagger$ acts.

$$\begin{aligned} a_j^\dagger \psi_{j,0} &= (c_1 y_j - c_2 \frac{\partial}{\partial y_j}) \psi_{j,0} \qquad (c_1, c_2 \text{ defined by } (\mathbf{??})) \\ &= \sigma C y_j e^{-\kappa y_j^2} = \sigma y_j \psi_{j,0}. \end{aligned} \tag{1.80}$$

The second equality holds, because the derivative with respect to y_j also gives us a term proportional to $y_j e^{-\kappa y_j^2}$.

We will now insert this into equation (1.75). But we have to keep in mind that in (1.75) the creation operator acts on the product wave function $|0\rangle = \prod_{j'} \psi_{j^{prime},0}(y_{j'})$ and that only one single $\psi_{j,0}$ is changed by the operator. We therefore get

$$|q\rangle(t) = \frac{1}{\sqrt{\mathcal{N}}} \sum_j e^{i(qx-\omega_q t)} \sigma y_j C e^{-\kappa y_j^2} \prod_{j' \neq j} C e^{-\kappa y_{j'}^2}. \tag{1.81}$$

The relative phase factor $e^{i(qx-\omega_q t)}$ is important. If we have, for instance, a difference of

$$x_2 - x_1 = \frac{\pi}{q} \tag{1.82}$$

between two oscillators, they will have a phase difference of π. Furthermore, this relative phase between two oscillators is constant in time.

Well, this is now a good moment to discuss the meaning of the quasi-momentum q. In equation (1.82) we see, that q plays the role of a wave number, and as we set $\hbar = 1$, this is equal to a momentum. So a phonon with momentum q is not a localized particle somewhere in the lattice, traveling with a velocity that corresponds to the given momentum. It can be better understood as the vibration of the whole lattice. *Every* atom within the lattice is oscillating, and we have fixed phase relations between them, corresponding to the wave number (equals momentum) of the phonon. The frequency of the oscillation of an atom is given by ω, which is a quantity that depends on q, but also on the properties of the lattice.

We could even ask more questions on the interpretation of phonons. One would be: What happens, if we have two phonons with the same quasi-momentum? Well, they will cause the same type of oscillation, but the lattice sites will oscillate with a bigger amplitude. More difficult situations, e.g. excitations of different q-modes or propagating phonons (so a system with next neighbor interaction) are not discussed or interpreted here.

To finish this paragraph, we make some additional remarks:

- The difference $\Delta x = \frac{\pi}{q}$ can be transformed into a difference Δ_j (number of lattice sites):

$$\frac{\pi}{q} = \frac{\pi}{2\pi k/L} = \frac{\mathcal{N}a}{2k} \Rightarrow \Delta_j = \frac{\mathcal{N}}{2k}. \tag{1.83}$$

- We have constant phase for $qx = \omega_q t$.
- The phase velocity is $v_{ph} = \frac{\omega_q}{q}$.

Correlation Function in q-Mode

We are now coming to the last point in the discussion of solids: the *correlation function*. Let's first define it for our very particular case (we will define it more generally later):

$$F(\Delta j) := \langle q | Q_j Q_{j+\Delta j} | q \rangle. \tag{1.84}$$

In order to interpret this quantity, we compute it for our one-phonon state.

$$\begin{aligned} F(\Delta j) &= \langle q | Q_j Q_{j+\Delta_j} | q \rangle \\ &= \frac{1}{\mathcal{N}} \sum_{k,k'} e^{-i(qak-\omega_q t)} e^{i(qak'-\omega_q t)} \langle 0 | a_k Q_j Q_{j+\Delta_j} a^\dagger_{k'} | 0 \rangle \\ &= \frac{1}{\mathcal{N}} \sum_{k,k'} e^{iqa(k'-k)} \sigma^2 \int y_k y_{k'} y_j y_{j+\Delta_j} \prod_i \left(C^2 e^{-2\kappa y_i^2} dy_i \right) \end{aligned} \tag{1.85}$$

The integral is non-zero only if the integrand is not antisymmetric in any of the integration variables. This is only realized for $k = j, k' = j + \Delta_j$ or $k = j + \Delta_j, k' = j$. So we get

$$\begin{aligned}
F(\Delta_j) &= \frac{2\sigma^2}{\mathcal{N}} \sum_{k,k'} \cos(qa[k'-k])\delta_{k,j}\delta_{k',j+\Delta_j} \int y_j^2 y_{j+\Delta_j}^2 \prod_i \left(C^2 e^{-2\kappa y_i^2} dy_i\right) \\
&= \frac{2}{\sigma^2 \mathcal{N}} \int dy_j \sigma^2 C^2 y_j^2 e^{-2\kappa y_j^2} \int dy_{j+\Delta_j} \sigma^2 C^2 y_{j+\Delta_j}^2 e^{-2\kappa y_{j+\Delta_j}^2} \cos(qa\Delta_j) \\
\Rightarrow F(\Delta_j) &= \frac{2}{\mathcal{N}\sigma^2} \cos(qa\Delta_j). \qquad (1.86)
\end{aligned}$$

In the last step we used the normalization of the first excited states.

Let us come to the interpretation: The correlation function is a cosine with maximum values for $qa\Delta j = q\Delta x = 2\pi m$. These are those lattice sites which are in exactly the same phase as lattice site j. We call this a "coherent excitation". Remember that this has nothing to do with the coupling between the atoms—we have considered an uncoupled system here! The correlation is just due to the fact, that we have an oscillation of the whole lattice with fixed phase relations between the lattice sites.

If we do the same calculation for the ground state, we get

$$\langle 0|Q_j Q_{j+\Delta j}|0\rangle = 0 \qquad (1.87)$$

for every $\Delta j \neq 0$.

But this is not the case for a more complex ground state (vacuum). We will later see examples where the correlation function is non-zero for $\Delta j \neq 0$. So we see that the correlation function is a good probe for the properties of the ground state (and also for the excited states).

Exercise: How does the correlation function look like for a 1D system with $B \neq 0$?

1.4 Non-Relativistic Many-Body Systems 2: Atom Gas

1.4.1 Identical Bosonic Atoms in a Box

We discuss the behavior of a gas of Spin 0 particles like ^{4}He atoms. By "many atoms" we mean at least $N = 10^5$, but N could be much larger, like $N = 10^{26}$. Applications are e.g. Bose-Einstein condensates (BEC) and macroscopic waves.

We impose periodic boundary conditions

$$\begin{aligned}
\psi(x_1 + L, x_2, x_3) &= \psi(x_1, x_2, x_3), \\
\psi(x_1, x_2 + L, x_3) &= \psi(x_1, x_2, x_3), \\
\psi(x_1, x_2, x_3 + L) &= \psi(x_1, x_2, x_3). \qquad (1.88)
\end{aligned}$$

Therefore the momenta in each of the three directions, $p = (p_1, p_2, p_3)$, can only have certain discrete values. This can be seen by looking for separable solutions $\psi(x_1, x_2, x_3) =$

$\psi_1(x_1)\psi_2(x_2)\psi_3(x_3)$. Applying the boundary conditions to the general solutions gives:

$$e^{ip_1x_1} = e^{ip_1(x_1+L)} \Rightarrow e^{ip_1L} = 1 \Rightarrow p_1L = 2\pi k_1 \text{ with } k_1 \in \mathbb{Z} \tag{1.89}$$

Same procedure for the other two directions:

$$p = (p_1, p_2, p_3) = \frac{2\pi}{L}(k_1, k_2, k_3) = \frac{2\pi}{L}k. \tag{1.90}$$

We want to consider atoms in continuous space, but for technical reasons we first put them on a lattice. In this way, there will only be a finite number of points in our box where the atoms can be. We do that because now our system only has a finite number of degrees of freedom $\mathcal{N}$ and everything is well-defined.

Having this well-defined system, we can make the **continuum limit** by

$$a \to 0, \quad N, L \text{ fixed}, \quad k^{max} \to \infty, \quad \mathcal{N} \to \infty. \tag{1.91}$$

However, the resulting theory is only an **effective theory** of the atoms. The reason is that they are treated as point-like particles, but of course real atoms will have a finite size and therefore the theory will not make any sense at scales smaller than the atom size. Going beyond this size, it is required to build a more complicated theory, describing the interactions of the electrons with the nucleus or even the interactions between the single protons and neutrons. According to the uncertainty principle, this minimum size in the theory corresponds to a maximum momentum, which gives as a so-called **ultraviolet cutoff** Λ. This means that we only consider momenta $|p| < \Lambda$. This is a very typical situation in QFT, that there is an effective theory valid until a certain UV-cutoff. In this case we know where to apply the cutoff, because we know the size of the atoms, however there may be situations where we do not know the right cutoff, i. e. on which scales the theory is valid. This is why physical meaningful results should be independent of Λ. In practice, this can be a difficult problem and the predictions of effective theories will depend on Λ.

To summarize: In QFT one usually works with effective theories, either because the "true" theory is unknown or because you want to use a simple model where you can do calculations. That one has to perform some kind of UV-cutoff simply reflects the fact that the theory has a limited range of validity. The art of QFT is to do the UV-cutoff right, i.e. in a way to get the right physics. These methods are called **renormalization** techniques.

Now we can also do the **infinite volume limit:**

$$L \to \infty, \quad \mathcal{N} \to \infty. \tag{1.92}$$

As long as L was finite, the size of the box corresponded to a maximum length scale, i. e. a minimal momentum. It served as a so-called infrared-cutoff. Now this cutoff goes to zero. Of course, to have a well-defined limit, physical results may not depend on this infrared-cutoff, but must be independent of L.

1.4.2 N-Atom States

The Hamiltonian for a free gas of N atoms with mass M is

$$H_0 = \sum_{i=1}^{N} \frac{1}{2M} p_i^2 = \sum_{i=1}^{N} \frac{1}{2M} (p_{i,1}^2 + p_{i,2}^2 + p_{i,3}^2). \tag{1.93}$$

We have bosons, so the wave function is symmetric, and the basis of momentum eigenstates of H_0 is given by

$$\begin{aligned} N = 1: &\quad |p\rangle, \\ N = 2: &\quad \frac{1}{\sqrt{2}} \left(|p_1\rangle |p_2\rangle + |p_2\rangle |p_1\rangle \right), \\ N = 3: &\quad \frac{1}{\sqrt{6}} \left(|p_1\rangle |p_2\rangle |p_3\rangle + \cdots + |p_3\rangle |p_2\rangle |p_1\rangle \right), \\ N = 10^5, &\quad N = 10^{26}, \quad \ldots \text{ well } \ldots . \end{aligned} \tag{1.94}$$

It is inefficient to consider the momenta of individual atoms. This is just like in classical statistical mechanics, where you would use a momentum distribution instead of describing every atom.

Occupation Number Representation

How many atoms have momentum $p_1, p_2, \ldots$? Let μ label all the possible values of momenta (more generally, μ labels the degrees of freedom, $\mu = 1, \ldots, \mathcal{N}$).

$$|\psi\rangle = |n_1, n_2, \ldots, n_{\mathcal{N}}\rangle = |\{n_\mu\}\rangle \tag{1.95}$$

We have annihilation a_μ and creation $a_\mu^\dagger$ operators with

$$[a_\nu, a_\mu^\dagger] = \delta_{\nu\mu}, \quad \hat{n}_\mu = a_\mu^\dagger a_\mu, \quad \hat{n}_\mu |\psi\rangle = n_\mu |\psi\rangle. \tag{1.96}$$

In our case

$$\mu = p = (p_1, p_2, p_3) \text{ and the operators are } a_p, a_p^\dagger. \tag{1.97}$$

We neglect the additive constant $\mathcal{N}/2$ in the Hamiltonian and get

$$H_0 = \sum_p \frac{p^2}{2M} a_p^\dagger a_p. \tag{1.98}$$

The vacuum is represented by

$$|0\rangle = |0, 0, \ldots, 0\rangle \tag{1.99}$$

and in this case has no energy,

$$H_0 |0\rangle = 0. \tag{1.100}$$

The one particle state for an atom with momentum p is given by

$$a_p^\dagger|0\rangle = |p\rangle. \tag{1.101}$$

This treatment is analogous to the treatment of phonons, although the physics is very different (sound waves vs atoms). Again particles are excitations above the vacuum, the ground state. For phonons we had a vacuum structure, an ether, because they live in crystals. This ether is now gone.

The strength of QFT is that such different systems can be treated with the same formalism.

Again we could do the Fourier transform to coordinate space. There we ask whether an atom is in cell j and use the operators a_j and so on ....

1.4.3 Continuum Limit

Notation

In the discrete case we had

$$a_j \text{ with } [a_i, a_j^\dagger] = \delta_{ij}. \tag{1.102}$$

Now we introduce a continuum notation, i. e. we formulate the problem in terms of continuous variables $x = aj$ instead of discrete lattice sites j. We define

$$\hat{\phi}(x) = a^{-3/2} a_j. \tag{1.103}$$

(Notice that the atom separation a and the operator a_j only share the same letter, but otherwise are totally different things. Unfortunately both notations are so common that we will also use them.) The normalization factor is obtained by looking at the total particle number operator,

$$\hat{N} = \sum_j a_j^\dagger a_j = \int d^3x \hat{\phi}^\dagger(x)\hat{\phi}(x). \tag{1.104}$$

We will use the notation

$$\int_x \quad \equiv \quad \int d^3x \quad \equiv \quad a^3 \sum_j . \tag{1.105}$$

$\hat{\phi}^\dagger(x)\hat{\phi}(x)$ is the operator for the atom number density. The *field operator* $\hat{\phi}$ has dimension length$^{-3/2}$ = mass$^{3/2}$. The field commutator follows as

$$[\hat{\phi}(y), \hat{\phi}^\dagger(x)] = a^{-3}[a_i, a_j^\dagger] = a^{-3}\delta_{ij} \equiv \delta(x-y). \tag{1.106}$$

Check:

$$\int_x \delta(x-y) = a^3 \sum_j a^{-3}\delta_{ij} = 1. \tag{1.107}$$

For the moment $\hat{\phi}$ is only defined at the lattice points. Later when we let $a \to 0$, it will really be a field in space. We try to define our notation in such a way that everything looks the same in the discrete and continuum case.

Fourier Transform of $\hat{\phi}$

We define the Fourier transform

$$\hat{\phi}(q) = \int_x e^{-iqx}\hat{\phi}(x) = a^3 \sum_j e^{-iqaj} a^{-3/2} a_j = a^{3/2} \sum_j e^{-iqaj} a_j. \tag{1.108}$$

We call the number of degrees of freedom in one direction $\mathcal{N}'$, thus

$$L = \mathcal{N}' a \quad \text{and} \quad \mathcal{N} = \mathcal{N}'^3. \tag{1.109}$$

By definition of a_q we then have

$$\hat{\phi}(q) = a^{3/2}\mathcal{N}'^{3/2} a_q = L^{3/2} a_q = V^{1/2} a_q. \tag{1.110}$$

The commutator in momentum space is

$$[\hat{\phi}(q), \hat{\phi}^\dagger(q')] = V\delta_{qq'} = \delta(q - q') \equiv (2\pi)^3 \delta^3(\mathbf{q} - \mathbf{q}'). \tag{1.111}$$

Because we don't want to write 2π factors all the time we define integration and delta function in momentum space as follows:

$$\int_q \equiv \frac{1}{(2\pi)^3} \int d^3q, \quad \text{and} \quad \int_q \delta(q - q') = 1. \tag{1.112}$$

These definitions are motivated by the following equations:

$$\int_q \delta(q - q') = \frac{1}{(2\pi)^3} \int d^3q (2\pi)^3 \delta^3(\mathbf{q} - \mathbf{q}') = 1, \tag{1.113}$$

$$d^3q = \frac{(2\pi)^3}{a^3} = \left(\frac{2\pi}{L}\right)^3 \mathcal{N}'^3, \tag{1.114}$$

$$\int_q 1 = \frac{1}{a^3}, \text{ which is conjugate to } \int_x 1 = L^3 = V. \tag{1.115}$$

<u>Exercise:</u> Show $dq = \frac{1}{(2\pi)^3} d^3q$ and $\sum_k = V \int_q$.

Proof that the 2π's are ok:

$$\begin{aligned}
\hat{\phi}(x) &= \int_q e^{iqx}\hat{\phi}(q) = \frac{1}{(2\pi)^3} \int d^3\mathbf{q} e^{i\mathbf{qx}} \hat{\phi}(\mathbf{q}) \\
&= \frac{1}{(2\pi)^3} \int d^3\mathbf{q} e^{i\mathbf{qx}} \int d^3\mathbf{y} e^{-i\mathbf{qy}} \hat{\phi}(\mathbf{y}) \\
&= \int d^3y \hat{\phi}(y) \frac{1}{(2\pi)^3} \int d^3\mathbf{q} e^{i\mathbf{q}(\mathbf{x}-\mathbf{y})} \\
&= \hat{\phi}(x).
\end{aligned} \tag{1.116}$$

Continuum limit

It is now straightforward to the perform the continuum limit $a \to 0$. We can write the commutator relations in the same way:

$$[\hat{\phi}(q), \hat{\phi}^\dagger(q')] = (2\pi)^3 \delta^3(\mathbf{q} - \mathbf{q}') = \delta(q - q'),$$
$$[\hat{\phi}(y), \hat{\phi}^\dagger(x)] = \delta^3(\mathbf{x} - \mathbf{y}) = \delta(x - y). \tag{1.117}$$

Please note that though the notation is the same, we have to interpret it in a slightly different way. $\hat{\phi}$ and $\hat{\phi}^\dagger$ are now defined over all the space, and of course now we need to consider the 3-dimensional Delta-function in continuum. In fact one can show that $\delta(x-y) = \delta^3(\mathbf{x} - \mathbf{y})$ and $\delta(p-q) = (2\pi)^3\delta^3(\mathbf{p} - \mathbf{q})$, where $\delta^3(x)$ is the 3-dimensional Delta-function in continuum, which we know for instance from electrodynamics. Of course, in this limit no a or L is appearing.

So $\hat{\phi}(x)$ is now an operator valued function of x, it is called the *quantum field operator* or simply the *quantum field*.

Why do we start with a lattice and then perform the limit to the continuum instead of starting with the continuum in the first place?
Because this is a useful preparation for *functional integrals*. There we will have several new concepts, so we try to separate these new concepts. Here we showed how to do the limit from the discrete to the continuum case.

Remark on the continuum limit: When you think about it, in physical theories only dimensionless ratios have physical meaning. When you say some length is 3 meters you mean that the length is three times the length of some other object, which defines the meter. Typically in an experiment you have some characteristic length l. To perform the continuum limit means to take $\frac{l}{a} \to \infty$. This can mean

$$\begin{aligned} &\text{either } l \text{ fixed}, \quad a \to 0, \\ &\text{or } a \text{ fixed}, \quad l \to \infty. \end{aligned} \tag{1.118}$$

In a practical case, a may be fixed from a natural grid, but concentrating on low wavelength is equivalent to making the continuum limit.

1.4.4 Quantum Fields - Summary

Atoms on a Lattice with Finite Volume

Creation operators $a_j^\dagger$, $a_q^\dagger$.
Canonical commutator relation:

$$[a_i, a_j^\dagger] = \delta_{ij} \tag{1.119}$$

Atoms in Continuum and Infinite Volume

Creation operators $\hat{\phi}^\dagger(x)$, $\hat{\phi}^\dagger(q)$
Canonical commutator relation:

$$
\begin{aligned}
\left[\hat{\phi}(y), \hat{\phi}^\dagger(x)\right] &= \delta(x-y) = \delta^{(3)}(\mathbf{x}-\mathbf{y}), \\
\left[\hat{\phi}(q), \hat{\phi}^\dagger(q')\right] &= \delta(q-q') = (2\pi)^3\delta^{(3)}(\mathbf{x}-\mathbf{y}), \\
\int_x &= \int d^3x, \quad \int_q = \int \frac{d^3q}{(2\pi)^3}
\end{aligned}
\tag{1.120}
$$

Limit procedure:

$$
\begin{aligned}
\hat{\phi}^\dagger(x) &= \lim_{a\to 0} a^{-3/2} a_j^\dagger, \\
\hat{\phi}^\dagger(q) &= \lim_{V\to\infty} V^{-1/2} a_q^\dagger
\end{aligned}
\tag{1.121}
$$

Density operator $\hat{n}(x) = \hat{\phi}^\dagger(x)\hat{\phi}(x)$

1.4.5 Atom Gas

We consider an atom gas of bosonic atoms. The free Hamiltonian only has a kinetic term, so it is given by a sum over all q-modes and their kinetic energy $\frac{\mathbf{q}^2}{2M}$, multiplied by the corresponding number operator $\hat{n}_q = a_q^\dagger a_q$:

$$
\begin{aligned}
H_0 &= \sum_q \frac{\mathbf{q}^2}{2M} a_q^\dagger a_q = \int_q \frac{\mathbf{q}^2}{2M} \hat{\phi}^\dagger(q)\hat{\phi}(q) \\
&= \int_x \frac{1}{2M} \nabla\hat{\phi}^\dagger(x)\nabla\hat{\phi}(x),
\end{aligned}
\tag{1.122}
$$

where we have transformed to position space in the last step. As we know from quantum mechanics, the momentum operator corresponds to the ∇-operator in position space. Now we imagine that our atoms are in a local trap, which can be described by an appropriate potential $V_l(x)$. Therefore, we have to add a term

$$
H_V = \int d^3x V_l(x)\hat{n}(x) = \int_x V_l(x)\hat{\phi}^\dagger(x)\hat{\phi}(x). \tag{1.123}
$$

We also introduce a local point-like interaction between the atoms, which means that there is an interaction if there are two atoms at the same point. Like in the case of the self-interaction of electric charges, we assume that this interaction is approximately proportional to $n^2(x)$. More precisely, the interaction Hamiltonian is given by

$$
H_{int} = \int d^3x \frac{\lambda}{2} \hat{\phi}^\dagger(x)\hat{\phi}^\dagger(x)\hat{\phi}(x)\hat{\phi}(x). \tag{1.124}
$$

In operator notation, we notice that $a_j^\dagger a_j^\dagger a_j a_j = a_j^\dagger a_j a_j^\dagger a_j - a_j^\dagger a_j = \hat{n}_j^2 - \hat{n}_j$. So for one-atom states, there is no contribution from this term. We assume $\lambda > 0$, corresponding to a repulsive interaction. This can be seen in the following way. First we assume a two-atom-state with one atom at y, one at x, $y \neq x$. Then $H_{int}\hat{\phi}^\dagger(y)\hat{\phi}^\dagger(x)|0\rangle = 0$. However for two atoms at x, we have $H_{int}\hat{\phi}^\dagger(x)\hat{\phi}^\dagger(x)|0\rangle = \lambda$. So it is energetically preferred to have the atoms at different places.

Up to know we have assumed that the number of atoms N in our trap is fixed, which gives us the additional constraint

$$\int_x \hat{\phi}^\dagger(x)\hat{\phi}(x)|\Psi\rangle = N|\Psi\rangle \tag{1.125}$$

Now as in statistical mechanics, we drop this constraint and introduce the chemical potential μ. Now the total Hamiltonian is given by

$$\begin{aligned} H_\mu &= H - \mu\hat{N} \\ &= \int_x \left\{ \hat{\phi}^\dagger(x)\,\Big[-\frac{\Delta}{2M} - \mu + V_l(x)\Big]\,\hat{\phi}(x) + H_{int}\right\}. \end{aligned} \tag{1.126}$$

As we know from statistical mechanics, the system is now determined by the partition function, given by

$$Z \propto tr e^{-\beta H_\mu}. \tag{1.127}$$

1.4.6 From Quantum Field Theory to Quantum Mechanics for a One-Atom State

By now, we have used concepts from quantum mechanics and extended them to build up a quantum theory of fields, the quantum field theory. Now we want to show that we can also go the way back and that we can recover quantum mechanics by considering a one-atom state. Such a state has to fulfill the constraint equation

$$\hat{N}|\Psi\rangle = |\Psi\rangle = \int_x \hat{\phi}^\dagger(x)\hat{\phi}(x)|\Psi\rangle. \tag{1.128}$$

A general one-atom state is given by a superposition of one-atom states, i. e.

$$|\Psi\rangle(t) = \int_x \Psi(x,t)\hat{\phi}^\dagger(x)|0\rangle. \tag{1.129}$$

As we will see, $\Psi(x,t)$ is the Schrödinger wave function we know from quantum mechanics. In fact (1.129) is the most general one-atom state. This can be seen in the following way. A general physical state can be expressed as

$$\begin{aligned} |\Psi\rangle(t) = \psi_0|0\rangle + \int_x \Psi(x,t)\hat{\phi}^\dagger(x)|0\rangle + \int_{x,y} \Psi_2(x,y)\hat{\phi}^\dagger(x)\hat{\phi}^\dagger(y)|0> \\ + \int_{x,y,z} \Psi_3(x,y,z)\hat{\phi}^\dagger(x)\hat{\phi}^\dagger(y)\hat{\phi}^\dagger(z)|0\rangle + \ldots \end{aligned} \tag{1.130}$$

Now let's consider the following commutators:

$$\begin{aligned}\left[\hat{N}, \hat{\phi}^\dagger(x)\right] &= \hat{\phi}^\dagger(x), \\ \left[\hat{N}, \hat{\phi}^\dagger(x)\hat{\phi}^\dagger(y)\right] &= 2\hat{\phi}^\dagger(x)\hat{\phi}^\dagger(y), \ldots\end{aligned} \tag{1.131}$$

Now if we let these operators act on the vacuum, we can see that for a one particle state there are no terms in the superposition with more than one creation operator. Additionally we also cannot add a term proportional to the ground state$|0\rangle$, since we want to consider an eigenstate of $\hat{N}$. Now the time evolution of a non-relativistic physical state is given by the Schrödinger equation

$$\begin{aligned}i\partial_t|\Psi\rangle &= H|\Psi\rangle \\ &= \int_y \left\{\hat{\phi}^\dagger(y)\left[-\frac{\Delta}{2M} + V_l(y)\right]\hat{\phi}(y)\right\}|\Psi\rangle \\ &\quad + \int_y \frac{\lambda}{2}\hat{\phi}^\dagger(y)\hat{\phi}^\dagger(y)\hat{\phi}(y)\hat{\phi}(y)|\Psi\rangle.\end{aligned} \tag{1.132}$$

We insert (1.129) in the last equation and use the canonical commutator relation for $\hat{\phi}(y)$ and $\hat{\phi}^\dagger(x)$. Since (1.129) describes a one-atom state, the interaction term vanishes and we end up with

$$\begin{aligned}H|\Psi\rangle &= \int_x \left[-\frac{\Delta_x}{2M} + V_l(x)\right]\Psi(x)\hat{\phi}^\dagger(x)|0\rangle \\ &= \int_x i\partial_t\Psi(x,t)\hat{\phi}^\dagger(x)|0\rangle = i\partial_t|\Psi\rangle\end{aligned} \tag{1.133}$$

So indeed we can see that Ψ is the wave function we know from quantum mechanics, which fulfills the Schrödinger equation

$$i\partial_t\Psi(x,t) = (-\frac{\Delta}{2M} + V_l(x))\Psi(x,t). \tag{1.134}$$

In contrast to typical evolution equations in Quantum Field Theory, (1.134) is a linear equation for the wave function. In QFT, we usually have non-linear operator equations with non-zero interaction terms, but as shown here, one can always go back to quantum mechanics by considering only one-atom states.

1.4.7 Heisenberg Picture for Field Operators

In the Schrödinger picture we have used so far, the physical states depend on t and their evolution is given by the Schrödinger equation (1.132), whereas the operators do not depend on time (unless there is an explicit time dependence, for instance if we want to assume that our atoms are caught in a trap with a time-dependent potential. However in the usual QFT problems, we will have no explicit time dependence.)

Now in the Heisenberg picture, there is no time evolution for the physical states, but the operators will depend on time. Given an operator $\hat{A}_S$ from the Schrödinger picture, we can switch to the Heisenberg picture by the following transformation:

$$\hat{A}(t) = e^{iHt}\hat{A}_S e^{-iHt}. \tag{1.135}$$

In the usual case where the Schrödinger operator does not depend explicitly on time, the time evolution for the corresponding Heisenberg operator is given by

$$i\partial_t \hat{A} = -[H, \hat{A}]. \tag{1.136}$$

From now on we will use the Heisenberg picture if not stated otherwise, since it is much more convenient to describe QFT in this picture. The reason is that now field operators depend on space and time, so space and time are treated in the same way. This is important when we go to relativistic situations, where space and time are no longer independent, but rotated into each other by Lorentz-transformations.

1.4.8 Field Equation for $\hat{\phi}(x,t)$

For fixed t, the Heisenberg operators $\hat{\phi}(x), \hat{\phi}^\dagger(x)$ obey the same canonical commutator relations as in the Schrödinger picture:

$$\begin{aligned}
\left[\hat{\phi}^\dagger(y), \hat{\phi}(x)\right] &= -\delta(x-y) \\
\left[\hat{\phi}^\dagger(y)\hat{\phi}^\dagger(y), \hat{\phi}(x)\right] &= -2\delta(x-y)\hat{\phi}^\dagger(y)
\end{aligned} \tag{1.137}$$

According to (1.136), the evolution equation for the field $\hat{\phi}(x,t)$ is given by

$$\begin{aligned}
i\partial_t\hat{\phi}(x,t) &= -[H, \hat{\phi}(x,t)] \\
&= -\left[\int_y \left\{\hat{\phi}^\dagger(y,t)\left[-\frac{\Delta}{2M} + V_l(y) - \mu\right]\hat{\phi}(y,t) + H_{int}\right\}, \hat{\phi}(x,t)\right] \\
&= -\int_y \left\{\left[\hat{\phi}^\dagger(y,t), \hat{\phi}(x,t)\right]\left(-\frac{\Delta_y}{2M} + V_l(y,t) - \mu\right)\hat{\phi}(y,t)\right\} - \\
&\quad -\int_y \frac{\lambda}{2}\left[\hat{\phi}^\dagger(y,t)\hat{\phi}^\dagger(y,t), \hat{\phi}(x,t)\right]\hat{\phi}(y,t)\hat{\phi}(y,t) \\
\Rightarrow i\partial_t\hat{\phi}(x,t) &= \left(-\frac{\Delta_x}{2M} + V_l(x) - \mu\right)\hat{\phi}(x,t) + \lambda\hat{\phi}^\dagger(x,t)\hat{\phi}(x,t)\hat{\phi}(x,t)
\end{aligned} \tag{1.138}$$

In contrast to the quantum mechanical Schrödinger equation (1.134), this equation is a highly nonlinear operator differential equation. This is a typical situation for the complications occurring in QFT.

Expectation Values

The equation (1.138) is valid for any arbitrary state in the Heisenberg picture. We can define the expectation value for the field operator $\hat{\phi}$:

$$\langle\hat{\phi}(x,t)\rangle = \langle\psi|\hat{\phi}(x,t)|\psi\rangle, \tag{1.139}$$

and with more operators ...

$$\langle\hat{\phi}^\dagger(x,t)\hat{\phi}(x,t)\hat{\phi}(x,t)\rangle = \langle\psi|\hat{\phi}^\dagger(x,t)\hat{\phi}(x,t)\hat{\phi}(x,t)|\psi\rangle \tag{1.140}$$

Remarks on the Phrase 'The Second Quantization'

Until now, we have seen the system of a one particle state, described by the Schrödinger equation. We have also derived the time evolution equation (1.138) for a many particle state. Some authors refer to quantum mechanics as the first quantization, then precede to call the transition $\phi_{QM}(x) \to \hat{\phi}_{QFT}(x)$ the second quantization. But this is generally wrong, due to the fact, that the Schrödinger equation is linear in $\phi(x)$, while the time evolution equation is *not* linear in $\hat{\phi}(x)$, simply because of the interactions between the particles in $|\Psi\rangle$.

Comments on interpretations

- We know now that the vacuum is described by the ground state $|0\rangle$, which is not 0, but can be rather complex. The particles are described as excitations of the ground state, $\hat{\phi}^\dagger(x,t)|0\rangle$, with the creation operator $\hat{\phi}^\dagger$. The number density operator is defined by $\widehat{n}(x,t) = \hat{\phi}^\dagger(x,t)\hat{\phi}(x,t)$. So a rather weak interpretation of $\hat{\phi}$ is

  $$\hat{\phi}(x,t)\text{='Square root of the density } \widehat{n}(x,t)$$

- **Analogy to continuum mechanics**

  In classical mechanics, one has the observables $q_i(t), p_i(t)$ for systems with few degrees of freedom. Changing to systems with any degrees of freedom, that is changing to statistical mechanics, we then desire to look at the density field $\rho(x,t)$.

  In quantum mechanics, we have the hermitian operators $Q_i(t), P_i(t)$, for one particle systems. Just like in the classical view, we can change to a system with many particles, and look at the density operator $\hat{\phi}^\dagger(x,t)\hat{\phi}(x,t)$ in quantum field theory. Like in statistical mechanics, one can recover QM from QFT.

  In QM, the probability density of a one particle state described by the wave function $\Psi(x,t)$ is given by $\Psi^*\Psi$. As we know, this density is normalized to 1. In QFT one has the number density from above, which is normalized to N, the number of particles in a given state ($\langle\Psi|\hat{\phi}^\dagger\hat{\phi}|\Psi\rangle = N$)

1.5 Correlation Functions, Propagator

1.5.1 One Particle States

To see what a correlation function is, we will look at a one particle nonrelativistic, bosonic state.

Schrödinger Picture

On the lattice, the operator $a_j^\dagger$ creates an atom at site j. The normalization is $\langle 0|a_j a_j^\dagger|0\rangle = 1$. So with the number operator $\widehat{n}_i = a_i^\dagger a_i$, we get $\widehat{n}_i a_j^\dagger|0\rangle = \delta_{ij} a_j^\dagger|0\rangle$. This means $a_j^\dagger|0\rangle$ is an eigenvector of $\widehat{n}_i$, with eigenvalue δ_{ij}

In the continuum we have an atom at a specific point x, described by $\hat{\phi}^\dagger(x)|0\rangle$, but in what sense? Well if we look at $\langle 0|\hat{\phi}(x)\hat{\phi}^\dagger(x)|0\rangle$, we see that this is $\delta(x)$, meaning that the state is normalized to one. Now applying the number operator $\hat{n}(y)$ to $\hat{\phi}^\dagger(x)|0\rangle$ we get

$$\hat{n}(y)\hat{\phi}^\dagger(x)|0\rangle = \delta(x-y)\hat{\phi}^\dagger(x)|0\rangle \tag{1.141}$$

So we see, $\hat{\phi}^\dagger(x)|0\rangle$ is an eigenvector of $\hat{n}(y)$ with the eigenvalue $\delta(x-y)$. This also tells us, in our state $\hat{\phi}^\dagger(x)|0\rangle$ we have one particle.

There is a major fault in the Schrödinger picture: our state $\hat{\phi}^\dagger(x)|0\rangle$ is only given at *t=0*. Generally the particle will move, and at $t \neq 0$ it will be at y. This means $\hat{\phi}^\dagger(y)|0\rangle$ is not an eigenstate of $\hat{n}(x)$, because $[\hat{n}(x), H] \neq 0$, due to the $\nabla\hat{\phi}^\dagger\nabla\hat{\phi}$ term in H. This is why we turn to the …

Heisenberg Picture

In this picture, the operators are time dependant, and the states are time independent. The Heisenberg operator is given by

$$\hat{\phi}_H^\dagger(x,t) = e^{iHt}\hat{\phi}_S^\dagger(x)e^{-iHt} \tag{1.142}$$

The states are given by $|x;t\rangle = \hat{\phi}^\dagger(x,t)|0\rangle$, for all t. This state is TIME INDEPENDENT! The notion $|x;t\rangle$ is to be read like: *An atom created at x, at the time t. Thus t does* **not** *denote a time dependence of the state in the Heisenberg picture.*

In this picture, our number operator $\hat{n}(x,t) = \hat{\phi}^\dagger(x,t)\hat{\phi}(x,t)$ acts upon a state like

$$\hat{n}(y,t)|x,t\rangle = \delta(x-y)|x,t\rangle \tag{1.143}$$

The normalization is like usual $\langle y,t|x,t\rangle = \delta(x-y)$. The Fourier transform of $|x;t\rangle$ is $|p;t\rangle = \hat{\phi}^\dagger(p,t)|0\rangle = \int_x e^{-ipx}\hat{\phi}^\dagger(x,t)|0\rangle = \int_x e^{-ipx}|x;t\rangle$, so we find out: $\langle p',t|p,t\rangle = \delta(p'-p)$

1.5.2 Transition Amplitude

We are now interested in calculating the transition probability, for a particle moving from x, at time t, to x', at time t'.This is given by the overlap of the states $|x;t\rangle$ and $|x';t'\rangle$ and we define for $t' \geq t$

$$\langle x',t'|x,t\rangle = \langle 0|\hat{\phi}(x',t')\hat{\phi}^\dagger(x,t)|0\rangle = G(x',t',x,t) \tag{1.144}$$

This function is called the *propagator* (also correlation function, Green's function, two-point function, correlator). It appears when one describes scattering processes, e.g. those described by the graphs

1.5.3 Completeness

The completeness statement $\int_x |x,t\rangle\langle x,t| = \mathbf{1}$, is in general only true for one particle states. A proof for such a state can be sketched by proving
$\int_x \langle z,t|x,t\rangle\langle x,t|y,t\rangle \equiv \delta(z-y)$. One does this, by showing $\int_x \langle\Psi'|x,t\rangle\langle x,t|\Psi\rangle = \langle\Psi'|\Psi\rangle$ for an arbitrary state $|\Psi\rangle = \int_y \Psi(y)|y,t\rangle$. One then reverts back to the lattice, and knowing that the completeness relation is valid on the lattice, one then let's the lattice spacing $a \to 0$.

1.5.4 Huygens Principle

We know from Huygens principle, that any state $|x',t'\rangle$ can be expressed as a superposition of a complete set $\{\ |x,t\rangle\ \}$ via:

$$|x',t'\rangle = \int_x |x,t\rangle\langle x,t|x',t'\rangle = \int_x |x,t\rangle G^*(x',t',x,t) \tag{1.145}$$

Looking at the state $|\Psi\rangle = \int_y \Psi(y)|y,t\rangle$, the coefficients are given by $\Psi(x,t) = \langle x,t|\Psi\rangle$. This leads to

$$\Psi(x',t') = \langle x',t'|\Psi\rangle = \int_x G(x',t',x,t)\Psi(x,t) \tag{1.146}$$

This means in words: *If Ψ is known at t, then $\Psi' = \Psi(x',t')$ is also known at t' if one knows G.*

This is what makes G so unique in QFT. Important problems in QFT are solved if one has found G, which is definitely not an easy task. For this reason, we will first calculate G for free particles

1.5.5 The Propagator G

The propagator G obeys for $t' \geq t$

$$G(x',t',x,t) = \langle 0|\hat{\phi}(x',t')\hat{\phi}^\dagger(x,t)|0\rangle \quad = \langle 0|e^{iHt'}\hat{\phi}_S(x')e^{-iHt'}e^{iHt}\hat{\phi}_S^\dagger(x)e^{-iHt}|0\rangle. \tag{1.147}$$

Using $H|0\rangle = 0$ we get

$$G(x',t',x,t) = \langle 0|\hat{\phi}_S(x')e^{-iH(t'-t)}\hat{\phi}_S^\dagger(x)|0\rangle \tag{1.148}$$

and we recover for $t' = t$:

$$G(x',t,x,t) = \delta(x-x') \tag{1.149}$$

1.5.6 Free Non-Relativistic Propagator

For simplicity we consider non-interacting atoms without a potential.

$$H = \int_p \frac{p^2}{2M}\hat{\phi}^\dagger(p)\hat{\phi}(p) \tag{1.150}$$

In momentum space the free propagator is particularly simple.

$$\begin{aligned} G(p',t',p,t) &= \langle 0|\hat{\phi}(p',t')\hat{\phi}^\dagger((p,t)|0\rangle \\ &= \langle 0|\hat{\phi}_S(p')e^{-iH(t'-t)}\hat{\phi}_S^\dagger(p)|0\rangle \end{aligned} \tag{1.151}$$

with the commutator relations

$$\begin{aligned} [H,\hat{\phi}^\dagger(p)] &= \frac{p^2}{2M}\hat{\phi}^\dagger(p) \\ [H^2,\hat{\phi}^\dagger(p)] &= \left(\frac{p^2}{2M}\right)^2\hat{\phi}^\dagger(p) + \frac{p^2}{M}\hat{\phi}^\dagger(p)H \\ &\vdots \end{aligned} \tag{1.152}$$

Of course the Hamilton function of the vacuum gives zero.

$$H|0\rangle = 0 \tag{1.153}$$

This way we can move the exponential function to the right to get an explicit expression for the Green's function.

$$G(p',t',p,t) = \langle 0|\hat{\phi}_S(p')\hat{\phi}_s^\dagger(p)e^{-\frac{ip^2}{2M}(t'-t)}|0\rangle \tag{1.154}$$

or

$$\boxed{G(p',t',p,t) = e^{\frac{-ip^2}{2M}(t'-t)}\delta(p'-p)} \tag{1.155}$$

Exactly as one would expect we only gain an additional phase factor but have no change in momentum.

To get the propagator in coordinate space we have to do a Fourier transform for both momenta, p and p'

$$\begin{aligned} G(x',t',x,t) &= \int_p\int_{p'} e^{-ip'x'}e^{ipx}G(p',t',p,t) \\ &= \int_p e^{-ip(x'-x)}e^{-i\frac{p^2}{2M}(t'-t)}. \end{aligned} \tag{1.156}$$

To solve this integral we bring the exponent to the form $(p+\alpha)^2$ which gives

$$\begin{aligned} G(x',t',x,t) &= \int_p \exp\left(-i\frac{t'-t}{2M}\left(p+\frac{(x'-x)M}{t'-t}\right)^2 + i\frac{t'-t}{2M}\left(\frac{(x'-x)M}{t'-t}\right)^2\right) \\ &= \exp\left(i\frac{M}{2}\frac{(x'-x)^2}{t'-t}\right)\cdot\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}y\, e^{-i\frac{t'-t}{2M}y^2}\right)^3. \end{aligned} \tag{1.157}$$

In the last step we did the variable transform $y := p + \frac{(x'-x)M}{t'-t}$ with one integral for each component of p. The integral is called the Fresnel's integral its solution is

$$\int_{\infty}^{\infty} \mathrm{d}y\, e^{-i\alpha y^2} = \sqrt{\frac{\pi}{2\alpha}}(1-i) \tag{1.158}$$

(for a proof see section 1.5.6). Thus we get for $\tau = i(t'-t)$

$$\boxed{G = \left(\frac{M}{2\pi\tau}\right)^{\frac{3}{2}} e^{-\frac{M}{2\tau}(x'-x)^2}.} \tag{1.159}$$

To verify our calculation we check if G becomes a delta function in the limit $\tau = i(t'-t) \to 0$. We get

$$\lim_{\tau\to 0} G = \prod_{i=1}^{3} \sqrt{\frac{M}{2\pi\tau}} e^{-\frac{M(x_i'-x_i)^2}{2\tau}} = \delta^3(x'-x) \tag{1.160}$$

which confirms our result.

In position space propagators are not easy objects (waves get broadened and position changes), so better avoid it. On the other hand operators are diagonal and not changing momentum in momentum space. This makes calculations much easier.

Proof of the Fresnel Integral (Not from Lecture)

Fresnel's integral is $\int_0^\infty e^{-it^2}\,\mathrm{d}t$.

Let $f(z) := e^{-z^2}$. The function f is holomorphic in $\mathbb{C}$ and the integral from one point to another is path independent because $\mathbb{C}$ is a star domain. This means

$$\int_{\gamma_1} f\,\mathrm{d}z + \int_{\gamma_2} f\,\mathrm{d}z = \int_{\gamma_3} f\,\mathrm{d}z \tag{1.161}$$

as pictured in figure 1.1.

1. Now, we consider the integral of f along γ_2. For $\gamma_2(t) = r + it$, $t \in [0, r]$ follows

$$\begin{aligned} & |f(\gamma_2(t))| = e^{-r^2+t^2} \le e^{-r^2} e^{rt} \\ \Rightarrow\quad & \left|\int_{\gamma_2} f\,\mathrm{d}z\right| \le \int_0^r |f(\gamma_2(t))|\,\mathrm{d}t \\ & \qquad \le e^{-r^2}\int_0^r e^{rt}\,\mathrm{d}t < \frac{1}{r} \\ \Rightarrow\quad & \lim_{r\to\infty}\int_{\gamma_2} f\,\mathrm{d}z = 0. \end{aligned} \tag{1.162}$$

With equation (1.161) this leads to

$$\lim_{r\to\infty}\int_{\gamma_3} f\,\mathrm{d}z = \lim_{r\to\infty}\int_{\gamma_1} f\,\mathrm{d}z \tag{1.163}$$

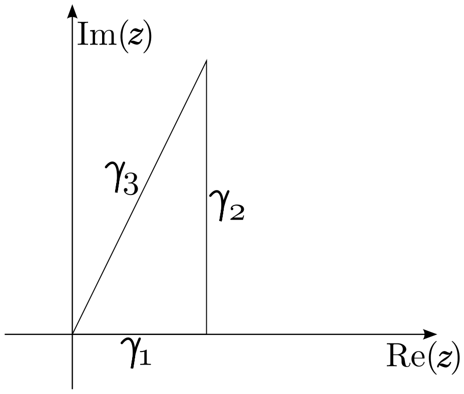


Figure 1.1: Scetch for the proof of the Fresnel integral

2. The integral along γ_1 is a Gaussian integral

$$\lim_{r\to\infty}\int_{\gamma_1} f\,\mathrm{d}z = \int_0^\infty e^{-t^2}\,\mathrm{d}t = \frac{1}{2}\sqrt{\pi} \tag{1.164}$$

3. Now, we consider the integral along γ_3.

$$\begin{aligned}\lim_{r\to\infty}\int_{\gamma_3} f\,\mathrm{d}z &= (1+i)\int_0^\infty e^{-(1+i)^2t^2}\,\mathrm{d}t\\ &= (1+i)\int_0^\infty e^{-2it^2}\,\mathrm{d}t\\ &= \frac{1+i}{\sqrt{2}}\int_0^\infty e^{i\tau^2}\,\mathrm{d}\tau\end{aligned} \tag{1.165}$$

Because of the identity (1.163) the Fresnel integral exists and has the value

$$\boxed{\int_0^\infty e^{i\tau^2}\,\mathrm{d}\tau = \frac{\sqrt{2\pi}}{4}(1-i)} \tag{1.166}$$

1.5.7 Time Dependence

G only depends on $\Delta t = t' - t$ and has been defined so far only for $t' \geq t$:

$$G(p', t', p, t) = G(p, \Delta t)\delta(p' - p) \tag{1.167}$$

There are different definitions for how to extend a Green's function to $t' < t$. One possibility continues the definition (1.144) for all times t':

$$\begin{aligned}G_S &= \langle 0|\hat{\phi}(x', t)\hat{\phi}^\dagger(x, t)|0\rangle\\ &= \langle 0|[\hat{\phi}(x', t)\hat{\phi}^\dagger(x, t)]|0\rangle\end{aligned} \tag{1.168}$$

We make a Fourier transform from time into frequency space.

$$\begin{aligned} G_S(p,\omega) &= \int_{-\infty}^{\infty} e^{i\omega\Delta t} G_S(p,\Delta t)\,\mathrm{d}\Delta t \\ &= \int_{-\infty}^{\infty} e^{i\Delta t(\omega-\frac{p^2}{2M})}\,\mathrm{d}\Delta t \\ &= 2\pi\delta\left(\omega-\frac{p^2}{2M}\right) \end{aligned} \tag{1.169}$$

The spectral function

$$G_S(p,\omega) = 2\pi\delta\left(\omega-\frac{p^2}{2M}\right) \tag{1.170}$$

gives information about the particle content. Delta functions generally denote stable particles. Unstable particles are characterized by resonance peaks with their decay width.

1.5.8 Higher Correlation Functions

We consider the scattering of two incoming particles with momentum p_1 and p_2 into two outgoing particles with momentum p_3 and p_4. The transition amplitude for this event is

$$\langle 0|\hat{\phi}(p_3,t')\hat{\phi}(p_4,t')\hat{\phi}^\dagger(p_1,t)\hat{\phi}^\dagger(p_2,t)|0\rangle. \tag{1.171}$$

Here the incoming particles states refer to $t \to -\infty$ (i.e. an incoming two particle state present long times before the scattering event) and outgoing ones to $t' \to \infty$.

We get a four-point function because we have two particles.

We introduce the index notation

$$\begin{aligned} &\hat{\phi}_\alpha(p,t), \qquad \alpha = 1,2 \\ &\hat{\phi}_1(p,t) = \hat{\phi}(p,t), \quad \hat{\phi}_2(p,t) = \hat{\phi}^\dagger(p,t) \end{aligned} \tag{1.172}$$

We furthermore consider n times with $t_n \geq t_{n-1} \geq \cdots \geq t_1$ and define

$$\begin{aligned} &G^{(n)}_{\alpha_n\ldots\alpha_1}(p_n,t_n;p_{n-1},t_{n-1};\ldots;p_2,t_2;p_1,t_1) \\ &= \langle 0|\hat{\phi}_{\alpha_n}(p_n,t_n)\ldots\hat{\phi}_{\alpha_2}(p_2,t_2)\hat{\phi}_{\alpha_1}(p_1,t_1)|0\rangle \end{aligned} \tag{1.173}$$

1.5.9 Time Ordered Correlation Functions

We introduce the time ordering operator, it puts the <u>l</u>ater t to the <u>l</u>eft:

$$T\{O(t_1)O(t_2)\} = \begin{cases} O(t_1)O(t_2) \text{ if } t_1 > t_2 \\ O(t_2)O(t_1) \text{ if } t_1 < t_2 \end{cases} \tag{1.174}$$

This operator is only well defined if $t_1 \neq t_2$ or for $t_1 = t_2$ only if $[O(t_1), O(t_2)] = 0$.

With the use of the time ordering operator we get

$$\begin{aligned}
&G^{(n)}_{\alpha_1\ldots\alpha_2}(p_n,t_n;p_{n-1},t_{n-1};\ldots;p_2,t_2;p_1,t_1) \\
&\quad= \langle 0|T\{\hat{\phi}_{\alpha_n}(p_n,t_n)\ldots\hat{\phi}_{\alpha_1}(p_1,t_1)\}|0\rangle
\end{aligned} \tag{1.175}$$

which defines the Green's function for arbitrary ordering of times. The time ordering operator erases the information of the initial time ordering of the operators which provides for much easier calculations. The Green's function is now symmetric under the exchange of indices

$$(\alpha_j,p_j,t_j) \leftrightarrow (\alpha_k,p_k,t_k). \tag{1.176}$$

This symmetry reflects the bosonic character of the scattered particles. For fermions it will be replaced by antisymmetry.

$$\boxed{G^n \text{ is the key to QFT.}} \tag{1.177}$$

In future we will only compute time ordered Green's functions.

1.5.10 Time Ordered Two-Point Function

As an example for the time ordered correlation functions we write down the time ordered two-point function using this formalism.

$$\begin{aligned}
G(x',t',x,t) &= \langle 0|T\{\hat{\phi}(x',t')\hat{\phi}^\dagger(x,t)\}|0\rangle \\
&= \begin{cases} G_S \text{ for } t'>t \\ 0 \text{ for } t'<t \end{cases} \\
&= G_S(x',t',x,t)\Theta(t'-t)
\end{aligned} \tag{1.178}$$

Notice that the limit $t' \to t$ is simple for the spectral function but not a simple limit for the time ordered correlation function since it is ill defined.

For the time ordered operator products we have the identities

$$\begin{aligned}
T\{[\hat{A}(t'),\hat{B}(t)]\} &= 0, \\
T\{\hat{A}(t')\hat{B}(t)\} &= \frac{1}{2}T\{\hat{A}(t')\hat{B}(t)\} + \frac{1}{2}T\{\hat{B}(t)\hat{A}(t')\} \\
&= T\{\frac{1}{2}\{\hat{A}(t'),\hat{B}(t)\}_+\}.
\end{aligned} \tag{1.179}$$

2 Path Integrals

2.1 Path Integral for a Particle in a Potential

At this point we take one step back and only consider a one-dimensional one-particle problem in classical quantum mechanics without explicit time dependency. We can later easily generalize it to 3D bosonic systems.

2.1.1 Basis of Eigenstates

In the Heisenberg picture we have the operators $Q(t)$ and $P(t)$ with the commutator relation

$$[Q(t), P(t)] = i \tag{2.1}$$

and the Hamiltonian

$$H = \frac{P^2}{2M} + V(Q). \tag{2.2}$$

We introduce a basis of eigenstates $|q,t\rangle$ with

$$Q(t)|q,t\rangle = q(t)|q,t\rangle. \tag{2.3}$$

Note that the basis $|q,t\rangle$is only a basis of eigenstates of $Q(t)$ at time t, it is not an eigenstate of $Q(t')$ for $t' \neq t$. Don't confuse this with the Schrödinger picture, where the states are time dependent. Here we work in the Heisenberg picture where $|q,t\rangle$ and $|q,t'\rangle$ are two different basis sets of time - independent states, one eigenstates of $Q(t)$, the other of $Q(t')$. The states $|q,t\rangle$ are normalized at equal time to

$$\langle q',t|q,t\rangle = \delta(q'-q). \tag{2.4}$$

and the basis is complete

$$\int \mathrm{d}q\,|q,t\rangle\langle q,t| = 1 \tag{2.5}$$

We also introduce a basis of eigenstates in momentum space $|p,t\rangle$with

$$P(t)|p,t\rangle = p(t)|p,t\rangle. \tag{2.6}$$

Again $|p,t\rangle$is only a basis of eigenstates at time t, it is not an eigenstate of $P(t')$ for $t' \neq t$. The relations

$$\langle p', t|p,t\rangle = 2\pi\delta(p'-p) \qquad \text{and} \qquad \int \frac{\mathrm{d}p}{2\pi}|p,t\rangle\langle p,t| = 1 \tag{2.7}$$

are similar to those for the position space.

The transition from the basis in position space to the basis in momentum space is defined through the relations

$$\begin{aligned}\langle p,t|q,t\rangle &= e^{-ipq},\\ \langle q,t|p,t\rangle &= e^{ipq}\end{aligned} \tag{2.8}$$

To avoid confusion we straighten out the connection of these states to the Schrödinger picture. The state $|q\rangle$ of the Schrödinger picture is equivalent to the state $|q,t=0\rangle$. To get the state $|q,t\rangle$we need to time evolve the state $|q\rangle$ of the Schrödinger picture to get $|q,t\rangle = e^{iHt}|q\rangle$. Summarizing this we have

$$\begin{aligned}|q\rangle &= |q,t=0\rangle & p &= |p,t=0\rangle\\ |q,t\rangle &= e^{iHt}|q\rangle & |p,t\rangle &= e^{iHt}|p\rangle.\end{aligned} \tag{2.9}$$

Let's check the relations mentioned above. We calculate the eigenvalue of $\hat{Q}(t)$for a ket $|q,t\rangle$by transforming into the Schrödinger picture and back again. The calculation

$$\begin{aligned}Q(t)|q,t\rangle &= Q(t)e^{iHt}|q\rangle\\ &= e^{iHt}Q_S e^{-iHt}e^{iHt}|q\rangle\\ &= e^{iHt}Q_S|q\rangle\\ &= e^{iHt}q|q\rangle\\ &= q|q,t\rangle\end{aligned} \tag{2.10}$$

leads to the desired result. It is also immediately obvious that

$$\langle p,t,|q,t\rangle = \langle p|q\rangle = e^{-ipq} \tag{2.11}$$

2.1.2 Transition Amplitude

The probability amplitude for a transition from an eigenstate of $Q(t)$ to an eigenstate of $Q(t')$ is given by the transition amplitude:

$$\begin{aligned}G(q',t',q,t) &= \langle q',t'|q,t\rangle\\ &= \langle q',t|e^{-iH(t'-t)}|q,t\rangle\end{aligned} \tag{2.12}$$

(We use here the symbol G since we will later see the analogy to the correlation function when $Q(t)$ is replaced by $\hat{\phi}(x,t)$.) Our aim is now to give $G(q',t',q,t)$ a path integral expression. In order to do this, we will compute the transition amplitude for an infinitesimal time step dt, which is actually the only one that can be computed explicitly. In the end, we will make the limit procedure $dt \to 0$.

2.1.3 Infinitesimal Transition Amplitude

We are now interested in the infinitesimal transition amplitude

$$\langle q', t + dt | q, t\rangle = \langle q', t| e^{-iH\cdot dt} |q, t\rangle. \tag{2.13}$$

If we use the Taylor expansion of the exponential function, we get

$$\langle q', t + dt | q, t\rangle = \langle q', t| \mathbf{1} - iH dt |q, t\rangle. \tag{2.14}$$

Although the Taylor expansion of the exponential function up to first order is very often used in theoretical physics without worry to much about this, one usually has to show, that terms of higher order are *really* unimportant in the limit $dt \to 0$. This is mathematically *very* complicated and so we will not deal with this problem here.

We insert now the completeness relation $\mathbf{1} = \int \frac{dp}{2\pi} |p, t\rangle\langle p, t|$ into (2.14). We get

$$\langle q', t + dt | q, t\rangle = \int \frac{dp}{2\pi} \langle q', t| \mathbf{1} - iH dt |p, t\rangle\langle p, t|q, t\rangle \tag{2.15}$$

We now want to restrict ourselves to Hamiltonians of the form

$$H = \frac{\left(P^2(t)\right)^2}{2M} + V(Q(t)). \tag{2.16}$$

The time dependence of the operators P and Q tells us that we will work in the Heisenberg picture.

Actually, Hamiltonians that are given by (2.16) have a big advantage, because we can now easily compute the matrix element of H appearing in equation (2.15):

$$\langle q', t| H |p, t\rangle = \langle q', t| \frac{(P(t))^2}{2M} |p, t\rangle + \langle q', t| V(Q(t)) |p, t\rangle \tag{2.17}$$

This is now very simple, because we can use the eigenstate properties of $\left(P(t)\right)^2$ to the ket vector and the eigenstate properties of $V(Q(t))$ to the bra vector. The result is

$$\begin{aligned}\langle q', t| H |p, t\rangle &= \left(\frac{p^2}{2M} + V(q')\right)\langle q', t|p, t\rangle \\ &= H(q', p)\langle q', t|p, t\rangle,\end{aligned} \tag{2.18}$$

where q' and p are now the position space and momentum eigenvalues to the operators $Q(t)$ and $P(t)$. Inserting this into equation (2.15) we get

$$\langle q', t | q, t + dt\rangle = \int \frac{dp}{2\pi} \left(1 - iH(q', p)dt\right) \langle q', t|p, t\rangle\langle p, t|q, t\rangle. \tag{2.19}$$

For the term $(1 - iH(q', p)dt)$ we can now write again the exponential function. Furthermore, the scalar products as well give exponential functions, so our infinitesimal transition amplitude can be written as

$$\langle q', t + dt | q, t\rangle = \int \frac{dp}{2\pi} \exp\left(ip(q' - q) - iH(q', p)dt\right) \tag{2.20}$$

Please remember that this result is only valid for Hamiltonians that can be written as $H = \frac{\left(P(t)\right)^2}{2M} + V\big(Q(t)\big)$ and for really infinitesimal time steps, where terms proportional to dt^2 can be neglected. Imagine the difficulties we would be faced with, if we have an H^2: in this case we could *not* compute the matrix element just by using the eigenstate properties. It would be necessary to commute $\widehat{P}$ and $\widehat{Q}$ terms first.

Nevertheless, we are of course interested in transition amplitudes for *finite* time steps. Getting this out of our result for infinitesimal time steps will be the task of the next paragraph.

2.1.4 Split of Amplitudes in Product of Infinitesimal Amplitudes

a) Split Time Interval

The basic idea is to split up a finite time interval $t' - t$ ($t' > t$) into $N + 1$ infinitesimal time steps. Therefore we insert N "lattice points" $\tau_i, i = 1 \ldots N$ in time, so that we get

$$t < \tau_1 < \tau_2 < \ldots < \tau_{N-1} < \tau_N < t'. \tag{2.21}$$

The time distance from each τ_i to the neighboring points is $d\tau$. In the end we will do the limit procedure $N \to \infty$ what corresponds to $d\tau \to 0$.

b) Insert Completeness Relation

The transition amplitude we want to compute is

$$\langle q', t' | q, t \rangle. \tag{2.22}$$

For every time point τ_i within the interval $[t, t']$, we have the completeness relation

$$\int dq_i |q_i, \tau_i\rangle\langle q_i, \tau_i| = \mathbf{1}. \tag{2.23}$$

Inserting this completeness relation for *every* τ_i gives us

$$\langle q', t' | q, t \rangle = \int dq_1 dq_2 \ldots dq_N \langle q', t' | q_N, \tau_N \rangle \langle q_N, \tau_N | q_{N-1}, \tau_{N-1} \rangle \langle q_2, \tau_2 | q_1, \tau_1 \rangle \langle q_1, \tau_1 | q, \tau \rangle \tag{2.24}$$

Remark that we have inserted $\mathbf{1}$ operators as an integration over position space variables q_i, not as an integration over momentum space variables p_i like we did in paragraph 2.1.3, so there is no 2π missing here.

Our interim result is, that we can write our transition amplitude as a product of $N+1$ infinitesimal time evolution steps, with integration over the N intermediate $q(\tau_i)$.

c) Infinitesimal Amplitudes

We have now reached the point, where we can use the result of the last paragraph. Every infinitesimal transition amplitude is given by

$$\langle q_{j+1}, \tau_{j+1} | q_j, \tau_j \rangle = \int \frac{dp_{j+1}}{2\pi} \exp\left(i[p_{j+1}(q_{j+1} - q_j)] - iH(q_{j+1}, p_{j+1}) d\tau\right) \tag{2.25}$$

We will put this expression now into equation (2.24). Notice that this gives us now $N+1$ integrations over p_j, but that we still only have N integrations over q_j. Furthermore, we remind ourselves that we could rewrite the appearing product of $N+1$ exponential functions (one for every infinitesimal amplitude) as an exponential function of $N+1$ summands. So we have now

$$\langle q', t' | q, t \rangle = \int \prod_{i=1}^{N} dq_i \int \prod_{j=1}^{N+1} \frac{dp_j}{2\pi} \exp\left(i \left[\sum_{k=1}^{N+1} p_k(q_k - q_{k-1}) - H(q_k, p_k) d\tau \right] \right), \tag{2.26}$$

where $q_0 \equiv q$ and $q_{N+1} \equiv q'$. The 2π factor belongs to the product, so it appears $N+1$ times in this equation.

d) Notation

In order to write equation (2.26) a little bit more elegantly, we define

$$\begin{aligned} \dot{q}_k &= \frac{q_k - q_{k-1}}{d\tau}, \\ \dot{q}(\tau) &= \frac{q(\tau) - q(\tau - d\tau)}{d\tau}. \end{aligned} \tag{2.27}$$

Here we used the additional definition $\tau \equiv t + kd\tau$ (what implies $t + (k-1)d\tau \equiv \tau - d\tau$). This looks reasonable, as q_k is a position variable at time $t + kd\tau$ and q_{k-1} is a position variable at time $t + (k-1)d\tau$. So in the limit $d\tau \to 0$ that we will perform later, our defined $\dot{q}_k$ should have the meaning of a velocity (what we already imply here by choosing the notation $\dot{q}$).

Anyway, for the moment we will just use equation (2.27) to simplify equation (2.26). We get

$$\langle q', t' | q, t \rangle = \int \prod_{i=1}^{N} dq_i \int \prod_{j=1}^{N+1} \frac{dp_j}{2\pi} \exp\left(id\tau \sum_{k=1}^{N+1} p_k \dot{q}_k - H(q_k, p_k) \right) \tag{2.28}$$

2.1.5 Path Integral

With equation (2.28) we are just one step away from the path integral. We define it by the limit procedure

$$\int \mathcal{D}q \equiv \lim_{N \to \infty} \int \prod_{i=1}^{N} dq_i \tag{2.29}$$

and

$$\int \mathcal{D}p \equiv \lim_{N\to\infty} \int \prod_{j=1}^{N+1} dp_j. \tag{2.30}$$

Let us now discuss these equations a little bit:

- The integration $\int \mathcal{D}q$ means, that for every intermediate time point τ_i our particle may be *everywhere*, because we are integrating over all possible values of q_i. Only the endpoints are fixed: $q(t) = q$, $q(t') = q'$. To come from one endpoint to another, all *paths* are allowed.

- Every path can be written as a function $q(t)$. We are integrating over all these functions. That's why we will sometimes call our integrals "functional integrals".

- Our paths don't need to be very smooth. For all intermediate points, every value is allowed, so we could have arbitrary strong oscillations.

- The integration $\int \mathcal{D}p$ is, for the moment, without a further interpretation. It came into our calculation just as integration variable. Nevertheless, we can already guess that it will have something to do with the canonical momentum.

- For all calculations, we can only work with a large, but finite number of variables. Even if we use a computer, all data will be discrete and finite (and should be, unless we don't want to wait for the results infinitely long).

- Anyway, the use of finite $d\tau$ should not play a role, if $d\tau$ is sufficiently small - we cannot resolve time arbitrary accurately by observations, e.g. nobody has observed the Planck time $t_p = 10^{-42}s$ yet.

- Furthermore, in the limit $d\tau \to 0$ nothing interesting should happen, as all physical observables should better have smooth limits. If a computation of a physical observable shows no smooth limit, it is most likely wrong, because otherwise it could be used to resolve arbitrary small $d\tau$.

2.1.6 Action

Let us now perform the p integration appearing in the expression for the transition amplitude (2.28) in the case that

$$H = \frac{P^2}{2M} + V(Q) \tag{2.31}$$

Well, actually it is already *implied* that H can be written in this form, because this was an assumption we made to get our infinitesimal amplitude, that we used to come to (2.28).

First we rewrite the transition amplitude as

$$\langle q', t'|q, t\rangle = \int \mathcal{D}q\mathcal{A}\exp\left(-id\tau\sum_{k=1}^{N+1}V(q_k)\right) \tag{2.32}$$

with

$$\mathcal{A} = \int\prod_{j=1}^{N+1}\frac{dp_j}{2\pi}\exp\left(-id\tau\sum_{k=1}^{N+1}(\frac{p_k^2}{2M} - p_k\dot{q}_k)\right) = \prod_{j=1}^{N+1}\mathcal{A}_j. \tag{2.33}$$

Here $\mathcal{A}_j$ is defined as

$$\mathcal{A}_j = \int_{-\infty}^{\infty}\frac{dp}{2\pi}\exp\left(-id\tau\left[\frac{p^2}{2M} - p\dot{q}_j\right]\right) \tag{2.34}$$

Here it is no longer necessary to write p with an index. It is just an integration variable. Nevertheless, $\dot{q}_j$ must still be written *with* index, because every $\mathcal{A}_j$ depends on one special $\dot{q}_j$.

The exponent in equation (2.34) looks almost Gaussian. In order to get a binomial formula, we make the ansatz

$$\frac{p^2}{2M} - p\dot{q}_j = \frac{1}{2M}(p - \alpha\dot{q}_j)^2 - \frac{1}{2M}\alpha^2\dot{q}_j^2 = \frac{p^2}{2M} - \frac{\alpha}{M}p\dot{q}_j. \tag{2.35}$$

So we must set $\alpha = M$. With the variable substitution $p' = p - M\dot{q}_j$ equation (2.34) becomes

$$\mathcal{A}_j = \exp\left(-id\tau\left[\frac{M}{2}\dot{q}_j^2\right]\right)\cdot\int\frac{dp'}{2\pi}\exp\left(-id\tau\frac{p'^2}{2M}\right) \tag{2.36}$$

Well, whatever the integration over p' will give, it will just be a constant. We name this constant $\widetilde{c}$ and write

$$\mathcal{A}_j = \widetilde{c}\exp\left(-id\tau\left[\frac{M}{2}\dot{q}_j^2\right]\right) \tag{2.37}$$

Now it is quite easy to calculate $\mathcal{A}$:

$$\mathcal{A} = \mathcal{N}\exp(id\tau\sum_{k=1}^{N+1}\frac{M}{2}\dot{q}_k^2) \tag{2.38}$$

with $\mathcal{N} = \widetilde{c}^N$. Now we insert this in equation (2.32) and get

$$\begin{aligned}\langle q', t'|q, t\rangle &= \int\mathcal{D}q\mathcal{N}\exp\left(id\tau\left[\sum_{k=1}^{N+1} -V(q_k) + \frac{M}{2}\dot{q}_k^2\right]\right)\\ &= \int\mathcal{D}q\exp\left(id\tau\left[\sum_{k=1}^{N+1} -V(q_k) + \frac{M}{2}\dot{q}_k^2 + const\right]\right)\end{aligned} \tag{2.39}$$

Let us define the following quantity:

$$S = d\tau \left(\sum_{k=1}^{N+1} \frac{M}{2} \dot{q}_k^2 - V(q_k) + const \right). \tag{2.40}$$

Now we can write

$$\langle q', t' | q, t \rangle = \int \mathcal{D}q \;\; e^{iS} \tag{2.41}$$

Obviously, in the limit $d\tau \to 0$, and if we neglect the irrelevant constant, the quantity S is exactly the action of a particle in a potential, just as we know it from classical mechanics! There we have defined the action as

$$S = \int_t^{t'} d\tau \mathcal{L}(\tau), \tag{2.42}$$

with the Lagrangian

$$\mathcal{L} = \frac{M}{2} \dot{q}^2 - V(q), \qquad q \equiv q(\tau). \tag{2.43}$$

We call the action S a functional of $q(t)$ and write

$$S = S[q(t)] = S[q] = S[q_k]. \tag{2.44}$$

For a finite number of intermediate steps it depends on the N variables q_k and on the boundary conditions $q_0 \equiv q$ and $q_{N+1} \equiv q'$ (that's were the dependence of q and q' of our matrix element $\langle q', t' | q, t \rangle$ lies).

2.1.7 Interpretation of QM, Double Slit Experiment

The so called *path integral formulation of QM* is a method to calculate the probability for a particle, which is at time t at the point q, to be at the point q' at time $t' > t$.

The rule to compute that probability is as follows: Consider *every path* to get from q to q'. For every path $k = 1, 2, \ldots$ calculate a so called *probability amplitude* or simply *amplitude* ψ_k, which is a phase factor $\psi_k = e^{iS_k}$. Calculate the *total amplitude* as the sum of the amplitudes of all paths, $\psi = \sum_k \psi_k$. The probability for the particle to propagate from $|q; t\rangle$ to $|q', t'\rangle$ is then given by the square of the length of the complex number ψ.

This method is a generalization of the double slit experiment.

Here we have

$$\begin{aligned} \psi &= \psi_1 + \psi_2, \\ \psi_1 &= \psi_1(q') = \langle q', t' | q_1, \tau \rangle \langle q_1, \tau | q, t \rangle, \\ \psi_2 &= \psi_2(q') = \langle q', t' | q_2, \tau \rangle \langle q_2, \tau | q, t \rangle. \end{aligned} \tag{2.45}$$

This experiment can now be generalized in two ways:

1. Use more screens.

2. Cut more holes in each screen.

E.g. consider the following experiment with two screens and five holes.

Letting both the number of screens and the number of holes per screen go to infinity, we get the path integral formulation of QM. What is important is that the amplitude or phase factor of each path is given by e^{iS}.

Note that this is a radically new way to formulate QM. There is no Schrödinger equation and no operators. But of course the two formulations must be equivalent in the sense that they make the same physical predictions. We will later show how the old operator formulation of QM can be reconstructed.

But first let's consider the relation to Classical Mechanics. Since the classical Lagrangian $\mathcal{L}$ and action S appear, Classical Mechanics should be included in some limit.

2.1.8 Classical Path

We do a *saddle point approximation*, i.e. we expand the action S around the classical path $q_0(t)$.

$$S(q) = S(q_0) + \frac{1}{2} \left. \frac{\delta^2 S}{\delta q(t)^2} \right|_{q_0(t)} (q - q_0)^2(t) + \cdots \ . \tag{2.46}$$

There is no linear term since by definition $q_0(t)$ is an extremum:

$$\left. \frac{\delta S}{\delta q} \right|_{q_0(t)} = 0. \tag{2.47}$$

Remember that in classical mechanics one shows that this principle of stationary action is equivalent to the way to compute the path of a particle in Lagrangian formalism:

$$\begin{aligned} \frac{d}{dt}\frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial \mathcal{L}}{\partial q} &= 0, \\ M\ddot{q} + \frac{\partial V}{\partial q} &= 0. \end{aligned} \tag{2.48}$$

So the basic difference between Classical Mechanics and Quantum Mechanics is:

> Do not only consider the classical path, but also all other paths. (And include a phase factor.)

Obviously, for classical physics to be a good approximation, all higher terms have to be small in comparison to the quadratic one.

Comment: Definition of functional derivatives

If you are not sure how to work with functional derivatives, go back to q_n instead of $q(t)$. Then S is a normal function of the q_n instead of a functional of $q(t)$. When you have only finitely many n, the functional derivative becomes the gradient, i.e. a vector of partial derivatives, just many of them:

$$\begin{aligned} \frac{\delta S}{\delta q(t)} &\equiv \frac{\partial S}{\partial q_n}, \\ \frac{\delta S}{\delta q(t)} q(t) &\equiv \frac{\partial S}{\partial q_n} q_n, \\ \delta S &\equiv \sum_n \frac{\partial S}{\partial q_n} \delta q_n, \\ \frac{1}{2} \left. \frac{\delta^2 S}{\delta q(t)^2} \right|_{q_0(t)} (q - q_0)^2(t) &\equiv \sum_{n,k} \frac{1}{2} \left. \frac{\partial^2 S}{\partial q_n \partial q_k} \right|_{q_{0,n}} (q_n - q_0)(q_k - q_0). \end{aligned} \tag{2.49}$$

Then at the very end do the limit procedure from normal derivatives to the functional derivative. Let's not worry about that now.

The saddle point approximation is a key concept, the whole perturbation theory is based on it. That's why we want to motivate it some more:

(a) Let's first assume there is only one wall between the points q and q'. That leads us to the functional

$$I = \int_{-\infty}^{\infty} e^{if(x)}. \tag{2.50}$$

Assume that $f(x)$ is purely imaginary, i.e. $f(x) = ig(x)$ with some function $g(x)$ that has a minimum at x_0 and goes to infinity for $x \to \pm\infty$. Then

$$I = \int_{-\infty}^{\infty} e^{-g(x)} \tag{2.51}$$

converges, and the integral is dominated by the region around x_0.

But say $g(x) \to C$, i.e. $g(x)$ levels off on the right side. Then the integral will not converge.

To summarize: Under simple conditions, i.e. if $f(x)$ is purely imaginary and goes to infinity for $|x| \to \infty$ not too slowly, convergence will be ok.

(b) Now let's consider the case of many degrees of freedom $q(\tau)$ and the Euclidean action $S = iS_E$ There the saddle point approximation for

$$\int \mathcal{D}q \; e^{iS} = \int \mathcal{D}q \; e^{-S_E} \tag{2.52}$$

will often not converge.
But there is a trick: Use imaginary time, i.e. substitute $\tau \to i\tau$. Then analytically continue the result and go back to real time.

(c) In the case of the Minkowski action, which is a real quantity, the integrands

$$e^{iS} = \cos S + i \sin S \tag{2.53}$$

are oscillatory functions and convergence is a very subtle issue. Sometimes it does converge, sometimes it does not.

The upshot that you should take home is this: For almost all interaction theories the saddle point approximation never converges. Also, the theory of convergence of these integrals is a very complicated field of mathematics. Nevertheless, let's do saddle point approximations as a working method, although things might not be well defined.

2.1.9 Operators

We now show how to calculate expectation values of operators, not only transition amplitudes,

$$\mathcal{A} = \langle q'; t'|\hat{A}|q; t\rangle. \tag{2.54}$$

(a) $A = A(\tau) = f(Q(\tau), P(\tau)),\ t < \tau < t'$ where A is an arbitrary function of $Q(\tau)$ and $P(\tau)$ ordered such that all factors $P(\tau)$ are on the left of $Q(\tau)$.

We go back to the definition of functional integrals and insert the states:

$$\begin{aligned}
\mathcal{A} &= \int dq(\tau) \int \frac{dp(\tau)}{2\pi}\ \langle q'; t'|p(\tau); \tau\rangle\langle p(\tau); \tau|\hat{A}(\tau)|q(\tau); \tau\rangle\langle q(\tau); \tau|q; t\rangle \\
&= \int dq(\tau) \int \frac{dp(\tau)}{2\pi}\ A(q(\tau), p(\tau))\langle q'; t'|p(\tau); \tau\rangle e^{-ip(\tau)q(\tau)}\langle q(\tau); \tau|q; t\rangle \\
&= \int \mathcal{D}q\mathcal{D}p\ A(q(\tau), p(\tau))e^{i\int_t^{t'}\{p(\tau)\dot{q}(\tau)-H(p(\tau),q(\tau))\}}
\end{aligned} \tag{2.55}$$

(b) We consider the special case where $A(\tau)$ only depends on $Q(\tau)$. There we can carry out the P integration and find

$$\mathcal{A} = \int \mathcal{D}q\ A(q(\tau))e^{iS}. \tag{2.56}$$

Note that this case is not so restrictive as it may seem, because it includes derivative operators, e.g. $\dot{Q}(\tau)$, since they are sums of operators:

$$\dot{Q}(\tau) = \frac{Q(\tau + d\tau) - Q(\tau)}{d\tau}. \tag{2.57}$$

The expectation value depends linearly on operators, i.e. for sums we have

$$\langle q'; t'|\sum_k \hat{A}_k|q; t\rangle = \sum_k\langle q'; t'|\hat{A}_k|q; t\rangle = \int \mathcal{D}q\ A_k e^{iS}. \tag{2.58}$$

(c) Time ordered products $\hat{A} = \hat{A}_n(\tau_n)\ldots\hat{A}_2(\tau_2)\hat{A}_1(\tau_1)$ with $t < \tau_1 < \tau_2 < \cdots < \tau_n < t'$. For simplicity, let's say that the operators only depend on Q: $\hat{A}_k = A_k(Q(\tau_k))$. This can later be generalized to include a P dependence as well: $\hat{A}_k = \hat{A}_k(Q(\tau_k), P(\tau_k))$. Then

$$\mathcal{A} = \langle q'; t'|\hat{A}_n \ldots \hat{A}_1|q; t\rangle = \int \mathcal{D}q \; A_n(q_n, \tau_n)\ldots A_1(q_1, \tau_1)e^{iS}. \tag{2.59}$$

The path integral expression for $\mathcal{A}$ does not depend on the ordering of the factors $A_n(q_n, \tau_n)\ldots A_1(q_1, \tau_1)$. We have a path integral formula for arbitrary *time-ordered* n-point functions!

$$\boxed{\langle q'; t'|T\{\hat{A}_n(\tau_n)\ldots\hat{A}_1(\tau_1)\}|q; t\rangle = \int \mathcal{D}q \; A_n(\tau_n)\ldots A_1(\tau_1)e^{iS}} \tag{2.60}$$

The time ordering is crucial! This works because time-ordered products are commutative. We have arrived at a formulation that involves no q-numbers (i.e. operators), only c-numbers (i.e. complex numbers).
(Dirac invented these names to emphasize that one can most of the time calculate with functions, operators and any other mathematical object as if they were numbers, just that some of these things are commutative (then they are called c-numbers) and some are not (then they are called q-numbers).

2.1.10 Can One Construct QM from a Path Integral?

In the last section we have introduced the path integral formalism, starting from the usual quantum mechanical operator formalism. Now one may ask whether both formulations are really equivalent, i. e. if one can also derive the quantum mechanical operators from a path integral. In fact it is possible, but we will only sketch the proof here. The interested reader may try to formulate it in more detail. The most important result we derived previously is that we can express an operator expectation value through a path integral:

$$\langle q', t'|T\{\hat{A}_1(\tau_1)\ldots\hat{A}_n(\tau_n)\}|q, t\rangle = \int Dq \; A_1(\tau_1)\ldots A_n(\tau_n)e^{iS}, \qquad t' > t, \tag{2.61}$$

where $S = \int d\tau L(\tau)$, $L = L(q(\tau), \dot{q}(\tau), \ldots)$ is the action describing the problem. Note that the right-hand side does not depend on the order of the operators, since A_1, ..., A_n are only c-numbers, in contrast to $\hat{A}_1$, ..., $\hat{A}_n$ on the right-hand side. Now be $\hat{A}$ an arbitrary time-ordered operator, i. e. $\hat{A} = T\{\hat{A}\}$. Now as explained above, we have a prescription how to compute $\langle q', t'|\hat{A}|q, t\rangle$ in the case $t' > t$. This means that we can compute the matrix elements of $\hat{A}$ between two different bases, namely $|q(t)\rangle$ and $|q(t')\rangle$. What we want of course is to express $\hat{A}$ in one given basis $|q, t\rangle$. So we have to make a change of basis by

$$\langle q', \tau|\hat{A}|q, \tau\rangle = \int dq_1 \int dq_2 \langle q', \tau|q_2, t'\rangle\langle q_2, t'|\hat{A}|q_1, t\rangle\langle q_1, t|q, \tau\rangle, \tag{2.62}$$

where $t < \tau < t'$. On the right-hand side of the equation, there are three expectation values which can essentially be determined by the path integral formalism (in the case where the time value on the left hand side is smaller than the one on the right-hand side, we can use the formalism to compute the complex-conjugate). Then once we have determined an operator in a complete basis, we of course completely know the operator. Since the commutator of two operators is also an operator, they can be computed in the same way and we will find for instance $[Q(\tau), \dot{Q}(\tau)] \neq 0$. To find the momentum operator $\hat{P}$, we remember that it is defined classically by $p(\tau) = \frac{\partial L}{\partial \dot{q}(\tau)}$. In this way, we will get P as a function of $q(\tau)$ and $\dot{q}(\tau)$, which is often just $P = M\dot{Q}$. Inserting this expression in the path integral, we can determine the momentum operator in a complete basis. Additionally, one can derive the right canonical commutator relation $[Q(\tau), P(\tau)] = i$. The fact that we end up with non-vanishing commutators results from the fact that we go from integrals to matrix elements, and in general matrices do not commute.

2.1.11 Generalization to N Degrees of Freedom

To prepare the use of the path integral formalism in quantum field theory, we will generalize to $\mathcal{N}$ degrees of freedom. This is actually straight forward, we just add an index and define quantities $Q_j(t), P_j(t)$ with canonical commutators $[Q_i(t), P_j(t)] = i$. The integral will be generalized to $\int Dq_j(t)$ and the action will of course depend on all degrees of freedom, i. e. we have $S[q_j(t)]$.

Examples:

- One atom in 3D: $j = 1, 2, 3, \quad \mathcal{N} = 3, \quad$ and $Q_j(t)$ corresponds to a 3-vector $\mathbf{Q}(t)$.
- $\mathcal{N}$ atoms in d=1 lattice: $j = 1, \dots \mathcal{N}, \quad Q_j(t)$
- continuum notation: $\mathcal{N}, Q_j(t) \to \quad Q(x, t)$
- fields: $\mathcal{N} \to \infty$
- lattice in 3D, only one excitation direction: $Q(\mathbf{x}, t)$
- lattice in 3D, 3D excitations: $\mathbf{Q}(\mathbf{x}, t)$

Especially the fifth example is very important, since this will correspond to scalar fields in quantum field theory.

2.2 Functional Integral for Bosonic Many-Body Systems

2.2.1 Path Integral for QFT

Now of course we aim to use the derived functional integral formalism (i. e. the path integral formalism) in quantum field theory. There we have fields $\hat{\phi}(x, t)$, $\hat{\phi}^\dagger(x, t)$ and the canonical commutator relation $[\hat{\phi}(x',t),\hat{\phi}^\dagger(x,t)] = \delta(x-x')$. Then we can define position and momentum operators by

$$\begin{aligned}\hat{Q}(x,t) &= \frac{1}{\sqrt{2}}(\hat{\phi}(x,t)+\hat{\phi}^\dagger(x,t)),\\ \hat{P}(x,t) &= -\frac{i}{\sqrt{2}}(\hat{\phi}(x,t)-\hat{\phi}^\dagger(x,t))).\end{aligned} \tag{2.63}$$

As a simple exercise, the reader may show that

$$[Q(x',t),P(x,t)] = i\delta(x-x'). \tag{2.64}$$

Now we will consider a simple system of non-interacting bosonic atoms with a Hamiltonian

$$H = \int_x \left\{\frac{1}{2M}\nabla\hat{\phi}^\dagger(x,t)\nabla\hat{\phi}(x,t) + V(x)\hat{\phi}^\dagger(x,t)\hat{\phi}(x,t)\right\} \tag{2.65}$$

and derive the functional integral for this system. We use the inverse transformation of (2.63),(2.63) given by

$$\begin{aligned}\hat{\phi} &= \frac{1}{\sqrt{2}}(Q+iP),\\ \hat{\phi}^\dagger &= \frac{1}{\sqrt{2}}(Q-iP)\end{aligned} \tag{2.66}$$

where we have suppressed the arguments x and t. In the same way we can compute

$$\hat{\phi}^\dagger\hat{\phi} = \frac{1}{2}(Q-iP)(Q+iP) = \frac{1}{2}(Q^2+P^2) + i[P,Q] = \frac{1}{2}(Q^2+P^2) + const., \tag{2.67}$$

where we have introduced an infinite constant. However, this constant will drop out of the Hamiltonian anyway, since we are free to choose any zero-point of energy we consider appropriate. Now we can write the Hamiltonian as

$$H = \int_x \frac{1}{2}Q(x,t)(-\frac{\Delta}{2M}+V(x))Q(x,t) + \frac{1}{2}P(x,t)(-\frac{\Delta}{2M}+V(x))P(x,t). \tag{2.68}$$

Now let's have a look at transition amplitudes and the expectation values of operators: We introduce the notation $|q(x,t)\rangle = |q(x,t),t\rangle = |q,t\rangle$. The position operator Q will act on this basis as $Q(x,t)|q(x,t)\rangle = q(x,t)|q(x,t)\rangle$. The expectation value of a time-ordered product of operators can be expressed as usual by

$$\langle q'(x',t')|T\left\{\hat{A}_1(x_1,t_1),\ldots,\hat{A}_n(x_n,t_n)\right\}|q(x,t)\rangle = \int Dq\int DpA_1(x_1,t_1)\ldots A_n(x_n,t_n)e^{iS}, \tag{2.69}$$

where the action S is defined as $S=\int d\tau dx L(x,\tau)$ with the Lagrangian $L(x,\tau) = p(x,\tau)\dot{q}(x,t) - H(p(x,\tau),q(x,\tau))$. Further $\int Dq = \int Dq(x,t)$. In the case of finite degrees of freedom, this corresponds to integration over every degree of freedom. In the continuum case, we therefore integrate over infinitely many degrees of freedom. Now of course, we want to express the action in terms of the fields $\hat{\phi}$ and $\hat{\phi}^\dagger$. We remember the expressions (2.66),(2.66) and define $\int DqDp = \int D\phi D\phi^* = \int D\phi$. This can be understood by remembering that a complex field ϕ has two degrees of freedom, for example the real and the imaginary part. In the same way, one can also treat ϕ and ϕ^* independently. Now we are actually no longer integrating over paths, but we integrate over all possible configurations in space and time, each having a certain phase factor. This is in fact very similar to statistical mechanics. In the 3D Ising model, we have a cubic lattice with lattice sites $i = (n_1, n_2, n_3)$ with a certain spin $s_i = \pm 1$. The partition function is given by $Z = \sum_{s_i} Tre^{-\beta H}$, where we have to sum over all possible spin configurations. This is very similar to what we have in quantum field theory. In fact if we assume that our bosonic atoms are located on a grid, we have only a finite number of degrees on freedom in QFT and instead of the integral we will also have sums over all possible configurations in space. The other difference is that in statistical mechanics, the exponential factor is real, while it is imaginary in QFT. In fact we will later show that we can make a transformation $t \mapsto it$ in QFT so that the exponential factor will also become real.

Lagrangian Density in Terms of $\hat{\phi}$ and $\hat{\phi}^\dagger$

Now we wish to express the Lagrangian density $\mathcal{L}$ in terms of $\hat{\phi}$ and $\hat{\phi}^\dagger$. For this look at the Hamiltonian H, expressed in terms of $\hat{\phi}$ and $\hat{\phi}^\dagger$:

$$\begin{aligned} H =& \frac{1}{2} q(x,t) \left(-\frac{\Delta}{2M} + V(x) \right) q(x,t) + \frac{1}{2} p(x,t) \left(-\frac{\Delta}{2M} + V(x) \right) p(x,t) \\ =& \hat{\phi}^\dagger(x,t) \left(-\frac{\Delta}{2M} + V(x) \right) \hat{\phi}(x,t) \end{aligned} \tag{2.70}$$

$\mathcal{L}$ is calculated by

$$\mathcal{L} = p\dot{q} - H(p,q) \tag{2.71}$$

with

$$p\dot{q} = -\frac{i}{2} \left(\phi - \phi^* \right) \partial_t \left(\phi + \phi^* \right) = -\frac{i}{4} \partial_t \left(\phi^2 - \phi^{*2} + 2\phi\phi^* \right) + i\phi^* \partial_t \phi \tag{2.72}$$

When calculating the action S, the first term drops out, because it is a total time derivative. For S we therefore have

$$S = \int dtdx \left(i\phi^* \partial_t \phi - \phi^* \left(-\frac{\Delta}{2M} + V(x) \right) \phi \right) \tag{2.73}$$

This is the functional integral for bosonic atoms in a trap! Here we can see, indeed provokes an exponential decay, depending on the time dependence of $\hat{\phi}$!

2.2.2 Systems in Various Dimensions d

Up to now, we have been investigating systems in *real space* with dimension d=3. The cases d=2, d=1 just relate to QFT on the surface, on the line respectively, by adding constraints in d=3. The case d=0 is however somewhat special. Here the atoms are confined to points, the so called quantum-dots. Let's take a look at the action S for d=0:

$$S = \int dt \left(i\phi^*(t)\partial_t\phi(t) + \mu\phi^*(t)\phi(t) - \frac{\lambda}{2}\left(\phi^*(t)\phi(t)\right)^2 \right) \tag{2.74}$$

and compare it with the action in QM:

$$S_{QM} = \int dt \left(p(t)\dot{q}(t) - \frac{p^2(t)}{2M} - V(q(t)) \right) \to \int dt \left(\frac{1}{2}M\dot{q}^2(t) - V(q(t)) \right). \tag{2.75}$$

We see that although they are different actions, they have the same structure. So we can say for d=0:

$$QFT := QM \tag{2.76}$$

Another Comparison of QFT and QM

In QM there are, like you know only a finite number of degrees of freedom. $\mathbf{q}(t)$ describes a particle in a potential and $\phi(t)$ describes a quantum dot. By *adding more dimensions* to $\phi(t)$, that means looking at $\phi(\mathbf{x}, t)$, we enter QFT, and get infinite degrees of freedom. The same on the operator level:

$$\begin{aligned} \widehat{Q} &\leftrightarrow \widehat{\phi}(\mathbf{x}) && \text{(Schrödinger)} \\ \widehat{Q}(t) &\leftrightarrow \widehat{\phi}(\mathbf{x}, t) && \text{(Heisenberg)} \end{aligned} \tag{2.77}$$

2.2.3 In and Out States

Now we would like to look at a scattering experiment. In short: 2 or more particles arrive the interaction region, and several particles are scattered out. Before the scattering, we have well separated incoming particles (they don't influence each other!), and after the scattering also well separated outgoing particles.

We assume the interaction timescale $t_{int} = 0$. In experiments the timescale t_{exp} is finite, but since we look at times $t < 0$ with $|t| \gg t_{exp}$, and assume the incoming particles are well separated, we can also assume $t_{exp} \approx 0$.
At $t \to -\infty$, we have the incoming N-particle state, and at $t \to \infty$, the outgoing N-particle state. The incoming state is characterized by the occupation number N , the external properties of the particles (such as the momenta $p_1, \ldots, p_N$) and the internal properties (like the spins $j_1, \ldots, j_N$, the flavors, etc.)

$$|N, p_1, \ldots, p_N, j_1, \ldots, j_N\rangle \equiv |\alpha\rangle \tag{2.78}$$

where α is a multi index! The outgoing state is characterized by $|\beta\rangle$. These states are each a complete basis in Fock space. Now for the incoming state at some fixed t , we can also take an eigenbasis to the occupation operators $\widehat{n}_i(p,t)$, for example $\hat{\phi}_j^\dagger(p,t)|0;t\rangle$, or $\frac{1}{\sqrt{2}}\hat{\phi}_{j_1}^\dagger(p_1,t)\hat{\phi}_{j_2}^\dagger(p_2,t)|0;t\rangle$, but remember: the basis depends on t in a sense, that t indicates at which time the basis is an eigenbasis to the $\widehat{n}_i(p,t)$!

We label the incoming vacuum state $|0;t\rangle$, $t \to -\infty$ as $|0;in\rangle$, the outgoing state will be labeled $|0;out\rangle$.

The basis $|\alpha, in\rangle$ ($|\alpha, t\rangle$, $t \to -\infty$) is a **complete basis** of **in states**, and the basis $|\beta, out\rangle$ is a **complete basis** of **out states**, but they are not identical. They can have an overlap, which means there is a transition amplitude. This leads us to the ...

2.2.4 S-Matrix

The transition amplitude

$$S_{\beta\alpha} = \langle \beta, out|\alpha, in\rangle \tag{2.79}$$

is called the **S-matrix**. We have to study this basic concept because it is crucial for describing scattering experiments. It tells us how the system has evolved, with the existence (or nonexistence) of an interaction. If the system has no potential and interaction, we expect that $|\alpha, in\rangle$ and $|\beta, out\rangle$ are orthogonal. But what if there is an interaction? This interaction would certainly change the properties of the particles, and thus the state $|\alpha, in\rangle$. But there are of course conservation laws, like energy and momentum conservation, which as we will see be already implemented in $S_{\beta\alpha}$. In fact all the information of the physics in the interaction is contained in the S-matrix, wonderful, right? So let us explore $S_{\beta\alpha}$.

First of all the completeness of $|\alpha, in\rangle$ and $|\beta, out\rangle$ leads to the fact that S is unitary. Let's see why.
First we show $S^\dagger S = \mathbf{1}$:

$$\begin{aligned} S^\dagger S =& \sum_\beta \left(S^\dagger\right)_{\gamma\beta} S_{\beta\alpha} = \sum_\beta \langle \beta, out|\gamma, in\rangle^* \langle \beta, out|\alpha, in\rangle \\ =& \sum_\beta \langle \gamma, in|\beta, out\rangle \langle \beta, out|\alpha, in\rangle \\ =& \langle \gamma, in|\alpha, in\rangle = \delta_{\gamma,\alpha} \end{aligned} \tag{2.80}$$

In (2.80) we used the completeness of $|\beta, out\rangle$.

2.2.5 Functional Integral for the S-Matrix

By now, we know the functional integral for time ordered operators

$$\langle q(x',t')|T\{\widehat{A}_1(t_1)\dots\widehat{A}_n(t_n)\}|q(x,t)\rangle = \int \mathcal{D}\phi A_1(t_1)\dots A_n(t_n)e^{iS} \tag{2.81}$$

with $\widehat{A}_k(t_k) = \widehat{A}_k\{\hat{\phi}(t_k), \hat{\phi}^\dagger(t_k), \dot{\hat{\phi}}(t_k)\ldots\}$. But this is not yet the S-matrix. Now because we have $Q(x,t)|q(x,t)\rangle = q(x,t)|q(x,t)\rangle$ and $Q(x,t) = \frac{1}{\sqrt{2}}\left(\hat{\phi}(x,t) + \hat{\phi}^\dagger(x,t)\right)$, we can write the time ordered products as functions of $Q(x,t)$, and thus the integrals as functions of $q(x,t)$. To set up a functional integral for S, we just insert ones in the limits $\pm\infty$:

$$\begin{aligned}
S_{\beta\alpha} &= \langle\beta, out|\alpha, in\rangle \\
&= lim_{t\to\infty,t'\to-\infty} \int dq(x,t)dq(x',t')\langle\beta, out|q(x',t')\rangle\langle q(x',t')|q(x,t)\rangle\langle q(x,t)|\alpha, in\rangle \\
&= lim_{t\to\infty,t'\to-\infty} \int dq(x,t)dq(x',t')\langle\beta, out|q(x',t')\rangle\left(\int \mathcal{D}'\phi e^{iS}\right)\langle q(x,t)|\alpha, in\rangle
\end{aligned} \tag{2.82}$$

Now in (2.82) we have the path integral $\int\mathcal{D}'$ that still has the boundary conditions at q and q'. But now we integrate over these boundaries, and thus yield an unconstrained path integral:

$$S_{\beta\alpha} = lim_{t\to\infty,t'\to-\infty} \int \mathcal{D}\phi\langle\beta, out|q(x',t')\rangle\langle q(x,t)|\alpha, in\rangle \tag{2.83}$$

We would now like to investigate a $2\to 2$ scattering. The *in* and *out* states are given by

$$\begin{aligned}
|\alpha, in\rangle &= \hat{\phi}^\dagger(p_1,t)\hat{\phi}^\dagger(p_2,t)|0, in\rangle \\
\langle\beta, out| &= \langle 0, out|\hat{\phi}(p_3,t')\hat{\phi}(p_4,t').
\end{aligned} \tag{2.84}$$

The S-matrix is then a 4-point correlation function:

$$\begin{aligned}
S_{\beta\alpha} = \langle\beta, out|\alpha, in\rangle &= \langle 0, out|\hat{\phi}(p_3,t')\hat{\phi}(p_4,t')\hat{\phi}^\dagger(p_1,t)\hat{\phi}^\dagger(p_2,t)|0, in\rangle \\
&= \langle 0, out|T\left(\hat{\phi}(p_4,t')\ldots\hat{\phi}^\dagger(p_1,t)\right)|0, in\rangle.
\end{aligned} \tag{2.85}$$

For time ordered operators $\widehat{A}$ we want to find the matrix elements for the vacuum in and out states:

$$\begin{aligned}
&\langle 0, out|T\left(\widehat{A}\left[\hat{\phi}(x,t), \hat{\phi}^\dagger(x,t)\right]\right)|0, in\rangle \\
&= lim_{t\to-\infty,t'\to\infty} \int dq(x,t)dq(x',t')\langle 0, out|q(x',t')\rangle\langle q(x',t')|T\left(\widehat{A}\right)|q(x,t)\rangle\langle q(x,t)|0, in\rangle \\
&= \int \mathcal{D}\phi(x,t)A\left(\phi(x,t), \phi^*(x,t)\right)e^{iS-\eta}
\end{aligned} \tag{2.86}$$

where $e^{-\eta} = f^*(q(x',t'))f(q(x,t)) = \langle 0, out|q(x',t')\rangle\langle q(x,t)|0, in\rangle$ can be neglected. So we have, now in momentum space

$$\langle 0, out|T\left(\widehat{A}\left[\hat{\phi}(p,t), \hat{\phi}^\dagger(p,t)\right]\right)|0, in\rangle = \frac{1}{Z}\int \mathcal{D}\phi(p,t)A\left(\phi(p,t), \phi^*(p,t)\right)e^{iS[\phi]}. \tag{2.87}$$

Normalization

We calculate the matrix element of unity, and define it to be 1:

$$\langle 0, out|0, in\rangle = \frac{1}{Z}\int \mathcal{D}\phi e^{iS} = 1$$
$$\Rightarrow\ Z = \int \mathcal{D}\phi e^{iS}. \tag{2.88}$$

This actually means that the in and out states are the same! To see this remember that $|0,t\rangle = e^{iE_0 t}|0\rangle$!

So all in all the S-matrix of a time ordered operator $\widehat{A}$ is

$$\langle 0, out|T\left(\widehat{A}\right)|0, in\rangle = \frac{\int \mathcal{D}\phi A e^{iS}}{\int \mathcal{D}\phi e^{iS}}. \tag{2.89}$$

Summarizing our previous considerations, we can give an exact expression for the vacuum-expectation value of any time-ordered operator $T\{\hat{A}\}$ by

$$\langle 0|T\{\hat{A}\}|0\rangle = \frac{\int D\phi A e^{iS}}{\int D\phi e^{iS}}. \tag{2.90}$$

In the same way we can compute the S-matrix for 2-2 scattering by

$$S_{\beta\alpha} = Z^{-1}\int D\phi\phi(p_4,t')\phi(p_3,t')\phi^*(p_2,t)\phi^*(p_1,t)e^{iS}, \tag{2.91}$$

where we used the abbreviation $Z = \int D\phi e^{iS}$ and where we consider $t \to -\infty$ and $t' \to +\infty$.

2.2.6 Correlation Function

Now in the same way, we can express time ordered correlation functions in vacuum by

$$\langle 0|T\{\hat{\phi}_{\alpha_1}(t_1)\ldots\hat{\phi}_{\alpha_n}(t_n)\}|0\rangle = Z^{-1}\int D\phi\phi_{\alpha_1}\ldots\phi_{\alpha_n}(t_n)e^{iS[\phi]} =: \langle\phi_{\alpha_1}(t_1)\ldots\phi_{\alpha_n}(t_n)\rangle, \tag{2.92}$$

where we introduced the last expression as a simple convention. The index α used here is a multi index and includes:

- position or momentum variables as the argument for the operator
- internal indices
- whether we refer to $\hat{\phi}$ or $\hat{\phi}^\dagger$. In fact this can be interpreted as an additional internal index in the basis of real fields, having $\hat{\phi} = \frac{1}{\sqrt{2}}(\hat{\phi}_R + i\hat{\phi}_I)$.

So for a given action, the correlation functions can be computed. However one may ask a couple of questions, i. e.:

- How do we recover the concept of particles?
- What fields should be chosen? In an integral one can make variable transformations $\phi \to \phi'[\phi]$! For example, what is the normalization of ϕ? These questions may seem trivial in the examples we have considered so far, but they are very important in more complicated situations where the particles are not known from the beginning, like the pions in QCD!
- How is time-ordering realized in practice?

$$\langle \phi(p', t')\phi^*(p, t)\rangle \begin{array}{ll} \neq 0 & t' > t \\ = 0 & t' < t \end{array}$$

Now let's turn to the mathematical regularization of S: For this purpose we add a term $i\epsilon \int dt d^3x \phi^*(x)\phi(x)$. Then the phase factor in the functional integral transforms as $e^{iS} \to e^{iS}e^{-\epsilon \int \phi^*\phi}$. The limit $\epsilon \to 0_+$ will be done at the very end of the calculation, so that we always have well-defined integrals in the intermediate steps. This procedure can be seen in various ways: First of all, if the functional integral is well-defined, this limit should exist. On the other hand, if it is not, then we can just define the functional integral by this limit procedure. From the physical point of view, the reader may even remember that we had a similar term when we first derived the path integral for the S-matrix, this term was just very small and therefore neglected.

2.2.7 Two-Point Function in Free Theory

We consider a simple example, where the action in the momentum basis is given by

$$S_0 = \int dt \frac{d^3p}{(2\pi)^3} \left\{ i\phi^*(p, t)\partial_t\phi(p, t) - E(p)\phi^*(p, t)\phi(p, t) \right\} \tag{2.93}$$

with $E(p) = \frac{p^2}{2M}$. We can even simply this expression going to frequency space by

$$\phi(p, t) = \int \frac{d\omega}{2\pi} e^{-i\omega t}\phi(\omega, p). \tag{2.94}$$

Now we can write the action in frequency-momentum space, where it becomes diagonal (in time-momentum space, it involves a time derivative, which implies that values at different times are compared, though they are infinitely small in the continuum limit).

$$S = \int \frac{d\omega}{2\pi} \frac{d^3p}{(2\pi)^3} (\omega - E(p))\phi^*(\omega, p)\phi(\omega, p) \tag{2.95}$$

The functional integration in frequency-momentum space is defined by

$$\int \mathcal{D}\phi = \prod_{\omega, \mathbf{p}} \int_{-\infty}^{+\infty} d\phi(\omega, \mathbf{p})d\phi^*(\omega, \mathbf{p}). \tag{2.96}$$

This can be understood by going back to discrete time and space with torus boundary conditions at large t and $-t$ and a finite volume of space with periodic boundary conditions. In such a configuration, frequency-momentum space will also consist of a finite lattice of points $(\omega, \mathbf{p})$. Now we define the free propagator by

$$G_0(p', p) = \langle \phi(p')\phi^*(p)\rangle_0 = Z^{-1} \int D\phi\phi(p')\phi^*(p)e^{iS_0}, \tag{2.97}$$

using $p = (\omega, \mathbf{p})$. To compute the free propagator, we first need some Gaussian integrals:

$$\begin{aligned}
\int_{-\infty}^{+\infty} dx e^{-\alpha x^2} &= \sqrt{\frac{\pi}{\alpha}}, \quad \int d\phi d\phi^* e^{-\alpha\phi^*\phi} = \frac{\pi}{\alpha}, \\
\int d\phi d\phi^* \phi^*\phi e^{-\alpha\phi^*\phi} &= -\frac{\partial}{\partial\alpha}\int d\phi d\phi^* e^{-\alpha\phi^*\phi} = \frac{\pi}{\alpha^2}, \\
\frac{\int d\phi d\phi^* \phi^*\phi e^{-\alpha\phi^*\phi}}{\int d\phi d\phi^* e^{-\alpha\phi^*\phi}} &= \frac{1}{\alpha}, \\
\int d\phi d\phi^* \phi e^{-\alpha\phi^*\phi} &= \int d\phi d\phi^* \phi^* e^{-\alpha\phi^*\phi} = 0.
\end{aligned} \tag{2.98}$$

Now computing G_0, there are only contributions for $(\omega, \mathbf{p}) = (\omega', \mathbf{p}')$. Then we can use the above calculated Gaussian integrals by putting $\alpha = -i(\omega - E(p))$, yielding the very important result

$$G_0(p', p) = \langle \phi(p')\phi^*(p)\rangle = \frac{i}{\omega - E(p)}\delta(p' - p), \tag{2.99}$$

where $\delta(p' - p) = (2\pi)^4\delta(\omega' - \omega)\delta^3(\mathbf{p}' - \mathbf{p})$.

Time-Dependent Two-Point Function

Now we compute the time-dependent two-point function. For this purpose, we have to go from frequency space to time dependent functions. Then we can use the previous result and get

$$\begin{aligned}
\langle \phi(p', t')\phi^*(p, t)\rangle &= \int \frac{d\omega}{2\pi}\frac{d\omega'}{2\pi} e^{-i\omega' t'} e^{i\omega t} \langle \phi(\omega', p')\phi^*(\omega, p)\rangle \\
&= (2\pi)^3\delta^3(\mathbf{p} - \mathbf{p}') \int \frac{d\omega}{(2\pi)} e^{-i\omega(t'-t)} \frac{i}{\omega - E(p)} \\
&= (2\pi)^3\delta^3(\mathbf{p} - \mathbf{p}') e^{-iE(\mathbf{p})(t'-t)} A, \\
A &= \int \frac{d\tilde{\omega}}{2\pi} e^{-i\tilde{\omega}(t'-t)} \frac{i}{\tilde{\omega}},
\end{aligned} \tag{2.100}$$

where we defined $\tilde{\omega} = \omega - E(\mathbf{p})$. As we can see, A has a pole on the real axis. To regularize the integral, we introduce a shift $\omega \to \omega + i\epsilon$ with some positive ϵ. As we discussed previously, for a well-defined functional integral there should be a smooth limit $\epsilon \to 0_+$. Otherwise, we just define the functional integral by this limit. The shift in ω yields $\tilde{\omega} \to \tilde{\omega} + i\epsilon$ and therefore $e^{iS} \propto e^{i\omega\phi^*\phi \to e^{i\omega\phi^*\phi - \epsilon\phi^*\phi}}$. The pole in the expression for A is now below the real axis in the space of complex $\tilde{\omega}$. To evaluate the integral, we close the contour integral below the real axis for $t' > t$, and above the real axis for $t' < t$, yielding

$$A = \left\{ \begin{array}{ll} 1 & t' > t \\ 0 & t' < t \end{array} \right\} = \theta(t' - t) \tag{2.101}$$

according to the residue theorem. This already answers one of the questions we were asking above, i. e. how time ordering arises in practise. It is realized by the appropriate choice where to close the contour lines. As a result we get the useful formula

$$\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{i}{\omega - E(p) + i\epsilon} e^{-i\omega(t'-t)} = e^{-iE(p)(t'-t)} \theta(t' - t). \tag{2.102}$$

So we get the following result for the free propagator in time-momentum space, in agreement with our previous calculations:

$$\langle \phi(\mathbf{p}', t') \phi^*(\mathbf{p}, t) \rangle = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}') e^{-iE(p)(t'-t)} \theta(t' - t) = \langle 0 | T\{\hat{\phi}(p', t') \hat{\phi}^\dagger(p, t)\} | 0 \rangle. \tag{2.103}$$

2.2.8 S-Matrix Element in One-Particle Channel

Now we can compute the S-matrix in the one-particle channel, i. e. for one ingoing and one outgoing particle. It is given by

$$S_{p'p} = \delta(p' - p) e^{-iE(p)(t'-t)}. \tag{2.104}$$

We want to make some comments on this result:

1. The phase factor in the S-matrix element is irrelevant, we will see that only $|S|^2$ matters at the end.

2. The phase can be eliminated by multiplying $S_{\beta\alpha}$ with standard phase factors:
   - $e^{-iE_i(p_i)t}$ for every incoming particle,
   - $e^{iE_i(p_i)t'}$ for every outgoing particle.

3. This means that phase factors can be absorbed in a redefinition of the variables $\phi(p)$. With this convention, $S_{\beta\alpha}$ is normalized in comparison with free theory. This can be formally implemented in the general definition of $S_{\beta\alpha}$. Then the statement $S_{\beta\alpha} = \delta_{\beta\alpha}$ is true if and only if we have a free theory.

2.2.9 Reduced Transition Amplitude M

If we want to consider scattering of particles, we need to consider a deviation of S from unity. Therefore we define

$$S_{\beta\alpha} = \delta_{\beta\alpha} - i(2\pi)^4 \delta(E_f - E_i) \delta^3(\mathbf{p}_f - \mathbf{p}_i) M_{\beta\alpha}, \tag{2.105}$$

where the delta functions imply energy and momentum conservation. Let's consider an example of two incoming and several outgoing particles, then we have $\mathbf{p}_i = \mathbf{p}_1 + \mathbf{p}_2$ and $\mathbf{p}_f$ is the total momentum of the outgoing particles. Then we can compute the differential cross section from M by

$$d\sigma = \prod_f \frac{d^3 p_f}{(2\pi)^3} \frac{1}{|\mathbf{v}_1 - \mathbf{v}_2|} (2\pi)^4 \delta(E_f - E_i) \delta^3(\mathbf{p}_f - \mathbf{p}_i) |M(p_1, p_2 \to \{p_f\})|^2, \tag{2.106}$$

where $\mathbf{v}_1 - \mathbf{v}_2$ is the relative velocity of the incoming particles. More generally, M contains the dynamic information, but not the kinematics.

2.2.10 Classical Approximation for $2 \to 2$ Scattering

In the sections 2.2.7 and 2.2.8 we discussed the two-point function in free theory, thus the one-particle channel. Now we want to go a step further and compute the four-point function in the classical approximation, that is also called "Born Approximation" or "Tree Approximation" and simply means that we consider only pointlike interaction of two particles.

The action in time and position space is

$$S = \int d\tau \int d^3x \left(i\varphi^*(x,\tau)\partial_\tau \varphi(x,\tau) - \frac{1}{2M} \nabla\varphi^*(x,\tau)\nabla\varphi(x,\tau) - \frac{\lambda}{2}(\varphi^*(x,\tau)\varphi(x,\tau))^2 \right) \tag{2.107}$$

and we want to know the S-matrix elements

$$\begin{aligned} S_{\beta,\alpha} &= \langle \beta, out | \alpha, in \rangle \\ &= \langle \mathbf{p_4}, \mathbf{p_3}, out || \mathbf{p_1}, \mathbf{p_2}, in \rangle \\ &= \langle 0 | \varphi(\mathbf{p}_4, t')\varphi(\mathbf{p}_3, t')\varphi^\dagger(\mathbf{p}_2, t)\varphi^\dagger(\mathbf{p}_1, t) | 0 \rangle \end{aligned} \tag{2.108}$$

We know that this time ordered product of operators has the following path integral expression:

$$S_{\beta,\alpha} = f \; \frac{\int \mathcal{D}\varphi \varphi(\mathbf{p}_4, t')\varphi(\mathbf{p}_3, t')\varphi^*(\mathbf{p}_2, t)\varphi^*(\mathbf{p}_1, t) e^{iS}}{\int \mathcal{D}\varphi e^{iS}}. \tag{2.109}$$

f is a factor that is given by

$$f = e^{-i(E(\mathbf{p}_1,t)+E(\mathbf{p}_2,t))} e^{+i(E(\mathbf{p}_3,t')+E(\mathbf{p}_4,t'))} \tag{2.110}$$

and that will compensate some phases that come out of the calculation later. It is just the same here as it was in section 2.2.8, where we defined our S-matrix element.

Well, equation (2.109) is the basic problem that we will solve in this section. We will do this in two steps. First we will consider the free theory with $\lambda = 0$, and then we will turn on the interaction.

a) Free theory for $2 \to 2$ "Scattering"

Actually, the title of this paragraph is a little bit confusing. Of course, in a free theory with $\lambda = 0$ we expect no scattering at all.

The first thing that we have to do, is that we should use the representation of the action S in momentum space instead of (2.107), because the field variables also depend on momenta:

$$S = \int dt \int \frac{d^3p}{(2\pi)^3} \left(i\varphi^*(\mathbf{p},t)\partial_t \varphi(\mathbf{p},t) - E(\mathbf{p})\varphi^*(\mathbf{p},t)\varphi(\mathbf{p},t)\right) \tag{2.111}$$

The functional integrals in (2.109) are also to be understood as functional integrals over field variables, that depend on momenta and time or frequency

$$\int \mathcal{D}\varphi = \int \mathcal{D}\varphi(\mathbf{p},t) = \int \mathcal{D}\varphi(\mathbf{p},\omega) \tag{2.112}$$

Do you feel completely familiar with equation (2.109)? Do you know, what the different arguments of the functions tell us and where they came from? If not, read the following small insertion. If yes, proceed to the next paragraph that is called **Fourier transformation to frequency space** .

- Small insertion to discuss the meaning of equation (2.109)

  In section 2.1, we defined what a path integral is:

  $$\int \mathcal{D}q = \int \prod_{k=1}^{N} dq_k \tag{2.113}$$

  So it is an integral over all intermediate steps. As every q_k coordinate corresponds to a certain time, we could also write for example

  $$\int \mathcal{D}q = \int \prod_{k=1}^{N} dq(t_k) \tag{2.114}$$

  or, if we like

  $$\int \mathcal{D}q = \int \prod_{t} dq(t). \tag{2.115}$$

  So no matter how we write it, we always mean the same: A product of integrals over all intermediate steps. Remark, that for different t's, we simply mean different integration variables! This will be extremely important later on.

  So far, we only considered quantum mechanical path integrals, or, if we want to say it in the words of 2.2.2, a 0-dimensional Quantum Field Theory. If we go to infinitely many degrees of freedom, our path integral function q depends not only on t, but now on x and t:

  $$\int \mathcal{D}q = \int \prod_{\mathbf{x},t} dq(\mathbf{x},t) \tag{2.116}$$

  where we mean the integration over all intermediate steps in space and time. But if x is the "real" space coordinate, one may ask the question what is the meaning of q? To answer this question remember, that $q(\mathbf{x}, t)$ is the eigenfunction to the Operator $\widehat{Q}(\mathbf{x}, t)$! The corresponding classical quantity was $Q(\mathbf{x}, t)$, which was in the solid-picture the distance of the oscillator at space position $\mathbf{x}$ at time t to its equilibrium position. Of course, this is not an explanation of what it is in the case of a “real” vacuum without an underlying substructure of atoms like we have it in the solid. But anyway you should keep in mind, that in the QFT-path integral the real space coordinate is x, and not the integration variable q.

Again, you should remark, that for different $(\mathbf{x}, t)$ we mean different integration variables q.

Of course we had a similar expression for momenta p:

$$\int \mathcal{D}p = \int \prod_{\mathbf{x},t} dp(\mathbf{x}, t). \tag{2.117}$$

The next step is now to “exchange” our integration variables $q(\mathbf{x}, t)$ and $p(\mathbf{x}, t)$ into field variables $\varphi(\mathbf{x}, t)$ and $\varphi^*(\mathbf{x}, t)$. Ignoring the arguments for a short while, this is according to

$$\begin{aligned} q &= \frac{1}{\sqrt{2}}(\varphi + \varphi^*), \\ p &= i\frac{1}{\sqrt{2}}(-\varphi + \varphi^*) \end{aligned} \tag{2.118}$$

just a rotation with Jacobian 1. Thus, we have now

$$\int \mathcal{D}q(\mathbf{x}, t) \int \mathcal{D}p(\mathbf{x}, t) = \int \mathcal{D}\varphi(\mathbf{x}, t) \int \mathcal{D}\varphi^*(\mathbf{x}, t). \tag{2.119}$$

The vacuum expectation value of a time-ordered product of operators $T\{\widehat{A}(\varphi(\mathbf{y}, t), \varphi^\dagger(\mathbf{y}, t))\}$ is given by the following path integral, where we write now once all dependencies:

$$\langle 0|T\{\widehat{A}(\varphi(\mathbf{y}, t), \varphi^\dagger(\mathbf{y}, t))\}|0\rangle = \frac{\int \mathcal{D}\varphi(\mathbf{x}, t) \int \mathcal{D}\varphi^*(\mathbf{x}, t) A(\varphi(\mathbf{y}, t'), \varphi^*(\mathbf{y}, t')) e^{iS[\varphi(\mathbf{x},t), \varphi^*(\mathbf{x},t)]}}{\int \mathcal{D}\varphi(\mathbf{x}, t) \int \mathcal{D}\varphi^*(\mathbf{x}, t) e^{iS[\varphi(\mathbf{x},t), \varphi^*(\mathbf{x},t)]}} \tag{2.120}$$

Please note that the difference between the $\mathbf{x}$ and $\mathbf{y}$ is important (and so is the difference between t and t')! The operator $\widehat{A}$ consists of creators and annihilators, that create and annihilate particles at particular points in space $\mathbf{y}$, while the $\mathbf{x}$ are arguments of the integration variables! Anyway, equation (2.120) is not formal perfect. Please imagine that any φ and φ^* acts at different times and at different points in space, and of course not all at time t and at the same position $\mathbf{y}$, and that we have to order the product of operators with respect to the different times t_i when they act.

Well, we have now almost explained equation (2.109). What remains is the transition from position space to momentum space. Unfortunately we are once more confronted with a lack of variable names. So we name our integration variable $\mathbf{p}$, although it is *not* the same p that appeared a few lines above in equation (2.117). That p corresponded to q, while our $\mathbf{p}$ that we have now corresponds to $\mathbf{x}$.

Anyway, under the assumption that the transition

$$\int \mathcal{D}\varphi(\mathbf{x}, t) \int \mathcal{D}\varphi^*(\mathbf{x}, t) \to \int \mathcal{D}\varphi(\mathbf{p}, t) \int \mathcal{D}\varphi^*(\mathbf{p}, t) \tag{2.121}$$

has Jacobian 1, we finally get our equation (2.109), if we set $\widehat{A}$ to be the operator that corresponds to the four-point function that we want to compute:

$$S_{\beta,\alpha} = f \quad \frac{\int \mathcal{D}\varphi(\mathbf{p},t) \int \mathcal{D}\varphi^*(\mathbf{p},t)\varphi(\mathbf{p}_4,t_4)\varphi(\mathbf{p}_3,t_3)\varphi^*(\mathbf{p}_2,t_2)\varphi^*(\mathbf{p}_1,t_1)e^{iS[\varphi(\mathbf{p},t),\varphi^*(\mathbf{p},t)]}}{\int \mathcal{D}\varphi(\mathbf{p},t) \int \mathcal{D}\varphi^*(\mathbf{p},t)e^{iS[\varphi(\mathbf{p},t),\varphi^*(\mathbf{p},t)]}}. \tag{2.122}$$

In contrast to (2.109), we used t_i so that we don't mix up the integration variables t with the special times t_1 and t_2 before and t_3 and t_4 after the scattering process.

Fortunately a possible double use of times will now have an end. Because here, our small excursion ends and the next step is the...

<u>Fourier transformation to frequency space</u>

The Fourier transformation from time to frequency space is quite simple. As we already used

$$\varphi(\mathbf{x},t) = \int \frac{d^3p}{(2\pi)^3} e^{i\mathbf{p}\mathbf{x}} \varphi(\mathbf{p},t) \tag{2.123}$$

the transformation to frequency space is of course

$$\varphi(\mathbf{p},t) = \int \frac{d\omega}{2\pi} e^{-i\omega t} \varphi(\mathbf{p},\omega) \tag{2.124}$$

so the overall transformation is

$$\varphi(\mathbf{x},t) = \int \frac{d^3p d\omega}{(2\pi)^4} e^{i\mathbf{p}\mathbf{x}-i\omega t} \varphi(\mathbf{p},\omega). \tag{2.125}$$

To shorten the notation, we will write this very often as

$$\varphi(\mathbf{x},t) = \int \frac{d^4p}{(2\pi)^4} e^{ipx} \varphi(\mathbf{p},\omega), \tag{2.126}$$

with four-vectors $p = (\omega, \mathbf{p})$ and $(px) = -p^0x^0 + \vec{p}\vec{x} = -\omega t + \vec{p}\vec{x}$.

For the functional integral we again assume that the Jacobian is 1, so we have

$$\int \mathcal{D}\varphi(\mathbf{p},t) = \int \mathcal{D}\varphi(\mathbf{p},\omega) \tag{2.127}$$

If we describe everything in momentum space, we should do the same with the action. This becomes

$$S = \int \frac{d^4p}{(2\pi)^4} (\omega - E(\mathbf{p}))\varphi^*(p)\varphi(p). \tag{2.128}$$

Before we compute now the S-matrix element in the free theory, we make another small excursion.

- Let's play with a toy action!

  We want to work first with some kind of toy action, that has no physical meaning but has the advantage to be even more simple:

$$S = \int \frac{d^4p}{(2\pi)^4} \varphi^*(p)\varphi(p). \tag{2.129}$$

The two point function in the toy action is

$$\begin{aligned}\langle \varphi(p_2)\varphi^*(p_1)\rangle &= \frac{1}{Z}\int \prod_p d\varphi(p)d\varphi^*(p)\,[\varphi(p_2)\varphi^*(p_1)]\, e^{i\int \frac{d^4p}{(2\pi)^4}\varphi(p)\varphi^*(p)} \\ &= \frac{\int \prod_p \left(d\varphi(p)d\varphi^*(p)e^{i\frac{d^4p}{(2\pi)^4}\varphi(p)\varphi^*(p)}\right)\varphi^*(p_1)\varphi(p_2)}{\int \prod_p \left(d\varphi(p)d\varphi^*(p)e^{i\frac{d^4p}{(2\pi)^4}\varphi(p)\varphi^*(p)}\right)}\end{aligned} \tag{2.130}$$

Here we wrote the exponential factor to the product, with the consequence that there is not anymore an integral sign in the exponential function.

To solve this integral it is now important to know the difference between p and p_i and to remind that for different "product-p's" the integration variables φ are also different! Remembering the Gaussian Integrals of (2.98) to (2.98) we see now immediately that our two point function will be non-zero only if $p_1 = p_2$. If this condition is fulfilled, we have a lot of integrals that cancel with the normalization, and one single of the type

$$\frac{\int dz d\overline{z}\; z\overline{z} e^{-\alpha z\overline{z}}}{\int dz d\overline{z} e^{-\alpha z\overline{z}}} = \frac{1}{\alpha} \tag{2.131}$$

So here we get

$$\langle \varphi(p_2)\varphi^*(p_1)\rangle = \frac{i}{\frac{d^4p}{(2\pi)^4}} \tag{2.132}$$

For the four-point function in our toy action $\langle \varphi(p_4)\varphi(p_3)\varphi^*(p_2)\varphi^*(p_1)\rangle$ it is not much more complicated. The only difference is that we need to combine our p's such that we get two integrals of the type (2.131). As we need to combine always one φ^* with one φ, the result is zero whenever $p_1 \neq p_3$ and $p_1 \neq p_4$.

Only if $p_1 = p_3$ *and* $p_2 = p_4$ or if $p_1 = p_4$ *and* $p_2 = p_3$, we get a contribution, namely

$$\langle \varphi(p_4)\varphi(p_3)\varphi^*(p_2)\varphi^*(p_1)\rangle = \left(\frac{i}{\frac{d^4p}{(2\pi)^4}}\right)^2 = -\frac{(2\pi)^8}{(d^4p)^2} \tag{2.133}$$

And in the limit that the volume element goes $d^4p \to 0$ we get Dirac functions

$$\begin{aligned}\langle \varphi(p_4)\varphi(p_3)\varphi^*(p_2)\varphi^*(p_1)\rangle &= -(2\pi)^8\,(\delta(p_1-p_3)\delta(p_2-p_4) + \delta(p_1-p_4)\delta(p_2-p_3)) \\ &= \langle \varphi(p_3)\varphi^*(p_1)\rangle\langle \varphi(p_4)\varphi^*(p_2)\rangle + \langle \varphi(p_4)\varphi^*(p_1)\rangle\langle \varphi(p_3)\varphi^*(p_2)\rangle \\ &= \langle \varphi(p_3)\varphi^*(p_1)\rangle\langle \varphi(p_4)\varphi^*(p_2)\rangle + 1\ \textit{permutation}\end{aligned} \tag{2.134}$$

At this point it is necessary to say that the arguments of the δ-functions are four-vectors and that for this single section our δ-functions are defined without factors of 2π!

This result can easily be generalized to the $2N$-point function. The result is

$$\langle \varphi_1 \dots \varphi_n \varphi^*_{1'} \dots \varphi^*_{n'} \rangle = \langle \varphi_1 \varphi^*_{1'} \rangle \cdots \langle \varphi_n \varphi^*_{n'} \rangle + \ N \ permutations \tag{2.135}$$

This is called *Wick's theorem.*

With this, our short excursion with the toy action ends.

Let's stop playing and return to real physics Well, actually the real physical action is not much more complicated then our "toy action". The only difference was a $\omega - E(\mathbf{p})$. So if we go through our calculation again, the only change in the result is, that the factor α in (2.131) will now be

$$\alpha = \frac{-i}{\frac{d^4p}{(2\pi)^4}\big(\omega - E(\mathbf{p})\big)}$$

and so the two contributions are not completely identical, but differ in ω_i and $\mathbf{p}_1$. So we have:

$$\langle \varphi(p_4)\varphi(p_3)\varphi^*(p_2)\varphi^*(p_1)\rangle = \frac{i}{\omega_1 - E(\mathbf{p}_1) + i\epsilon}\ \frac{i}{\omega_2 - E(\mathbf{p}_2) + i\epsilon}\delta(p_1 - p_3)\delta(p_2 - p_4) \\ +1 \ permutation(\mathbf{p}_1 \leftrightarrow \ \mathbf{p}_2) \tag{2.136}$$

This is now the spectral Green's function. To get the scattering matrix we need to do

- the reverse Fourier transform to time
- and multiply the result with the phases f.

$$S_{\beta,\alpha} = -f \int \frac{d\omega_1}{2\pi}\frac{d\omega_2}{2\pi}\frac{d\omega_3}{2\pi}\frac{d\omega_4}{2\pi} e^{-i(\omega_3+\omega_4)t'} e^{i(\omega_1+\omega_2)t} \cdot \\ \left(\frac{\delta(p_1 - p_3)\delta(p_2 - p_4)}{(\omega_1 - E(\mathbf{p}_1) + i\epsilon)(\omega_2 - E(\mathbf{p}_2) + i\epsilon)} + 1 \ permutation(\mathbf{p}_1 \leftrightarrow \ \mathbf{p}_2)\right). \tag{2.137}$$

Now we split up our four-vector δ-function

$$\delta(p_1 - p_3) = (2\pi)^4 \delta(\mathbf{p}_1 - \mathbf{p}_3)\delta(\omega_1 - \omega_3)$$

and perform the very easy ω_3 and ω_4 integration. We get

$$S_{\beta,\alpha} = f \int \frac{d\omega_1}{2\pi} e^{-i\omega_1(t'-t)} \frac{i}{\omega_1 - E(\mathbf{p}_1)} \int \frac{d\omega_2}{2\pi} e^{-i\omega_2(t'-t)} \frac{i}{\omega_2 - E(\mathbf{p}_2)} \\ \cdot (2\pi)^6 \left(\delta(\mathbf{p}_1 - \mathbf{p}_3)\delta(\mathbf{p}_2 - \mathbf{p}_4) + (\mathbf{p}_1 \to \mathbf{p}_2)\right) \tag{2.138}$$

To solve the ω_1 and ω_2 integrations we need the "$i\epsilon$-regularization". The appearing phase factors are exactly canceled by the factor f that we still have in front of all our integrals. Furthermore we use the obviously correct relation for Θ-functions

$$\Theta^2(t' - t) = \Theta(t' - t) \tag{2.139}$$

and employ $t' > t$. The final result for the S-matrix element is

$$S = (2\pi)^6 \left(\delta(\mathbf{p}_1 - \mathbf{p}_3)\delta(\mathbf{p}_2 - \mathbf{p}_4) + (\mathbf{p}_1 \to \mathbf{p}_2)\right) \\ = \delta_{\beta\alpha} \tag{2.140}$$

The last line should be read as the definition for $\delta_{\beta\alpha}$.

b) Include Interaction for $2 \leftrightarrow 2$ Scattering

Now we come to the real physical interesting part of true scattering processes with interaction.

Our action S is given by

$$S = S_0 + S_{int} \tag{2.141}$$

where S_0 is the free action that we had in case a). The interacting part of the action is given by

$$S_{int} = -\frac{\lambda}{2} \int dt \int d^3x (\varphi^* \varphi)^2 \tag{2.142}$$

just as we had it already at the very beginning of this section 2.2.10. We are again interested in the spectral Green's function

$$G(p_1, p_2, p_3, p_4) = \langle \varphi(p_4)\varphi(p_3)\varphi^*(p_2)\varphi^*(p_1)\rangle \\ = \frac{\int \mathcal{D}\varphi \varphi^*(p_1)\varphi^*(p_2)\varphi(p_3)\varphi(p_4)e^{iS}}{\int \mathcal{D}\varphi e^{iS}} \tag{2.143}$$

As everything is already written here in frequency and momentum space, we will of course have to calculate our S_{int} also in momentum space. But before we do that, let us simplify our problem (2.143).

Our ansatz is, that we don't try to solve the full problem (2.143), but an easier one. First, we expand our exponential function of S_{int} to

$$e^{iS} = e^{iS_0}(1 + iS_{int} + \mathcal{O}(\lambda^2)) \tag{2.144}$$

and use this for the numerator. For the denominator, we neglect even the first order and work simply with e^{iS_0}. We get

$$G(p_1, p_2, p_3, p_4) = G_0 + \Delta G^{(4)} \tag{2.145}$$

where $\Delta G^{(4)}$ is the first order correction to the spectral Green's function and is given by the following equation:

$$\Delta G^{(4)} = -\frac{i\lambda}{2} \frac{\int \mathcal{D}\varphi \varphi^*(p_1)\varphi^*(p_2)\varphi(p_3)\varphi(p_4)\hat{S}_{int}e^{iS_0}}{\int \mathcal{D}\varphi e^{iS_0}} \tag{2.146}$$

We already mentioned that it will be necessary to use the frequency-momentum representations of S_{int}. We use the variable name q for these Fourier transforms and get

$$\hat{S}_{int} = \int \frac{d^4q_1}{(2\pi)^4}\frac{d^4q_2}{(2\pi)^4}\frac{d^4q_3}{(2\pi)^4}\frac{d^4q_4}{(2\pi)^4}(2\pi)^4\delta^4(q_1+q_2-q_3-q_4)\varphi(q_1)\varphi(q_2)\varphi^*(q_3)\varphi^*(q_4). \tag{2.147}$$

We insert this and get

$$\Delta G^{(4)} = -\frac{i\lambda}{2}\int\prod_{i=1}^{4} dq_i\delta(q_1+q_2-q_3-q_4)\langle\varphi(q_1)\ldots\varphi^*(q_4)\varphi^*(p_1)\ldots\varphi(p_4)\rangle_{S_0} \tag{2.148}$$

The expectation value is to be taken with the free action S_0. So here appears an eight-point function of the free theory!

Let us compute it in the case of a *true* scattering event, what requires that the momenta of all outgoing particles are different from the incoming ones. In order to get a non-zero result, we need to combine the q's and p's in such a way, that we get four integrals of the kind (2.131). So we need to combine "non-$*$-q's" with "$*$-p's" and vice versa. This is only the case if we choose

- $p_1 = q_1,\ p_2 = q_2,\ p_3 = q_3,\ p_4 = q_4$
- $p_1 = q_2,\ p_2 = q_1,\ p_3 = q_3,\ p_4 = q_4$
- $p_1 = q_1,\ p_2 = q_2,\ p_3 = q_4,\ p_4 = q_3$
- $p_1 = q_2,\ p_2 = q_1,\ p_3 = q_4,\ p_4 = q_3$

Now it is very convenient to use Wick's theorem. So we get

$$\Delta G^{(4)} = \frac{-i\lambda}{2}\int\prod_{i=1}^{4} dq_i\delta(q_1+q_2-q_3-q_4)[G_0(p_1,q_1)G_0(p_2,q_2)G_0(p_3,q_3)G_0(p_4,q_4) \\ +3\ permutations] \tag{2.149}$$

Every G_0 is just the two-point function of the free theory, e.g.

$$G_0(p_1,q_1) = \frac{i}{\omega_1 - E(\mathbf{p}_1)}\delta(q_1-p_1). \tag{2.150}$$

With this we come to the relation

$$\Delta G^{(4)} = \frac{-i\lambda}{2}\int\prod_{i=1}^{4} dq_i\delta(q_1+q_2-q_3-q_4) \\ \cdot\left[\frac{i\delta(q_1-p_1)}{\omega_1-E(\mathbf{p}_1)}\cdot\ldots\ldots\cdot\frac{i\delta(q_4-p_4)}{\omega_4-E(\mathbf{p}_4)}+3\ permutations\right] \tag{2.151}$$

With all the δ-functions, the q-integrations become trivial. After performing the integration the permutations give all the same result, that's why we get a factor of 4 in the following expression:

$$\Delta G^{(4)} = -4\frac{i\lambda}{2}\frac{\delta(p_1+p_2-p_3-p_4)}{(\omega_1-E(\mathbf{p}_1))(\omega_2-E(\mathbf{p}_2))(\omega_3-E(\mathbf{p}_3))(\omega_4-E(\mathbf{p}_4))} \tag{2.152}$$

To get the first order correction of the S-matrix, we have again to do the reverse Fourier transformation to time and to multiply with f

$$\Delta S_{\beta,\alpha} = -2i\lambda f\int\frac{d\omega_1}{2\pi}\cdots\frac{d\omega_4}{2\pi}\frac{\delta(p_1+p_2-p_3-p_4)e^{i\omega_1 t+\ldots-\ldots-i\omega_4 t'}}{(\omega_1-E(\mathbf{p}_1))\cdot\ldots\cdot\ldots\cdot(\omega_4-E(\mathbf{p}_4))} \tag{2.153}$$

Splitting up the δ-function in momentum and frequency part and using

$$\delta(\omega_1+\omega_2-\omega_3-\omega_4) = \int d\tau e^{-i(\omega_1+\omega_2-\omega_3-\omega_4)\tau} \tag{2.154}$$

we get

$$\begin{aligned}\Delta S_{\beta,\alpha} = -2i\lambda f(2\pi)^4\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4)\int d\tau &\left(\int\frac{d\omega_1}{2\pi}\frac{e^{-i\omega_1(t-\tau)}}{\omega_1-E(\mathbf{p}_1)}\right)\cdots\\ &\left(\int\frac{d\omega_4}{2\pi}\frac{e^{-i\omega_4(\tau-t')}}{\omega_4-E(\mathbf{p}_4)}\right).\end{aligned} \tag{2.155}$$

The solution of the ω-integrations with $i\epsilon$ regularization is

$$\begin{aligned}\int d\omega_1\frac{e^{-i\omega_1(t-\tau)}}{\omega_1-E(\mathbf{p}_1)} &= \frac{2\pi}{i}e^{-iE(\mathbf{p}_1)(\tau-t)}\Theta(\tau-t),\\ \int d\omega_4\frac{e^{-i\omega_4(\tau-t')}}{\omega_4-E(\mathbf{p}_4)} &= \frac{2\pi}{i}e^{-iE(\mathbf{p}_4)(t'-\tau)}\Theta(t'-\tau)\end{aligned} \tag{2.156}$$

Note the difference in the argument of the Θ function!

The $e^{\pm iE(\mathbf{p}_i)t}$ factors cancel with the f factor. What remains is the τ-integration:

$$\int d\tau\left[\Theta(\tau-t)\Theta(t'-\tau)\right]^2 e^{-i\tau(E(\mathbf{p}_1)\cdots-E(\mathbf{p}_4))} = \Theta(t'-t)\delta(E(\mathbf{p}_1)\ldots-E(\mathbf{p}_4)) \tag{2.157}$$

Thus, the final result for first order correction to the S-matrix is

$$\Delta S_{\beta,\alpha} = -2i\lambda(2\pi)^4\delta(\mathbf{p}_1+\mathbf{p}_2-\mathbf{p}_3-\mathbf{p}_4)\delta(E(\mathbf{p}_1)+E(\mathbf{p}_2)-E(\mathbf{p}_3)-E(\mathbf{p}_4)) \tag{2.158}$$

Now we can easily see the reduced transition amplitude or amputated, connected Green's function, according to (2.105):

$$M_{\beta,\alpha} = 2\lambda \tag{2.159}$$

Comments

- after the ω-integration, the 'external propagators' $\frac{i}{\omega_i - E(p_i)}$ serve to put the energy *on shell*: $\omega \to E(p)$. $M_{\beta\alpha}$ does not contain propagators for the incoming and outgoing particles anymore. This is what the word *amputated* means

- there is always a function $\delta(\sum_i p_{in_i} - \sum_j p_{out_j})$ in $S_{\beta,\alpha}$ counting for conservation of the total energy and momentum

- The interaction is given by

$$S_{int} = -\frac{\lambda}{2} \int \frac{d^4 q_1}{(2\pi)^4} \cdots \frac{d^4 q_4}{(2\pi)^4} \phi^*(q_4) \ldots \phi(q_1)(2\pi)^4 \delta^4(q_1 + q_2 - q_3 - q_4). \quad (2.160)$$

In the classical approximation one has

$$M_{cl}\delta(p_1 + p_2 - p_3 - p_4) = -\frac{\delta^4 S}{\delta\phi^*(p_4) \ldots \delta(p_1)} \quad (2.161)$$

2.3 Generating Functionals

In this section we introduce a powerful method to calculate correlation functions. At the end we will have a formula, which we can directly use in perturbation calculations. To start, we take a one dimensional Gaussian integral and look at it's n-th moment:

$$\langle x^n \rangle = \frac{\int dx x^n e^{-\alpha x^2}}{\int dx e^{-\alpha x^2}}. \quad (2.162)$$

In the exponent of the nominator of (2.162) we add a *source term* $-ijx$. Having done this, we can easily transform the equation:

$$\begin{aligned}\langle x^n \rangle &= \frac{\int dx x^n e^{-\alpha x^2 - ijx}}{\int dx e^{-\alpha x^2}} \,|_{j=0} \\ &= \frac{\left(i\frac{\partial}{\partial j}\right)^n \int dx e^{-\alpha x^2 - ijx}}{\int dx e^{-\alpha x^2}} \,|_{j=0} \\ &= \frac{\left(i\frac{\partial}{\partial j}\right)^n Z_0\,[j]\,|_{j=0}}{Z_0\,[0]}. \end{aligned} \quad (2.163)$$

In (2.163) we can see that we just need the partition function $Z_0\,[j]$ in order to calculate the momenta $\langle x^n \rangle$! This comes in handy, when we try to calculate the partition function, with the existence of a potential $V(x)$.

But first we explicitly calculate Z_0 by completion of the square:

$$\begin{aligned}\frac{1}{Z_0[0]}Z_0[j] &= \frac{1}{Z_0[0]}\int dx e^{-\alpha x^2 - ijx} \\ &= \frac{1}{Z_0[0]}\int dx e^{-\alpha(x+ij/(2\alpha))^2 - j^2/(4\alpha)} \\ &= \frac{1}{Z_0[0]}\int dx' e^{-\alpha x'} e^{-j^2/(4\alpha)} = e^{-j^2/(4\alpha)}.\end{aligned} \tag{2.164}$$

The partition function $Z[j]$, which includes a potential V, is given by

$$\begin{aligned}Z[j] &= \frac{1}{Z_0[0]}\int dx e^{-(\alpha x^2 + V(x)) + ijx} \\ &= \frac{1}{Z_0[0]} e^{V(i\frac{\partial}{\partial j})} Z_0[j] \\ &= e^{-V(i\partial_j)} e^{-j^2/(4\alpha)}.\end{aligned} \tag{2.165}$$

In (**??**) we use that $e^{-V(x)}$ can be expanded into a Taylor series of the monomials x^n. Then we just make use of (2.163). In (2.165) one can see how easy it is, to get a perturbation series in our interaction theory: we just have to expand $e^{-V(i\partial_j)}$ in the parameters of V.

Some Examples

Let's calculate some momenta $\langle x^n \rangle$

$V = 0$: Because we always set j=0, the odd momenta $\langle x^{2n+1}\rangle$ vanish, so we just need to calculate $\langle x^{2n}\rangle$. For this, we expand $e^{-j^2/(4\alpha)}$ in powers of $-j^2/(4\alpha)$. Because of setting $j = 0$, all powers higher than n vanish. So we get

$$\begin{aligned}\langle x^{2n}\rangle &= (i\partial_j)^{2n}\frac{1}{n!}\left(-\frac{j^2}{4\alpha}\right)^n \\ &= \frac{(2n)!}{n!}\left(\frac{1}{4\alpha}\right)^n\end{aligned} \tag{2.166}$$

$V = -\frac{\lambda}{2}x^4$**:** Now we'll calculate a deviation from the non-interacting $\langle x^4\rangle_0$ in first order of λ. Then we have $e^{\frac{\lambda}{2}\partial_j^4} \approx 1 + \frac{\lambda}{2}\partial_j^4$, so we get

$$\begin{aligned}\Delta\langle x^4\rangle &= (i\partial_j)^4\left(\frac{\lambda}{2}\partial_j^4\right)e^{-j^2/(4\alpha)} \\ &= \frac{\lambda}{2}\partial_j^8\left(\frac{1}{4!}\left(-\frac{j^2}{4\alpha}\right)^4\right) = \frac{\lambda}{2\cdot 4!}8!\left(\frac{1}{4\alpha}\right)^4 = \lambda\frac{3\cdot 5\cdot 7}{32\alpha^4}\end{aligned} \tag{2.167}$$

The Partition Function in the Path Integral

Now in the path integral formulation, we can do something similar to the above. Given the expression

$$Z = \int \mathcal{D}\varphi e^{iS[\varphi]} \tag{2.168}$$

for the partition function, we can add a source term

$$-\int \frac{d^4p}{(2\pi)^4} \left(J^*(p)\varphi(p) + J(p)\varphi^*(p)\right) \tag{2.169}$$

to the exponent of Z. In the free field theory ($V = 0$), the action $S[\varphi] = S_0[\varphi]$ takes the form

$$S_0[\varphi] = \int \frac{d^4p}{(2\pi)^4} \varphi^*(p) \left(\omega - E(\mathbf{p})\right) \varphi(p). \tag{2.170}$$

Together with (2.169), the partition function is

$$Z_0[J, J^*] = \int \mathcal{D}\varphi e^{i \int \frac{d^4p}{(2\pi)^4} \left(\varphi^*(p)(\omega - E(\mathbf{p}))\varphi(p) - J^*(p)\varphi(p) + J(p)\varphi^*(p)\right)}. \tag{2.171}$$

As usual, to get rid of the linear term in the exponent, we use the transformation $\varphi(p) = \varphi'(p) + \frac{J(p)}{\omega - E(\mathbf{p})}$. The exponent then transforms to

$$i \int \frac{d^4p}{(2\pi)^4} \left(\varphi'^*(p) \left(\omega - E(\mathbf{p})\right) \varphi'(p) - J^*(p) \frac{1}{\omega - E(\mathbf{p})} J(p)\right). \tag{2.172}$$

The partition function for the free field theory is therefore given by

$$Z_0[J, J^*] = Z_0[0]\, e^{-i \int \frac{d^4p}{(2\pi)^4} \left(J^*(p) \frac{1}{\omega - E(\mathbf{p})} J(p)\right)}. \tag{2.173}$$

For the existence of a potential V, we can use (2.173) as a generating functional. The action S is

$$\begin{aligned} S[\varphi] &= S_0[\varphi] + S_{int}[\varphi, \varphi^*], \\ S_{int}[\varphi, \varphi^*] &= \int d^4x V[\varphi^*(x), \varphi(x)]. \end{aligned} \tag{2.174}$$

Expanding $S_{int}[\varphi, \varphi^*]$ in powers of φ and φ^*, we can use the same argumentation, as for (2.165). For the partition function, we then get

$$Z[J, J^*] = e^{S_{int}\left[i\frac{\delta}{\delta J}, i\frac{\delta}{\delta J^*}\right]} Z_0[J, J^*]. \tag{2.175}$$

3 Fermions

3.1 Fermionic Quantum Fields

3.1.1 Pauli Principle

We want to generalize the machinery we have developed so far for bosons to *fermions*. Examples of fermions are free electrons or nonrelativistic atoms with spin $\frac{1}{2}$.

A one particle state can be denoted by

$$|\mathbf{p}, s\rangle, \text{ with spin } s = \pm 1 \ \leftrightarrow \ s_z = \pm\frac{\hbar}{2}, \tag{3.1}$$

a two particle state by

$$|\mathbf{p}_1, s_1, \mathbf{p}_2, s_2\rangle. \tag{3.2}$$

We can write the two particle state in terms of one particle states if we keep in mind the *antisymmetry*,

$$|\mathbf{p}_1, s_1, \mathbf{p}_2, s_2\rangle = \frac{1}{\sqrt{2}}\left(|\mathbf{p}_1, s_1\rangle|\mathbf{p}_2, s_2\rangle - |\mathbf{p}_2, s_2\rangle|\mathbf{p}_1, s_1\rangle\right). \tag{3.3}$$

The *Pauli principle* states that no two fermions can be in the same state, so if their only degrees of freedom are momentum $\mathbf{p}$ and spin s, it states

$$|\mathbf{p}, s, \mathbf{p}, s\rangle = 0. \tag{3.4}$$

Remember that we can also denote states in the *occupation number basis*,

$$\{n_{\mathbf{p},s}\}, \text{ where } n_{\mathbf{p},s} = 1 \text{ or } 0 \text{ (Pauli principle).} \tag{3.5}$$

3.1.2 Symmetries and Normalization of N-Fermion States

We introduce yet another useful shortcut notation (no new physics),

$$j = (\mathbf{p}, s), \tag{3.6}$$

with a "collective index" j, which we for now assume to be discrete.

Now a two particle state can be denoted by

$$|i, j\rangle := \varepsilon|n_i = 1; n_j = 1; n_k = 0 \text{ for } k \neq i, j; i \neq j\rangle, \tag{3.7}$$

where $\varepsilon = \pm 1$ is a "phase" to realize

$$|i,j\rangle = -|j,i\rangle. \tag{3.8}$$

In the occupation number notation with a fixed ordering of i, j, etc. this dependence on the ordering of i and j is not needed.

We have the *normalization*

$$\langle k,l|i,j\rangle = \delta_{ki}\delta_{lj} - \delta_{kj}\delta_{li}, \tag{3.9}$$

which is antisymmetric as it should be.

An N particle state is denoted as

$$|j_1, \ldots, j_N\rangle, \tag{3.10}$$

which is totally antisymmetric under the exchange of two indices j_k, j_l.

As the normalization we get a sum over all $N!$ permutations with a sign $+$ for an even permutation and a $-$ for an odd permutation.

3.1.3 Annihilation and Creation Operators

$$\begin{aligned} &\text{Creation operators:} \qquad \hat{a}^\dagger_{\mathbf{p},s}|\ldots, n_{\mathbf{p},s}, \ldots\rangle = \begin{cases} 0 & \text{if } n_{\mathbf{p},s} = 1 \\ \varepsilon|\ldots, 1, \ldots\rangle & \text{if } n_{\mathbf{p},s} = 0 \end{cases} \\ &\text{Annihilation operators:} \qquad \hat{a}_{\mathbf{p},s}|\ldots, n_{\mathbf{p},s}, \ldots\rangle = \begin{cases} 0 & \text{if } n_{\mathbf{p},s} = 0 \\ \varepsilon|\ldots, 0, \ldots\rangle & \text{if } n_{\mathbf{p},s} = 1 \end{cases} \end{aligned} \tag{3.11}$$

We need the ε here to account for the fact that

$$\hat{a}^\dagger_{\mathbf{p},s}\hat{a}^\dagger_{\mathbf{p}',s'} = -\hat{a}^\dagger_{\mathbf{p}',s'}\hat{a}^\dagger_{\mathbf{p},s}. \tag{3.12}$$

We give a simple matrix representation of these operators in the case $\mathcal{N} = 1$:

$$n = 0 \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad n = 1 \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \hat{a}^\dagger \leftrightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{a} \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \tag{3.13}$$

Exercise: Convince yourself that with this matrix representation we have

$$\hat{a}^\dagger \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} \beta \\ 0 \end{pmatrix}, \quad \hat{a} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ \alpha \end{pmatrix} \tag{3.14}$$

and

$$\{\hat{a}, \hat{a}^\dagger\} = \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} = 1 \quad \text{and} \quad \hat{a}^2 = \hat{a}^{\dagger 2} = 0. \tag{3.15}$$

Later on, we will compare an explicit representation of the *Grassmann variables* with this representation.

The generalization to $\mathcal{N} > 1$ is

$$\begin{aligned} \{\hat{a}_i, \hat{a}_j^\dagger\} &= \delta_{ij}, \\ \{\hat{a}_i, \hat{a}_j\} &= 0, \\ \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} &= 0. \end{aligned} \tag{3.16}$$

For different i, j the creation and annihilation operator *anticommute*. It especially follows that

$$\hat{a}_i{}^2 = \hat{a}_j^{\dagger 2} = 0. \tag{3.17}$$

We want to *motivate* these commutation relations. For one particle we have

$$\hat{a}_i^\dagger |0\rangle = |i\rangle, \tag{3.18}$$

and for two particles we have

$$\begin{aligned} \hat{a}_j^\dagger \hat{a}_i^\dagger |0\rangle &= |j, i\rangle, \\ -\hat{a}_i^\dagger \hat{a}_j^\dagger |0\rangle &= -|i, j\rangle. \end{aligned} \tag{3.19}$$

So $\{\hat{a}_i^\dagger, \hat{a}_j^\dagger\} = 0$ holds for the vacuum. This result is easily generalized to all states. $\{\hat{a}_i, \hat{a}_j\} = 0$ follows simply by Hermitian conjugation. $\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}$ can be motivated by a similar argument (which was not given in the lecture).

The *continuum normalization* is similar as for bosons, just that we now have anticommutators instead of commutators,

$$\{\hat{a}_{\mathbf{p},s}, \hat{a}^\dagger_{\mathbf{p}',s'}\} = \delta(\mathbf{p} - \mathbf{p}')\delta_{ss'} = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{p}')\delta_{ss'}. \tag{3.20}$$

3.1.4 Occupation Number, Hamiltonian

As usual, the number operator is given by

$$\hat{n}_{\mathbf{p},s} = \hat{a}^\dagger_{\mathbf{p},s} \hat{a}_{\mathbf{p},s}, \tag{3.21}$$

and the free Hamiltonian by

$$\hat{H}_0 = \sum_{\mathbf{p},s} \varepsilon(\mathbf{p}, s) \hat{a}^\dagger_{\mathbf{p},s} \hat{a}_{\mathbf{p},s} = \int \frac{d^3\mathbf{p}}{(2\pi)^3} \sum_{s=\pm 1} \varepsilon(\mathbf{p}, s) \hat{a}^\dagger_{\mathbf{p},s} \hat{a}_{\mathbf{p},s}, \tag{3.22}$$

where $\varepsilon(\mathbf{p}, s)$ is the *dispersion relation*. For free electrons or atoms it is given by

$$\varepsilon(\mathbf{p}, s) = \frac{\mathbf{p}^2}{2M}. \tag{3.23}$$

In general, a Fermi gas will have some other dispersion relation. Plus you have to add an interaction Hamiltonian $\sim \hat{a}^\dagger \hat{a} \hat{a}^\dagger \hat{a}$.

3.1.5 Fermion Field

We know the operator field already in momentum space. To get it in position space we Fourier transform it:

$$\begin{aligned}\hat{\psi}(\mathbf{x},s) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3}\hat{a}_{\mathbf{p},s}e^{i\mathbf{px}} = \int_{\mathbf{p}} \hat{a}_{\mathbf{p},s}e^{i\mathbf{px}},\\ \hat{\psi}^\dagger(\mathbf{x},s) &= \int \frac{d^3\mathbf{p}}{(2\pi)^3}\hat{a}^\dagger_{\mathbf{p},s}e^{-i\mathbf{px}} = \int_{\mathbf{p}} \hat{a}^\dagger_{\mathbf{p},s}e^{-i\mathbf{px}},\\ \{\hat{\psi}(\mathbf{x},s),\hat{\psi}^\dagger(\mathbf{x}',s')\} &= \delta^3(\mathbf{x}-\mathbf{x}')\delta_{ss'}.\end{aligned} \tag{3.24}$$

On the operator level, fermion fields are no more difficult than boson fields. The only difference is a little minus sign.

3.2 Path Integral for Fermionic Systems, Grassmann Variables

Why do we need a new mathematical object, the Grassmann variables, now? The answer is the same one why we use e.g. complex numbers or operators: *they are useful.*

As with complex numbers there is the *abstract definition* and there are simple *representations.* Let's start with a matrix representation:

From the two Pauli matrices

$$\tau_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \text{and} \quad \tau_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{3.25}$$

we define the following two linear combinations:

$$\begin{aligned}\tau_+ &:= \frac{1}{2}(\tau_1 + i\tau_2) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\\ \tau_- &:= \frac{1}{2}(\tau_1 - i\tau_2) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.\end{aligned} \tag{3.26}$$

Exercise: Check that

$$\tau_+^2 = 0, \qquad \tau_-^2 = 0, \qquad \{\tau_+,\tau_-\} = 1. \tag{3.27}$$

Now we switch to the abstract notation

$$\tau_- \to \theta, \qquad \tau_+ \to \bar{\theta}. \tag{3.28}$$

But instead of (3.27), we define the new Grassmann variables to have the properties

$$\theta^2 = 0, \qquad \bar{\theta}^2 = 0, \qquad \{\theta,\bar{\theta}\} = 0, \tag{3.29}$$

i.e. to be *anticommuting.* This is a new kind of product between θ and $\bar{\theta}$, different from the matrix product of τ_+ and τ_-.

Apart from multiplying Grassmann variables, one can also multiply them with real or complex numbers and add the, i.e. linear combinations

$$\alpha\theta + \beta\bar{\theta} \text{ are defined for } \alpha, \beta \in \mathbb{R} \text{ or } \mathbb{C}. \tag{3.30}$$

The product is distributive (i.e. linear in both factors):

$$\begin{aligned}(\alpha_1\theta + \beta_1\bar{\theta})(\alpha_2\theta + \beta_2\bar{\theta}) &= \alpha_1\alpha_2\theta^2 + \alpha_1\beta_2\theta\bar{\theta} + \beta_1\alpha_2\bar{\theta}\theta + \alpha_2\beta_2\bar{\theta}^2 \\ &= (\beta_1\alpha_2 - \alpha_1\beta_2)\bar{\theta}\theta.\end{aligned} \tag{3.31}$$

But wait, what kind of mathematical object is $\bar{\theta}\theta$ and these linear combinations?

By definition, the *Grassmann algebra* $\mathcal{G}$ is the set of all objects you can get by adding and multiplying the *Grassmann variables* $\theta, \bar{\theta}$ and taking multiples. It is obvious that

$$\{1, \theta, \bar{\theta}, \bar{\theta}\theta\} \text{ is a basis for } \mathcal{G}, \tag{3.32}$$

i.e. every element $g \in \mathcal{G}$ can be written as

$$g = \gamma_1 1 + \gamma_2\theta + \gamma_3\bar{\theta} + \gamma_4\bar{\theta}\theta, \tag{3.33}$$

with uniquely determined coefficients $\gamma_i \in \mathbb{R}$. (This is called a *real* Grassmann algebra. Later we will also consider the *complex* Grassmann algebra where we allow the coefficients to be complex.)

Mathematical Note (not from the lecture): In mathematics, an *algebra* is a vector space with a product that fulfills certain rules. In this sense the Grassmann algebra really is an algebra. (3.33) gives an isomorphism from the vector space $\mathcal{G}$ to the vector space $\mathbb{R}^4$. So mathematically the Grassmann algebra is something very simple: a four-dimensional vector space with a product that is determined by (3.29).

What is very strange is that Grassmann variables are called "variables" at all. Until now a variable x was something that could take on the values of some set, e.g. a real variable could have the value $2, \pi$ or $-\frac{1}{2}$. Grassmann variables are different, they are really just two fixed vectors. Everything happens in the coefficients.

Let's do a few exercises in translating statements from the abstract space $\mathcal{G}$ into the well known space $\mathbb{R}^4$:

The zero element is given by

$$g = 0 \quad \leftrightarrow \quad (\gamma_1, \gamma_2, \gamma_3, \gamma_4) = (0, 0, 0, 0). \tag{3.34}$$

Linear combinations in $\mathcal{G}$ are defined as expected,

$$g_3 = \alpha g_1 + \beta g_2 \quad \leftrightarrow \quad \gamma_{3,i} = \alpha\gamma_{1,i} + \beta\gamma_{2,i}. \tag{3.35}$$

And here's an example of how to evaluate a product of two Grassmann vectors (in lack of a better word):

$$\theta(\alpha\theta + \beta\bar{\theta}) = \alpha\theta^2 + \beta\theta\bar{\theta} = -\beta\bar{\theta}\theta \quad \leftrightarrow \quad (0, 0, 0, -\beta). \tag{3.36}$$

To summarize: Only θ and $\bar{\theta}$ are called Grassmann variables. The Grassmann algebra consists of all linear combinations of $1, \theta, \bar{\theta}, \bar{\theta}\theta$.

Compare the following three multiplication tables: (with $s_+ = 1, s_- = -1$ discrete variables of the Ising model)

$$
\begin{array}{c|cc} \cdot & \theta & \bar{\theta} \\ \hline \theta & 0 & -\bar{\theta}\theta \\ \bar{\theta} & \bar{\theta}\theta & 0 \end{array}
\qquad
\begin{array}{c|cc} \cdot & s_+ & s_- \\ \hline s_+ & s_+ & s_- \\ s_- & s_- & s_+ \end{array}
\qquad
\begin{array}{c|cc} \cdot & \hat{a} & \hat{a}^\dagger \\ \hline \hat{a} & 0 & 1-\hat{a}^\dagger\hat{a} \\ \hat{a}^\dagger & \hat{a}^\dagger\hat{a} & 0 \end{array}
\tag{3.37}
$$

The important point is that the product of Grassmann variables with the anticommutatior $\{\theta, \bar{\theta}\} = 0$ is different from the product of operators $\{\hat{a}^\dagger, \hat{a}\} = 1$.

It is easy to see how the multiplication table generalizes to products in $\mathcal{G}$, e.g.

$$\theta\bar{\theta}\theta = -\theta\theta\bar{\theta} = 0. \tag{3.38}$$

If there are n independent Grassmann variables (until now we had only $n = 2$), all products of m Grassmann variables with $m > n$ are 0. This is a direct mathematical representation of the Pauli principle.

We can not only define the "Grassmann product" of two Grassmann variables but also of any two elements of a Grassmann algebra. Below we compare the Grassmann product with the Clifford algebra which is generated by the matrices $1, \tau_-, \tau_+, \tau_+\tau_-$ and equivalent to the operator product generated by $1, \hat{a}, \hat{a}^\dagger, \hat{a}^\dagger\hat{a}$.

$$
\begin{array}{c|cccc} \cdot & 1 & \theta & \bar{\theta} & \bar{\theta}\theta \\ \hline 1 & 1 & \theta & \bar{\theta} & \bar{\theta}\theta \\ \theta & \theta & 0 & -\bar{\theta}\theta & 0 \\ \bar{\theta} & \bar{\theta} & \bar{\theta}\theta & 0 & 0 \\ \bar{\theta}\theta & \bar{\theta}\theta & 0 & 0 & 0 \end{array}
\qquad
\begin{array}{c|cccc} \cdot & 1 & \tau_- & \tau_+ & \tau_+\tau_- \\ \hline 1 & 1 & \tau_- & \tau_+ & \tau_+\tau_- \\ \tau_- & \tau_- & 0 & 1-\tau_+\tau_- & \tau_- \\ \tau_+ & \tau_+ & \tau_+\tau_- & 0 & 0 \\ \tau_+\tau_- & \tau_+\tau_- & 0 & \tau_+ & \tau_+\tau_- \end{array}
$$

Always keep in mind that the product of two Grassmann variables is not a Grassmann variable but only an element of the Grassmann algebra.

As a little preview of what will follow now, we write down the correspondence between operators and fields for bosons and fermions.

bosons	$a, a^\dagger \leftrightarrow \phi, \phi^*$ $a(x), a^\dagger(x) \leftrightarrow \phi(x), \phi^*(x)$
fermions	$a, a^\dagger \leftrightarrow \theta, \bar{\theta}$ $a(x), a^\dagger(x) \leftrightarrow \theta(x), \bar{\theta}(x)$

3.2.1 Several Grassmann Variables

Indices

To denote different Grassmann variables we use indices. For example, the index j in θ_j can denote spin up/down and thus have the value 1 or 2, or it can denote the sites on a lattice and run from 1 to $\mathcal{N}$. We will use the latter option to do the continuum limit

$\theta_j \to \theta(x)$ for fermions. Grassmann variables always anticommute, even if they have different indices.

$$\begin{aligned}
\{\theta_i, \theta_j\} &= 0, \\
\{\theta_i, \bar{\theta}_j\} &= 0, \\
\{\bar{\theta}_i, \bar{\theta}_j\} &= 0.
\end{aligned} \tag{3.39}$$

The same is true for Grassmann fields.

$$\{\theta(x), \theta(x')\} = 0 \tag{3.40}$$

Complex numbers on the other hand always commute with each other and commute with Grassmann variables.

Representation of Two Grassmann Variables as 4×4 Matrices

Unlike spin, Grassmann variables cannot be expressed as 2×2 matrices, but they have a representation as $2^n \times 2^n$ matrices, where n denotes the dimension of θ_j. We take a closer look at the case $n = 2$. Let

$$\theta_1 = \tau_- \otimes 1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{3.41}$$

and

$$\theta_2 = \tau_3 \otimes \tau_- = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \tag{3.42}$$

Let's verify that these matrices fulfill the product and commutation relations of the Grassmann variables.

$$\begin{aligned}
\theta_1\theta_2 &= \begin{pmatrix} \tau_- & 0 \\ 0 & \tau_- \end{pmatrix} \begin{pmatrix} 0 & 0 \\ \tau_3 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \tau_-\tau_3 & 0 \end{pmatrix}, \\
\theta_2\theta_1 &= \begin{pmatrix} 0 & 0 \\ \tau_3 & 0 \end{pmatrix} \begin{pmatrix} \tau_- & 0 \\ 0 & \tau_- \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ \tau_3\tau_- & 0 \end{pmatrix} = - \begin{pmatrix} 0 & 0 \\ \tau_-\tau_3 & 0 \end{pmatrix}, \\
\{\theta_1, \theta_2\} &= 0, \\
\theta_1^2 &= \begin{pmatrix} \tau_- & 0 \\ 0 & \tau_- \end{pmatrix} \begin{pmatrix} \tau_- & 0 \\ 0 & \tau_- \end{pmatrix} = 0, \\
\theta_2^2 &= \begin{pmatrix} 0 & 0 \\ \tau_3 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 \\ \tau_3 & 0 \end{pmatrix} = 0.
\end{aligned} \tag{3.43}$$

We have seen that we cannot represent Grassmann variables as simple τ matrices but if we go to higher dimensions a representation using matrices is possible. Grassmann multiplication then becomes normal matrix multiplication. One could set $\theta = \theta_1$ and $\bar{\theta} = \theta_2$ and this way express θ and $\bar{\theta}$ as 4×4 matrices.

The representation of n Grassmann variables as $2^n \times 2^n$ matrices is more convenient and will be used from now on.

Grassmann Algebra

The basis elements of the Grassmann algebra are all possible independent products of the Grassmann variables. For four independent Grassman variables, $j = 1 \dots 4$ we get

$$\begin{array}{r|l} 1, & 1 \\ \theta_1,\ \theta_2,\ \theta_3,\ \theta_4, & +4 \\ \theta_2\theta_1,\ \theta_3\theta_1,\ \theta_4\theta_1,\ \theta_3\theta_2,\ \theta_4\theta_2,\ \theta_4\theta_3, & +6 \\ \theta_3\theta_2\theta_1,\ \theta_4\theta_2\theta_1,\ \theta_4\theta_3\theta_1,\ \theta_4\theta_3\theta_2, & +4 \\ \theta_4\theta_3\theta_2\theta_1 & +1 \\ & \overline{16}. \end{array} \tag{3.44}$$

For n Grassmann variables there are 2^n basis elements for the Grassmann algebra.

If n Grassmann variables are represented by $2^n \times 2^n$ matrices, elements of the corresponding Grassmann algebra are also represented by $2^n \times 2^n$ matrices obtained by matrix multiplication. This Grassmann algebra has only 2^n independent basis elements, so it does only contain specific $2^n \times 2^n$ matrices!

3.2.2 Functions of Grassmann Variables

The functions

$$\begin{aligned} f(\theta_j):\ & \text{(Grassmann variables)} \ \rightarrow \ \text{(Grassmann algebra)} \\ f(g):\ & \text{(Grassmann algebra)} \ \rightarrow \ \text{(Grassmann algebra)} \end{aligned} \tag{3.45}$$

are only defined for polynomials, i.e. sums of products. The existence of a Taylor expansion around zero is sufficient for a definition of $f(\theta_j)$. Let $f(x_j)$ be defined by a Taylor expansion around $x_j = 0$. We define

$$\begin{aligned} f(\theta_j) &:= f(0) + \partial_j f(\theta_j)\big|_{\theta_j=0}\theta_j + \frac{1}{2}\partial_j\partial_k f(\theta_j,\theta_k)\big|_{\theta_j,\theta_k=0}\theta_j\theta_k + \cdots \\ \text{if } f(x_j) &= f(0) + \partial_j f(x_j)\big|_{x_j=0}x_j + \frac{1}{2}\partial_j\partial_k f(x_j,x_k)\big|_{x_j,x_k=0}x_j x_k + \cdots \end{aligned} \tag{3.46}$$

Obviously the Taylor expansion is cut off at order n because higher products always contain a square θ_j^2 of one of the variables, which makes the product zero. Note that in terms containing more than one Grassmann variable the Grassmann variables occur in all possible commutations but the relative minus sign is compensated because differentiation also anticommutes.

Examples for $n = 2$

Let's take a look at what some common functions become when we use Grassmann variables.

$$\exp(\bar{\theta}\theta) = 1 + \bar{\theta}\theta + \underbrace{\frac{1}{2}(\bar{\theta}\theta)^2 + \cdots}_{=0} = 1 + \bar{\theta}\theta \tag{3.47}$$

$$\frac{1}{1-\bar{\theta}\theta} = 1 + \bar{\theta}\theta + \underbrace{(\bar{\theta}\theta)^2 + \cdots}_{=0} = 1 + \bar{\theta}\theta \tag{3.48}$$

$$\ln(1+\bar{\theta}\theta) = \bar{\theta}\theta - \underbrace{\frac{1}{2}(\bar{\theta}\theta)^2 + \cdots}_{=0} = \bar{\theta}\theta \tag{3.49}$$

The functions $\frac{1}{1-\bar{\theta}\theta}$ and $\exp(\bar{\theta}\theta)$ are identical for Grassmann variables. Let's check how ln and exp work together.

$$e^{\ln(1+\bar{\theta}\theta)} = e^{\bar{\theta}\theta} = 1 + \bar{\theta}\theta \tag{3.50}$$

The logarithm still is the inverse of the exponential function. All operations with functions remain valid for functions of Grassmann variables provided that they are compatible with Taylor expansion.

Functions that have a pole at $x = 0$ are not defined for Grassmann variables. This includes common functions like $\frac{1}{\bar{\theta}\theta}$ and $\ln(\bar{\theta}\theta)$. The Grassmann algebra does not contain an inverse element of $\bar{\theta}\theta$!

3.2.3 Differentiation

For the differential operator of Grassmann variables we demand that

$$\frac{\partial}{\partial\theta_j} \begin{cases} \text{takes one factor } \theta_j \text{ in polynomials away if present.} \\ \text{ordering is important: } \frac{\partial}{\partial\theta_j}\theta_j\theta_i = \theta_i \neq \frac{\partial}{\partial\theta_j}\theta_i\theta_j = -\theta_i \\ \text{is zero if } \theta_j \text{ does not appear in the function to be differentiated.} \end{cases} \tag{3.51}$$

With these properties in mind we can write down the following relations:

$$\boxed{\frac{\partial}{\partial\theta_j}\theta_i = \delta_{ij}} \tag{3.52}$$

$$\frac{\partial}{\partial\theta_j}\underbrace{\theta_{a_1}\dots\theta_{a_m}}_{m}\theta_j\theta_{b_1}\dots\theta_{b_n} = (-1)^m\theta_{a_1}\dots\theta_{a_m}\theta_{b_1}\dots\theta_{b_n} \tag{3.53}$$

While differential operators for complex variables commute, differential operators for Grassmann variables anticommute like Grassmann variables themselves:

$$\boxed{\left\{\frac{\partial}{\partial\theta_i}, \frac{\partial}{\partial\theta_j}\right\} = 0} \tag{3.54}$$

We check this for $\theta_j\theta_i$ which gives the result

$$\frac{\partial}{\partial\theta_i}\frac{\partial}{\partial\theta_j}\theta_j\theta_i = -\frac{\partial}{\partial\theta_j}\frac{\partial}{\partial\theta_i}\theta_j\theta_i = \frac{\partial}{\partial\theta_i}\theta_i = 1. \tag{3.55}$$

Next we propose

$$\boxed{\left\{\frac{\partial}{\partial\theta_j}, \theta_i\right\} = \delta_{ji}.} \tag{3.56}$$

We can verify this proposal by letting the anticommutator act on a Grassmann variable. The calculation

$$\begin{aligned}\left(\frac{\partial}{\partial\theta_j}\theta_i + \theta_i\frac{\partial}{\partial\theta_j}\right)\theta_k &= \frac{\partial}{\partial\theta_j}\theta_i\theta_k + \theta_i\frac{\partial}{\partial\theta_j}\theta_k = \frac{\partial\theta_i}{\partial\theta_j}\theta_k - \frac{\partial\theta_k}{\partial\theta_j}\theta_i + \theta_i\frac{\partial}{\partial\theta_j}\theta_k \\ &= \delta_{ji}\theta_k - \delta_{jk}\theta_i + \delta_{jk}\theta_i = \delta_{ji}\theta_k \end{aligned} \tag{3.57}$$

shows that the proposal is correct.

Matrix Representation of Grassmann Differentiation

n Grassmann variables $\theta_1, \ldots, \theta_n$ can be represented by $2^n \times 2^n$ matrices, the Grassmann algebra that is generated by their products can also be represented by Grassmann $2^n \times 2^n$ matrices. We will give examples showing that the differential operator $\frac{\partial}{\partial\theta_j} : \mathcal{G} \to \mathcal{G}$ can also be represented as a $2^n \times 2^n$ matrix. In this representation the differentiation of Grassmann variables becomes an ordinary matrix multiplication.

In the case of only one Grassmann variable we have $\theta = \tau_-$ and $\frac{\partial}{\partial\theta} = \tau_+$ which fulfills the property $\{\frac{\partial}{\partial\theta}, \theta\} = \{\tau_+, \tau_-\} = 1$ of the Grassmann differentiation.

Things are slightly more complicated in the $n = 2$ case. We need the 4×4 matrices

$$\begin{aligned} \theta_1 &= \tau_- \otimes 1, & \theta_2 &= \tau_3 \otimes \tau_- \\ \frac{\partial}{\partial\theta_1} &= \tau_+ \otimes 1, & \frac{\partial}{\partial\theta_2} &= \tau_3 \otimes \tau_+ \end{aligned} \tag{3.58}$$

It is a simple exercise in matrix multiplication to show that these matrices represent the properties of differentiation of Grassmann variables in the form of a simple matrix multiplication. For example,

$$\frac{\partial}{\partial\theta_2}\theta_1 = \begin{pmatrix} 0 & \tau_3 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \tau_- & 0 \\ 0 & \tau_- \end{pmatrix} = (\tau_3\tau_-) \otimes \tau_+ = 0 \tag{3.59}$$

as expected.

Analogy between Bosons and Fermions

In quantum field theory we have the creation and annihilation operators. The correspondence for fermionic systems is

$$\begin{aligned} a_j &\leftrightarrow \theta_j \\ a_j^\dagger &\leftrightarrow \frac{\partial}{\partial\theta_j} \end{aligned} \tag{3.60}$$

3.2.4 Integration

For a integral over an asymptotically vanishing real function $f(x)$ we have

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \frac{\partial}{\partial x} f(x) = 0 \tag{3.61}$$

because the boundary terms vanish. Therefore we demand the relation

$$\int d\theta \frac{\partial}{\partial \theta} f(\theta) = 0 \tag{3.62}$$

for Grassmann integration. Also after the θ-integration the result should not depend on θ anymore and we require

$$\frac{\partial}{\partial \theta} \int d\theta f(\theta) = 0. \tag{3.63}$$

Grassmann differentiation satisfies the defining properties of Grassmann integration (3.62), (3.63). We can set

$$\boxed{\int \mathrm{d}\theta = \frac{\partial}{\partial \theta}}. \tag{3.64}$$

We find the properties

$$\begin{aligned} &1. \quad \int \mathrm{d}\theta \, 1 = \int \mathrm{d}\theta \, \frac{\partial}{\partial \theta} \theta = 0, \\ &2. \quad \int \mathrm{d}\theta \, \theta = 1. \end{aligned} \tag{3.65}$$

The first property corresponds to the fact that the Grassmann-differentiation is nilpotent

$$\left(\frac{\partial}{\partial \theta} \right)^2 = 0. \tag{3.66}$$

3.3 Functional integral with Grassmann variables

3.3.1 Partition function

The partition function is $Z = \int \mathcal{D}\Psi e^{iS[\Psi]}$ where the action $S[\Psi]$ is a functional of Ψ and $\bar{\Psi}$ and $\int \mathcal{D}\Psi$ is defined as

$$\int \mathcal{D}\Psi(x) = \int \mathcal{D}\Psi(x) \mathcal{D}\bar{\Psi}(x) = \prod_x \left[\int \mathrm{d}\Psi(x) \, \mathrm{d}\bar{\Psi}(x) \right]. \tag{3.67}$$

Here ordering matters and Ψ and $\bar{\Psi}$ satisfy the anti-commutation relations

$$\{\Psi(x), \bar{\Psi}(x')\} = \{\bar{\Psi}(x), \bar{\Psi}(x')\} = \{\Psi(x), \Psi(x')\} = 0. \tag{3.68}$$

because they are Grassmann variables, for example

$$\begin{aligned}\Psi(\mathbf{x},t) &= \int \frac{\mathrm{d}^3p}{(2\pi)^3} e^{i\mathbf{p}\mathbf{x}} \theta(\mathbf{p},t)\\ \bar{\Psi}(\mathbf{x},t) &= \int \frac{\mathrm{d}^3p}{(2\pi)^3} e^{-i\mathbf{p}\mathbf{x}} \bar{\theta}(\mathbf{p},t).\end{aligned} \tag{3.69}$$

The action can be expressed as

$$S[\psi] = \int \mathrm{d}t\, \mathrm{d}^3x\, \mathcal{L}[\Psi(\mathbf{x},t), \bar{\Psi}(\mathbf{x})]. \tag{3.70}$$

The non-relativistic Lagrangian for free fermions is

$$\mathcal{L}_0 = i\bar{\Psi}_\alpha \frac{\partial}{\partial t}\Psi_\alpha + \bar{\Psi}_\alpha \frac{\Delta}{2m}\Psi_\alpha. \tag{3.71}$$

Putting things together leaves us in Fourier space with

$$S[\Psi] = \int \mathrm{d}t \int_{\mathbf{p}} \left\{ i\bar{\Psi}_\alpha(\mathbf{p},t)\frac{\partial}{\partial t}\Psi_\alpha(\mathbf{p},t) - \frac{\mathbf{p}^2}{2m}\bar{\Psi}_\alpha(\mathbf{p},t)\Psi_\alpha(\mathbf{p},t) \right\}. \tag{3.72}$$

already included in this equation are the internal indices α (spin) which Ψ typically has. This is identical with the functional integral for non-relativistic bosons (2.93), only $\phi(\mathbf{x},t)$ and $\phi^*(\mathbf{x},t)$ are replaced by Grassmann variables $\Psi(\mathbf{x},t)$ and $\bar{\Psi}(\mathbf{x},t)$.

3.3.2 Correlation functions

Grassmann fields guarantee the anti-symmetry of the correlation functions required by Fermi statistics.

$$\begin{aligned}\langle \Psi_\alpha(\mathbf{x},t)\Psi_\beta(\mathbf{x}',t')\rangle &= H_{\alpha\beta}(\mathbf{x},t,\mathbf{x}',t')\\ &= Z^{-1}\int \mathcal{D}\Psi\, \Psi_\alpha(\mathbf{x},t)\Psi_\beta(\mathbf{x}',t')e^{iS}\\ &= -H_{\beta\alpha}(\mathbf{x}',t',\mathbf{x},t).\end{aligned} \tag{3.73}$$

Similarly, we get the fermion propagator if $\Psi_\beta(\mathbf{x},t)$ is replaced by $\bar{\Psi}_\beta(\mathbf{x},t)$:

$$G_{\alpha\beta}(\mathbf{x},t,\mathbf{x}',t') = \langle \Psi_\alpha(\mathbf{x},t)\bar{\Psi}_\beta(\mathbf{x}',t')\rangle. \tag{3.74}$$

This shows a great advantage of this formalism. The symmetry properties follow automatically from the properties of the Grassmann variables. For bosons the ordering does not matter (total symmetry), for fermions it only affects the over all sign (total anti-symmetry).

3.3.3 Simple Grassmann integrals

It is useful to get a little more acquainted with the properties of Grassmann integrals. The partition function will contain a term like

$$\int \mathrm{d}\Psi\,\mathrm{d}\bar{\Psi}\, e^{\lambda\bar{\Psi}\Psi} = \int \mathrm{d}\Psi\,\mathrm{d}\bar{\Psi}(1+\lambda\bar{\Psi}\Psi) = \lambda\frac{\partial}{\partial\Psi}\frac{\partial}{\partial\bar{\Psi}}\bar{\Psi}\Psi = \lambda. \tag{3.75}$$

This should be compared to a similar integral for complex numbers

$$\int \mathrm{d}\phi\,\mathrm{d}\phi^*\, e^{-\lambda\phi^*\phi} \propto \frac{1}{\lambda}. \tag{3.76}$$

With internal degrees of freedoms we get

$$\begin{aligned}
&\int \mathrm{d}\Psi_1\,\mathrm{d}\bar{\Psi}_1\ldots\mathrm{d}\Psi_n\,\mathrm{d}\bar{\Psi}_n\, e^{\lambda_1\bar{\Psi}_1\Psi_1}\ldots e^{\lambda_n\bar{\Psi}_n\Psi_n}\\
=&\int \mathrm{d}\Psi_1\,\mathrm{d}\bar{\Psi}_1\ldots\mathrm{d}\Psi_n\,\mathrm{d}\bar{\Psi}_n\{(1+\lambda_1\bar{\Psi}_1\Psi_1)(1+\lambda_2\bar{\Psi}_2\Psi_2)\cdots(1+\lambda_n\bar{\Psi}_n\Psi_n)\}\\
=&\lambda_1\ldots\lambda_n
\end{aligned} \tag{3.77}$$

because all terms that do not contain every variable vanish during Grassmann integration. The final result is

$$\boxed{\left(\prod_\alpha \int \mathrm{d}\Psi_\alpha\,\mathrm{d}\bar{\Psi}_\alpha\right) e^{\sum_\beta \lambda_\beta\bar{\Psi}_\beta\Psi_\beta} = \prod_\beta \lambda_\beta} \tag{3.78}$$

or with a matrix $\Lambda_{\beta\alpha}$

$$\boxed{\int \mathcal{D}\Psi\, e^{\bar{\Psi}_\beta\Lambda_{\beta\alpha}\Psi_\beta} = \det\Lambda}. \tag{3.79}$$

Note that there is no restriction on Λ from this expression since the eigenvalues are arbitrary complex numbers. They do not need to be real numbers as in the bosonic case because the Grassmann integral is always well defined for finite numbers of Grassmann variables.

The same way one can derive that

$$\int \mathrm{d}\Psi\,\mathrm{d}\bar{\Psi}\,\bar{\Psi}\Psi e^{\lambda\bar{\Psi}\Psi} = 1 \tag{3.80}$$

and

$$\int \mathcal{D}\Psi\,\bar{\Psi}_\gamma\Psi_\gamma e^{\sum_\beta \lambda_\beta\bar{\Psi}_\beta\Psi_\beta} = \prod_{\beta\neq\gamma}\lambda_\beta. \tag{3.81}$$

Hence we get

$$\langle\bar{\Psi}_\gamma\Psi_\gamma\rangle = \frac{\int \mathcal{D}\Psi\,\bar{\Psi}_\gamma\Psi_\gamma e^{\sum_\beta \lambda_\beta\bar{\Psi}_\beta\Psi_\beta}}{\int \mathcal{D}\Psi\, e^{\sum_\beta \lambda_\beta\bar{\Psi}_\beta\Psi_\beta}} = \frac{1}{\lambda_\gamma}. \tag{3.82}$$

3.3.4 Free Green's function for non-relativistic fermions

Using the results from above we can construct the free propagator for non-relativistic fermions. The factor λ_β is then

$$\lambda_\beta \mathrel{\widehat{=}} i\omega - i\epsilon(\mathbf{p}). \tag{3.83}$$

Green's function then is

$$G_{0,\alpha\beta}(\mathbf{p},\omega,\mathbf{p}',\omega') = \langle \Psi_\alpha(\mathbf{p},\omega)\bar{\Psi}_\beta(\mathbf{p}',\omega')\rangle = \frac{i}{\omega - \epsilon(\mathbf{p})}\delta(\mathbf{p}-\mathbf{p}')\delta_{\alpha\beta}. \tag{3.84}$$

It is exactly the same free propagator as we got for bosons in equation (2.97). The question arises if for a single propagating particle there is no difference between fermions and bosons. This is only true for a non-interacting theory. In an interacting theory there are vacuum fluctuations that introduce differences.

3.4 Functional integral for fermionic quantum systems

3.4.1 Correlation functions

For many particle fermionic systems the correlation function is given by

$$\boxed{\left\langle T\left\{a_{j_1}(t_1)a_{j_2}(t_2)\dots a^\dagger_{k_1}(t'_1)\dots a^\dagger_{k_m}(t'_m)\right\}\right\rangle \quad = Z^{-1}\int \mathcal{D}\Psi\, \Psi_{j_1}(t_1)\Psi_{j_2}(t_2)\dots\bar{\Psi}_{k_m}(t')e^{iS}\cdot\epsilon} \tag{3.85}$$

were $\epsilon = \pm 1$ is specified by the ordering of Grassmann variables in the correlation function and $Z = \int \mathcal{D}\Psi\, e^{iS}$.

S is related to the Hamiltonian via

$$S = \int \mathrm{d}t\{i\bar{\Psi}_j\partial_t\Psi_j - H[\bar{\Psi}_k,\Psi_k]\}. \tag{3.86}$$

The ordering of operators in H is for $H[a^\dagger,a]$ with $a^\dagger$ on the left. Then $H[\bar{\psi},\psi]$ follows from $H[a^\dagger,a]$ by replacing $a\to\psi$ and $a^\dagger\to\bar{\psi}$.

4 Relativistic Quantum Fields

4.1 Lorentz Transformations

4.1.1 Lorentz Group and Invariant Tensors

Lorentz Metric

The cartesian coordinates of spacetime are t and $\mathbf{x}$. They are denoted as the contravariant vector

$$x^\mu = (t, \mathbf{x}), \qquad t = x^0. \tag{4.1}$$

The corresponding covariant vector is

$$x_\mu = (-t, \mathbf{x}) = (-x^0, \mathbf{x}). \tag{4.2}$$

We can always lower and upper indices with the metric tensor $\eta_{\mu\nu}$ and its inverse $\eta^{\mu\nu}$, which are actually the same:

$$\eta_{\mu\nu} = \eta^{\mu\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4.3}$$

or, if we want to use a shorter notation, we can also say that our metric has the signature

$$(-, +, +, +). \tag{4.4}$$

The explicit transformation equations are

$$x_\mu = \eta_{\mu\nu} x^\nu \quad \textit{and} \quad x^\mu = \eta^{\mu\nu} x_\nu. \tag{4.5}$$

We want to know under which transformations $x^\mu \to x'^\mu = \Lambda^\mu{}_\nu x^\nu$ the quantity $x^\mu x_\mu$ is invariant. So we calculate

$$\begin{aligned} x'^\mu x'_\mu &= x'^\mu x'^\nu \eta_{\mu\nu} \\ &= \Lambda^\mu{}_\rho x^\rho \Lambda^\nu{}_\sigma x^\sigma \eta_{\mu\nu}. \end{aligned} \tag{4.6}$$

This is equal to $x^\mu x_\mu$ if the condition

$$\Lambda^\mu{}_\rho \Lambda^\nu{}_\sigma \eta_{\mu\nu} = \eta_{\rho\sigma}. \tag{4.7}$$

is fulfilled. Equation (4.7) is the defining equation for Λ. All transformations that fulfill (4.7) are called **Lorentz transformations**.

Transformation of Tensors

Let us consider the contravariant and covariant four-momenta:

$$\begin{aligned} p^\mu &= (E, \mathbf{p}) \\ p_\mu &= (-E, \mathbf{p}). \end{aligned} \tag{4.8}$$

As we already discussed, we can raise and lower indices of vectors with the metric tensor $\eta_{\mu\nu}$ and the inverse $\eta^{\mu\nu}$. As raising and lowering are inverse operations, the action of both tensors is the identity:

$$\eta^{\mu\nu}\eta_{\nu\rho} = \delta^\mu{}_\rho. \tag{4.9}$$

If we perform a Lorentz transformation

$$p'^\mu = \Lambda^\mu{}_\nu p^\nu \tag{4.10}$$

and lower indices on both sides, we get

$$\eta^{\mu\rho} p'{}_\rho = \Lambda^\mu{}_\nu \eta^{\nu\sigma} p_\sigma \tag{4.11}$$

We multiply with an inverse metric

$$p'_\kappa = \eta_{\kappa\mu}\Lambda^\mu{}_\nu \eta^{\nu\sigma} p_\sigma \tag{4.12}$$

Obviously, the tensor product on the right hand side should be

$$\Lambda_\kappa{}^\nu = \eta_{\kappa\mu}\Lambda^\mu{}_\nu \eta^{\nu\sigma} \tag{4.13}$$

So we obtained the result, that a covariant vector (lower index) transforms as

$$p'_\mu = \Lambda_\mu{}^\nu p_\nu \tag{4.14}$$

We can also use the metric tensor to raise and lower indices of tensors as wel as for $\Lambda_\mu{}^\nu$. A general example for the Lorentz transformation of a complicated tensor is:

$$A'^{\mu\nu\rho}{}_{\sigma\tau} = \Lambda^\mu{}_{\mu'}\Lambda^\nu{}_{\nu'}\Lambda^\rho{}_{\rho'}\Lambda_\sigma{}^{\sigma'}\Lambda_\tau{}^{\tau'} A^{\mu'\nu'\rho'}{}_{\sigma'\tau'} \tag{4.15}$$

Invariant Tensors

We already mentioned that Lorentz transformations are defined in such a way, that the metric tensor $\eta_{\mu\nu}$ is left invariant. Actually, there is only one more tensor that is invariant under Lorentz transformations, and this is $\epsilon_{\mu\nu\rho\sigma}$ - the generalization of the ϵ_{ijk} tensor. $\epsilon_{\mu\nu\rho\sigma}$ is defined by

$$\epsilon_{0123} = 1. \tag{4.16}$$

It is also 1 for all cyclic permutations of $(0, 1, 2, 3)$, and -1 for all anticyclic permutations. The ϵ-tensor with raised indices, $\epsilon^{\mu\nu\rho\sigma}$ has just the opposite signs, so e.g. $\epsilon^{0123} = -1$. So we can also say, that $\epsilon_{\mu\nu\rho\sigma}$ and $\epsilon^{\mu\nu\rho\sigma}$ are inverse tensors.

Let us prove our statement, that $\epsilon_{\mu\nu\rho\sigma}$ is invariant under Lorentz transformations. We the following lines, we will use the short hand notation $\Lambda_{\mu}{}^{\nu} \to \Lambda$, $\Lambda^{\mu}{}_{\nu} \to \Lambda^T$ and $\eta_{\mu\nu} \to \eta$.

First we consider

$$\Lambda\eta\Lambda^T = \eta \tag{4.17}$$

which we already know from (4.13). If we compute the determinant on both sides, we find

$$det(\Lambda) = \pm 1. \tag{4.18}$$

The determinant of Λ can also be calculated by

$$\begin{aligned} det(\Lambda) &= \frac{1}{4!}\Lambda_{\mu_1}{}^{\nu_1}\Lambda_{\mu_2}{}^{\nu_2}\Lambda_{\mu_3}{}^{\nu_3}\Lambda_{\mu_4}{}^{\nu_4}\epsilon_{\nu_1\nu_2\nu_3\nu_4}\epsilon^{\mu_1\mu_2\mu_3\mu_4} \\ &= \frac{1}{4!}\epsilon'{}_{\mu_1\mu_2\mu_3\mu_4}\epsilon^{\mu_1\mu_2\mu_3\mu_4} \end{aligned} \tag{4.19}$$

Here ϵ' is the Lorentz transformed tensor. We can verify that $\epsilon'_{\mu\nu\rho\sigma}$ is totally antisymmetric, thus $\epsilon'_{\mu\nu\rho\sigma} = c\epsilon_{\mu\nu\rho\sigma}$ with constant c. Using $\epsilon_{\mu\nu\rho\sigma}\epsilon^{\mu\nu\rho\sigma} = 4!$ we obtain

$$\epsilon'{}_{\mu_1\mu_2\mu_3\mu_4} = \det(\Lambda)\epsilon_{\mu\nu\rho\sigma} = \pm\epsilon_{\mu_1\mu_2\mu_3\mu_4} \tag{4.20}$$

Anyway, the obtained result is, that only those Lorentz transformations with $det(\Lambda) = +1$ will leave the ϵ-tensor invariant. We call these transformations **proper** Lorentz transformations, while those with $det(\Lambda) = -1$ are called **improper** Lorentz transformations.

Analogy to Rotations

Remember again equation (4.17). This looks very similar to orthogonal transformations O with

$$OIO^T = OO^T = I, \tag{4.21}$$

where I is the identity. In (4.17), the identity is simply replaced by the metric tensor. Furthermore, there are again two tensors that are left invariant, and these are the identity δ_{ij} and the ϵ-tensor ϵ_{ijk} (if we work in three dimensions).

The orthogonal transformations in $3D$ are denoted as $O(3)$. The analogy that we just discussed motivates the name "Pseudo orthogonal transformations" $O(1,3)$, where the separated 1 indicates the special role of time in special relativity.

Derivatives

The derivative with respect to a contravariant vector is a covariant vector:

$$\partial_\mu = \frac{\partial}{\partial x^\mu}. \tag{4.22}$$

For example we have

$$\partial_\mu x^\mu = 4. \tag{4.23}$$

The momentum operator is

$$\widehat{p}_\mu = -i\partial_\mu. \tag{4.24}$$

4D Fourier Transformations

We already used four-dimensional Fourier transformations in the previous chapters. For example, a function $\psi(x^\mu)$ can be written as

$$\psi(x^\mu) = \int_p e^{ip_\mu x^\mu} \psi(p^\mu). \tag{4.25}$$

With $p_\mu = (-\omega, \vec{p}),\ p_\mu x^\mu = (-\omega t + \vec{p}\vec{x})$ this reads

$$\psi(t, \vec{x}) = \int_\omega \int_{\vec{p}} e^{-i\omega t + i\vec{p}\vec{x}} \psi(\omega, \vec{p}) \tag{4.26}$$

Covariant equations

A covariant equation is e.g.

$$\partial_\mu F^{\mu\nu} = J^\nu, \tag{4.27}$$

in particular these are two of the four Maxwell equations.

4.1.2 Lorentz Group

Group Structure

If we have two elements g_1, g_2 that are elements of a group $\mathcal{G}$, the product of these two elements will still be an element of the group

$$g_3 = g_2 g_1 \in \mathcal{G}. \tag{4.28}$$

In particular, we can write for matrices

$$(\Lambda_3)^\mu{}_\nu = (\Lambda_2)^\mu{}_\rho (\Lambda_1)^\rho{}_\nu. \tag{4.29}$$

In a group, there is always a unit element e that satisfies

$$ge = eg = g \tag{4.30}$$

for a group element g. For matrices, this unit element is δ^ν_μ.

Furthermore we have an inverse element for every matrix $\Lambda^\mu{}_\nu$, because the determinant of Λ is ± 1 for proper resp. improper Lorentz transformations.

Discrete Symmetries

- Space reflection (parity)

  The space reflection transformation is $x^i \to -x^i$ for $i \in 1,2,3$ and $t \to t$. The corresponding matrix is

$$P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{4.31}$$

  The determinant of P is -1. The metric tensor $\eta_{\mu\nu}$ is kept invariant under space reflection: $P\eta P^T = \eta$

- time reflection

  The time reflection transformation is $x^i \to x^i$ for $i \in 1,2,3$ and $t \to -t$. The corresponding matrix is

$$T = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4.32}$$

  The determinant of T is the same as for P, $\det T = \det P = -1$. Both transformations change the sign of the ϵ-tensor and are therefore improper Lorentz transformations.

  Again, the metric tensor is invariant under $T\eta T^T = \eta$.

- space-time reflection

  The combination of both space and time reflection is

$$PT = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{4.33}$$

  This time the determinant is $+1$.

Continuous Lorentz Transformations

A continuous Lorentz transformation is the "product of infinitesimal" transformations. It always has a determinant $+1$, so we can immediately conclude that the discrete transformations P and T can't be described by continuous ones. As the product PT has a determinant $+1$, one could first think that this may be obtained by continuous transformations, but this is *not* the case. The reason is, that infinitesimal transformations will never change the sign in front of the time variable, but actually, PT does exactly this.

However, a discrete transformation that can be obtained by infinitesimal ones is the reflection of x and y, so the product P_1P_2 with

$$P_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, P_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

$$P_1P_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{4.34}$$

4.1.3 Generators and Lorentz Algebra

Infinitesimal Lorentz Transformations

Let us consider the difference δp^μ between a four-momentum and the transformed four-momentum

$$\begin{aligned} \delta p^\mu &= p'^\mu - p^\mu \\ &= (\Lambda^\mu{}_\nu - \delta^\mu{}_\nu)p^\nu \\ &= \delta\Lambda^\mu{}_\nu p^\nu \\ \Lambda^\mu{}_\nu &= \delta^\mu{}_\nu + \delta\Lambda^\mu{}_\nu \end{aligned} \tag{4.35}$$

Let us consider a pseudo orthogonal transformation in matrix representation:

$$\begin{aligned} \Lambda\eta\Lambda^T &= \eta \\ \Leftrightarrow (1+\delta\Lambda)\eta(1+\delta\Lambda)^T &= \eta \\ \Leftrightarrow \delta\Lambda\eta + \eta\delta\Lambda^T &= 0 \end{aligned} \tag{4.36}$$

In the last line we neglected the 2nd order term in $\delta\Lambda$. If we write down this equation in index notation, we have

$$\begin{aligned} \delta\Lambda_\mu{}^\rho\eta_{\rho\nu} + \eta_{\mu\rho}\delta\Lambda_\nu{}^\rho &= 0, \\ \delta\Lambda_{\mu\nu} + \delta\Lambda_{\nu\mu} &= 0. \end{aligned} \tag{4.37}$$

This equation tells us, that $\delta\Lambda_{\mu\nu}$ is antisymmetric, but note that $\delta\Lambda^\mu{}_\nu$ is *not* antisymmetric. However, but matrices have only six independent elements, what is obvious for $\delta\Lambda_{\mu\nu}$, because all diagonal elements are zero and for the off-diagonal elements we have the relation $\delta\Lambda_{\mu\nu} = -\delta\Lambda_{\nu\mu}$. The number of independent elements in a (antisymmetric) matrix is of course equal to the number of linear independent (antisymmetric) matrices we can build. The physical meaning of these six matrices is that they represent the possible *three rotations* and *three boosts*.

Generators

Let us write the infinitesimal transformation of the momentum vector in the following way:

$$\delta p^\mu = i\epsilon_z (T_z)^\mu{}_\nu p^\nu, \quad z = 1\ldots 6 \tag{4.38}$$

which simply means that we split up our infinitesimal Lorentz transformation into

$$\delta\Lambda^\mu{}_\nu = i\epsilon_z (T_z)^\mu{}_\nu. \tag{4.39}$$

So $\Lambda^\mu{}_\nu$ consists of a real, infinitesimal parameter ϵ_z, and the so-called **generator** $(T_z)^\mu{}_\nu$ (and a factor of i). Remember that we have six independent generators T_z of the Lorentz group and that we sum over all z.

Let us now write down all the generators that we have:

$$\begin{gathered} \textit{rotations}: \qquad (T_1)_{\mu\nu} = (T_1)^\mu{}_\nu = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \\ (T_2)_{\mu\nu} = (T_2)^\mu{}_\nu = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, \quad (T_3)_{\mu\nu} = (T_3)^\mu{}_\nu = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{gathered} \tag{4.40}$$

$$\begin{gathered} \textit{boosts}: \qquad (T_4)_{\mu\nu} = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (T_4)^\mu{}_\nu = \begin{pmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \\ (T_5)^\mu{}_\nu = \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (T_6)^\mu{}_\nu = \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \end{gathered} \tag{4.41}$$

Some remarks on these equations:

- T_1 is a rotation around the x-axis (only y and z components change). T_2 is a rotation around the y-axis and T_3 a rotation around the z-axis.
- For the rotation matrices, raising and lowering of indices doesn't change anything. The reason is that the metric tensor has a -1 only in the zero component and the rotation matrices are zero in the first row.
- For the boost matrices, raising of the first index changes the sign of the first row of the matrix (see T_4). After raising the index, the boost matrices are not any longer antisymmetric.

The calculation goes like this:

$$(T_4)^\mu{}_\nu = \eta^{\mu\rho}(T_4)_{\rho\nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{4.42}$$

- To see that T_1, T_2 and T_3 are really rotations, compare them to the well-known rotation matrix in 2D,

$$R = \begin{pmatrix} cos\phi & -sin\phi \\ sin\phi & cos\phi. \end{pmatrix} \tag{4.43}$$

If $\phi = \epsilon$ is infinitesimal, it becomes

$$R = \begin{pmatrix} 1 & -\epsilon \\ \epsilon & 1. \end{pmatrix} \tag{4.44}$$

The difference to the identity is

$$\delta R = \begin{pmatrix} 0 & -\epsilon \\ \epsilon & 0, \end{pmatrix} \tag{4.45}$$

But this is now equivalent to what we have (4.40) when we write $i\epsilon$ in front of the matrix.

- Similarly, you can convince yourself that T_4, T_5 and T_6 are really boosts in x, y and z direction.

Lorentz Algebra

In (**??**) we already mentioned that a product of two group elements will again be a group element. From this we can conclude, that also the commutator of two generators must again be a generator. In general we can therefore write

$$[T_x, T_y] = if_{xyz}T_z \tag{4.46}$$

The double appearance of z has (again) to be read as a summation. The f_{xyz} are called the **structure constants** of a group. Whenever one has to deal with groups, the structure constants are very important, because once we know them, we know all algebraic relations within this group.

Furthermore, whenever a set of generators fulfill one certain commutation relation, they all represent the *same group*, but only in different representations. This will be discussed further below.

Example
Let us consider a rotation in three dimensional space as an example. We want to rotate a system

- by an angle α around the y-axis,
- by an angle β around the x-axis,
- by an angle $-\alpha$ around the y-axis,
- and finally by an angle $-\beta$ around the x-axis.

The result is a product of infinitesimal rotations, which is of course nothing else than again an infinitesimal rotation,

$$\begin{aligned}(1 - i\beta T_x - \frac{1}{2}\beta^2 T_x^2)(1 - i\alpha T_y - \frac{1}{2}\alpha^2 T_y^2)(1 + i\beta T_x - \frac{1}{2}\beta^2 T_x^2)(1 + i\alpha T_y - \frac{1}{2}\alpha^2 T_y^2) \\ = 1 - \alpha\beta(T_x T_y - T_y T_x) \\ = 1 - i\alpha\beta T_z \end{aligned} \tag{4.47}$$

The first order is zero, and the terms $\propto T_x^2$ and $\propto T_y^2$ cancel, too. The product $\alpha\beta$ is the parameter of the resulting infinitesimal transformation.

For the special case of rotation in normal, three dimensional space, one could also show the commutation relation

$$[T_1, T_2] = iT_3 \tag{4.48}$$

by multiplication of matrices. More generally, we could show

$$[T_k, T_l] = i\epsilon_{klm} T_m \tag{4.49}$$

for $k, l, m \in \{1, 2, 3\}$.

The calculation of this example gives us already some commutation relations of the generators of the Lorentz group, if we consider the T_i as 4×4 matrices with zeros in all elements of the first column and row. This is of course not surprising, as the three dimensional rotations are a subgroup of the Lorentz group.

Of course, this is not all what we need to know about our Lorentz group, since up to now we did not yet determine those structure constants f_{xyz} where one element of x, y, z is 0. But as this is a little bit more complicated, this will be done later.

For the moment, we concentrate on another interesting fact: Remembering the Spin matrices and their commutation relations, we discover that it is exactly the same as for the generators of the rotation group $SO(3)$:

$$\begin{aligned}[s_k, s_l] &= i\epsilon_{klm} s_m, \\ [\frac{1}{2}\tau_k, \frac{1}{2}\tau_l] &= i\epsilon_{klm}\frac{1}{2}\tau_m. \end{aligned} \tag{4.50}$$

Note the difference between spin matrices s_i and Pauli matrices τ_i.

The important thing we learn here is that the spin matrices $\tau_i/2$ and the generators of rotations in $3D$ space have the same algebraic relations - and thus are *different representations of the same group.* The T_m are a three-dimensional and the $\tau_m/2$ are a two-dimensional representation of the group $(\mathcal{SO}(3))$.

4.1.4 Representations of the Lorentz Group (Algebra)

Representations and Matrices

Let us summarize what we know about the Lorentz group: It is $(\mathcal{SO}(1,3))$ and is generated by a set of 6 independent matrices T_z, which obey the commutation relations

$$[T_x, T_y] = i f_{xyz} T_z. \tag{4.51}$$

For $x, y, z \in \{1, 2, 3\}$ we know already that $f_{xyz} = \epsilon_{xyz}$. The dimension of the matrices T_z depends on the representation of the group: If we have a d-dimensional representation, the matrices will be $d \times d$.

For a vector, the dimension is of course 4, because we have three space and one time coordinate. But what happens if we want to transform a tensor? Well, if we have a symmetric tensor like the energy-momentum-tensor $T^{\mu\nu} = T^{\nu\mu}$, we know that it has 10 independent elements: 4 diagonal and 6 off-diagonal ones. Let us now forget for a while about tensors and write all independent elements into a 10-dimensional vector ψ^α. The generator T_z that transforms this vector into a new vector $\psi^\alpha + \delta\psi^\alpha$ (in complete analogy to the momentum p^μ that was transformed into $p^\mu + \delta p^\mu$) must now be a 10×10 matrix:

$$\delta\psi^\alpha = i\epsilon_z (T_z)^\alpha{}_\beta \psi^\beta \tag{4.52}$$

Finally, we remind ourselves that the elements of ψ have once been the elements of the energy-momentum tensor T. So we write

$$\delta T^{\mu\nu} = i\epsilon_z (T_z)^{\mu\nu}{}_{\mu'\nu'} T^{\mu'\nu'}. \tag{4.53}$$

Here $(\mu\nu) = (\nu\mu)$ is considered as a double index, $\alpha = (\mu\nu)$. In this equation, don't mix up the energy-momentum tensor and the generator! The elements of $(T_Z)^{\mu\nu}_{\mu'\nu'}$ can easily be computed from the known Lorentz transformation of a tensor.

Irreducible Representations

The treatment of the energy-momentum tensor T as a 10 component vector is more complicated as necessary. Actually we do not have to transform 10 elements, but only 9. The reason is, that we can decompose T into the trace and the remaining traceless part. So we have now

$$\widetilde{T}^{\mu\nu} = T^{\mu\nu} - \frac{1}{4}\theta\eta^{\mu\nu}. \tag{4.54}$$

θ is the trace of the energy-momentum tensor and $\widetilde{T}^{\mu\nu}$ is the traceless part. For the trace we can also write

$$\theta = T^{\mu}_{\mu} = \eta_{\nu\mu} T^{\mu\nu}. \tag{4.55}$$

The trace is a scalar and thus doesn't change under Lorentz transformations:

$$T'^{\rho}_{\rho} = T^{\rho}_{\rho}.. \tag{4.56}$$

Furthermore, the traceless tensor $\widetilde{T}$ remains traceless when it is transformed.

In this way, we have reduced the $10D$ representation to $9+1$. So the transformation of traceless, symmetric tensors is represented by a 9×9 matrix (generator).

As an intermediate result we can now summarize:

Representation	Dimension
scalar	1
vector	4
symmetric and traceless tensors	9
antisymmetric tensors	6
spinor	?

We will later see how complex andtisymmetric tensors can be reduced to two three dimensional representations, $6 \rightarrow 3+3$. We will find out later the dimension of the spinor representation.

4.1.5 Transformation of Fields

Scalar Field $\varphi(x)$

How do fields $\varphi(x)$ transform? Well, to answer this question, we go back to the transformation of space-time vector x^{μ}:

$$x'^{\mu} = \Lambda^{\mu}{}_{\nu} x^{\nu}, \quad x'^{\mu} = x^{\mu} + \delta x^{\mu} \tag{4.57}$$

To come to the transformation of the field, we have to do two steps:

$$\begin{aligned} \varphi(x) &= \varphi(x' - \delta x) \\ \Rightarrow \varphi'(x) &= \varphi(x - \delta x) \end{aligned} \tag{4.58}$$

So first we transform x to x' and then we use x for x' to get the transformed field. Furthermore we see that it is equivalent whether we change the coordinate system or the object (field). But note that the transformations are in opposite directions!

If we consider the x to be transformed, we call this an **passive transformation,** while if we change the field φ itself we are speaking about an **active transformation.**

The difference of the field $\delta\varphi$ is of course

$$\begin{aligned} \delta\varphi &= \varphi(x - \delta x) - \varphi(x) \\ &= -\partial_{\mu}\varphi(x)\delta x^{\mu} \end{aligned} \tag{4.59}$$

The second line comes from the definition of the derivative.

If we insert $\delta x^\mu = \delta\Lambda^\mu{}_\nu x^\nu$ we get

$$\begin{aligned}\delta\varphi &= -\delta\Lambda^\mu{}_\nu x^\nu \partial_\mu \varphi(x) \\ &= -i\epsilon_z (T_z)^\mu{}_\nu x^\nu \partial_\mu \varphi(x) \\ &= i\epsilon_z L_z \varphi(x)\end{aligned} \tag{4.60}$$

In the second to the last line we used (4.39) and in the last line we introduced the definition

$$L_z = -(T_z)^\mu{}_\nu x^\nu \partial_\mu. \tag{4.61}$$

For an easier notation, (4.39) is better written as

$$\delta\varphi = +x^\nu \delta\Lambda_\nu{}^\mu \partial_\mu \varphi(x) \tag{4.62}$$

To prove that this is true, lower one index of Λ and use the antisymmetry.

Note that in this case here the L_z are the generators and not T_z because (4.60) is of the form (4.38). Remark that the generators L_z contain a differential operator in this case!

The letter L was not chosen arbitrary, as L_1, L_2 and L_3 are the angular momenta. For instance, L_1 can be written as

$$L_1 = -(T_1)^\mu{}_\nu x^\nu \partial_\mu. \tag{4.63}$$

T_1 has only two non-zero elements: $(T_1)^2{}_3 = -i$ and $(T_1)^3{}_2 = i$, so

$$\begin{aligned}L_1 &= -ix^2 \frac{\partial}{\partial x^3} + ix^3 \frac{\partial}{\partial x^2} \\ &= -i(y\partial_z - z\partial_y).\end{aligned} \tag{4.64}$$

This is obviously the angular momentum as we know it from classical mechanics: $\mathbf{L} = \mathbf{r} \times \mathbf{p}$.

Vector Field $A^\mu(x)$

Contravariant vectors transform like this:

$$\begin{aligned}A^\mu(x) \quad \rightarrow \quad & A'^\mu(x) = A^\mu(x) + \delta A^\mu(x), \\ & \delta A^\mu(x) = \delta\Lambda^\mu{}_\nu A^\nu(x) + x^\rho \delta\Lambda_\rho{}^\sigma \partial_\sigma A^\mu(x).\end{aligned} \tag{4.65}$$

Here, $\delta\Lambda^\mu{}_\nu A^\nu$ is the usual transformation law for covariant vectors, and $x^\rho \delta\Lambda_\rho{}^\sigma \partial_\sigma A^\mu$ simply reflects the change of coordinates, this second term is always there, no matter what kind of field we are transforming.

Covariant vectors transform like that:

$$\delta A_\mu(x) = \delta\Lambda_\mu{}^\nu A_\nu(x) + x^\rho \delta\Lambda_\rho{}^\sigma \partial_\sigma A_\mu(x). \tag{4.66}$$

Examples

The **covariant derivative** is given by

$$
\begin{aligned}
\partial_\mu\varphi \quad &\rightarrow \quad \partial_\mu(\varphi(x)+\delta\varphi(x)) = \partial_\mu\phi(x)+\delta\partial_\mu\phi(x),\\
\delta\partial_\mu\phi(x) &= \partial_\mu\delta\phi(x) = \partial_\mu(x^\rho\delta\Lambda_\rho{}^\sigma\partial_\sigma\phi(x))\\
&= \delta\Lambda_\mu{}^\sigma\partial_\sigma\varphi(x)+(x^\rho\delta\Lambda_\rho{}^\sigma\partial_\sigma)(\partial_\mu\phi(x))
\end{aligned}
\tag{4.67}
$$

So $\partial_\mu\varphi$ transforms as a covariant vector!

$$
\delta(\partial^\mu\varphi(x)\partial_\mu\varphi(x)) = (x^\rho\delta\Lambda_\rho{}^\sigma\partial_\sigma)(\partial^\mu\varphi(x)\partial_\mu\varphi(x)),
\tag{4.68}
$$

i.e. $\partial^\mu\varphi(x)\partial_\mu\varphi(x)$ transforms as a scalar!

4.1.6 Invariant Action

This is a central piece, but with all the machinery we have developed it is almost trivial. Now our work pays off.

Let $f(x)$ be some (composite) scalar function

$$
\delta f = x^\rho\delta\Lambda_\rho{}^\sigma\partial_\sigma f,
\tag{4.69}
$$

examples are

$$
f=\varphi^2 \text{ or } f=\partial^\mu\varphi\partial_\mu\varphi.
\tag{4.70}
$$

It follows that

$$
S=\int d^4x\, f(x) \text{ is invariant, i.e. } \delta S=0.
\tag{4.71}
$$

Proof:

$$
\begin{aligned}
\delta S &= \int d^4x\, f(x)\\
&= \int d^4x\, x^\rho\delta\Lambda_\rho{}^\sigma\partial_\sigma f\\
&= \int d^4x\,\partial_\sigma(x^\rho\delta\Lambda_\rho{}^\sigma\partial_\sigma f) - \int d^4x\,\delta^\rho_\sigma\delta\Lambda_\rho{}^\sigma\partial_\sigma f\\
&= 0
\end{aligned}
\tag{4.72}
$$

The first integral is zero because there are no boundary contributions. Total derivatives in $\mathcal{L}$ will always be neglected, i.e. always $\int d^4x\,\partial_\mu A = 0$.
The second integral is zero because of the antisymmetry of $\Lambda_{\rho\sigma}$:

$$
\delta^\rho_\sigma\delta\Lambda_\rho{}^\sigma = \eta^{\rho\sigma}\delta\Lambda_{\rho\sigma}=0.
\tag{4.73}
$$

Examples

It is now very easy to construct quantum field theories!
Simply write down actions S that are Lorentz invariant.

We will consider actions of the form

$$S = \int d^4x \sum_k \mathcal{L}_k(x), \tag{4.74}$$

where L_k is a scalar field.
Here are some examples:

- $-\mathcal{L} = \partial^\mu \varphi^* \partial_\mu \varphi + m^2 \varphi^* \varphi$
  This is a **free charged scalar field**, it describes particles with mass m like e.g. pions $\pi^\pm$ with interactions neglected.
- $-\mathcal{L} = \frac{1}{4} F^{\mu\nu} F_{\mu\nu}, \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$
  F is the **electromagnetic field**. This describes free photons.
- $-\mathcal{L} = (\partial^\mu + ieA^\mu)\varphi^*(\partial_\mu - ieA_\mu)\phi + \frac{1}{4} F^{\mu\nu} F_{\mu\nu}$
  This describes a charged scalar field interacting with photons and is called **scalar QED**.
  (We need one more concept to do **QED**, we have to account for the spin of the electrons.)

The minus in front of the $\mathcal{L}$'s is a result of our $(-+++)$ metric convention.

4.1.7 Functional Integral, Correlation Functions

Measure

$$\int \mathcal{D}\varphi(x) \text{ is invariant.} \tag{4.75}$$

To prove this, we use the equivalence of active and passive transformations,

$$\varphi'(x) = \varphi(\Lambda^{-1}x). \tag{4.76}$$

For vectors we have

$$\int \mathcal{D}A^\mu = \int \mathcal{D}A'^\mu \cdot \text{Jacobian} \tag{4.77}$$

But the Jacobian is $\det \Lambda = 1$.

Comment: Is it always possible to find an invariant measure?
There is a possible conflict with regularization, i.e. with taking the continuum limit. E.g. lattice regularization is *not* Lorentz invariant.
The answer to that question is that in all experience physicists have so far, lattice QFTs do work. Without any proofs we assume that $\int \mathcal{D}\varphi$ is invariant.

Partition Function

$$Z = \int \mathcal{D}\varphi e^{iS} \text{ is invariant if } \int \mathcal{D}\varphi \text{ and } S \text{ are invariant.} \tag{4.78}$$

Correlation Function

$$\langle \varphi(x) | \varphi(x') \rangle = Z^{-1} \int \mathcal{D}\varphi \varphi(x) \varphi(x') e^{iS} \text{ transforms as } \varphi(x)\varphi(x'). \tag{4.79}$$

This is a *covariant construction*. This makes it easy to construct an invariant S-matrix. Thus e.g. scattering cross sections are Lorentz invariant.

Summary

Explicit Lorentz covariance is an important advantage of the functional integral formulation! This is not so for operators! Recall that H is not invariant, it is a three-dimensional object. S is a four-dimensional object. We will come back later to the question how operator-valued fields transform.

Before we can look at some theories and calculate their consequences, we need one more theoretical concept to account for spin: **spinors**

4.2 Dirac Spinors, Weyl Spinors

4.2.1 Spinor Representations of the Lorentz Group

Electrons have half-integer spin. We first look at the rotation group $SO(3)$, which is a subgroup of the Lorentz group. For *nonrelativistic* electrons this subgroup is all that matters.

We look at a two-dimensional representation of the rotation group:

$$\chi = \begin{pmatrix} \chi_1(x) \\ \chi_2(x) \end{pmatrix} = \begin{pmatrix} \chi_1 \\ \chi_2 \end{pmatrix}. \tag{4.80}$$

We omit the x-dependence since we are only interested in the group structure.

The rotations subgroup $SO(3)$ is given by

$$\begin{aligned} \delta\chi &= i\epsilon_z T_z \chi + \delta'\chi, \quad z = 1, 2, 3, \\ \delta'\chi(x) &= x^\rho \delta\Lambda_\rho{}^\sigma \partial_\sigma \chi(x). \end{aligned} \tag{4.81}$$

We will omit δ' from now on. Only for simplification of writing we set

$$\delta_{new} = \delta - \delta'. \tag{4.82}$$

The three matrices T_z are given by the Pauli matrices:

$$T_z = \frac{1}{2}\tau_z, \quad z = 1, 2, 3. \tag{4.83}$$

Comment: The $\chi(x)$ are Grassmann variables. But this is not relevant for symmetry transformations as long as .... Fields for relativistic electrons: needs field in representation of Lorentz group!

Now we ask the question for *relativistic* electrons:

- What are the spinor representations of the full Lorentz group, i.e. what are T_z for $z = 1, \dots, 6$?
- Are there two-dimensional representations, i.e. are there six 2×2 matrices that obey

$$[T_x, T_y] = i f_{xyz} T_z? \tag{4.84}$$

These questions belong to the mathematical field of **representation theory**. We do not attempt to find the representations ourselves. Dirac, Pauli and Weyl did that for us. We only give the representations and verify that they really are representations of the Lorentz group.

4.2.2 Dirac Spinors

By Dirac spinors we mean the four-dimensional representation

$$\psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix}, \tag{4.85}$$

with generators

$$i\varepsilon_z T_z = -\frac{i}{4}\varepsilon_{\hat{\mu}\hat{\nu}}\sigma^{\hat{\mu}\hat{\nu}}. \tag{4.86}$$

Note that there are still six generators σ, but they are now labeled by $\hat{\mu}\hat{\nu}$ instead of z, as T used to be. It's six generators because σ and ε are both antisymmetric,

$$\sigma^{\hat{\mu}\hat{\nu}} = -\sigma^{\hat{\nu}\hat{\mu}}, \quad \varepsilon_{\hat{\mu}\hat{\nu}} = -\varepsilon_{\hat{\nu}\hat{\mu}}. \tag{4.87}$$

We put the hats on $\hat{\mu}$ and $\hat{\nu}$ to avoid confusion: they are fixed 4×4 matrices and Lorentz transformations do *not* act on them as they do on fields. Once again: e.g. σ^{13} is itself a 4×4 matrix, $\hat{\mu}\hat{\nu} = 13$ is just a convenient label for this matrix, we could also have labeled it by $z = 5$.

The matrices $\sigma^{\hat{\mu}\hat{\nu}}$ are obtained as the commutators of yet other matrices,

$$\boxed{\sigma^{\hat{\mu}\hat{\nu}} = \frac{i}{2}\left[\gamma^{\hat{\mu}}, \gamma^{\hat{\nu}}\right].} \tag{4.88}$$

The γ-matrices are called **Dirac matrices**, they are complex 4×4 matrices and there are four of them:

$$\gamma^k = \begin{pmatrix} 0 & -i\tau_k \\ i\tau_k & 0 \end{pmatrix}, \quad k=1,2,3 \quad \text{and} \quad \gamma^0 = \begin{pmatrix} 0 & -i\mathbf{1} \\ -i\mathbf{1} & 0 \end{pmatrix}, \tag{4.89}$$

where the $\tau_k,\ k=1,2,3$ are the Pauli matrices. They are a generalization of the Pauli matrices.

In the following, we will omit the hat for γ^μ, but remember that Lorentz transformations act only on fields, whereas the matrices γ^μ are fixed.

If you compute the σ-matrices (exercise!), you will find that they are of the form

$$\sigma^{\mu\nu} = \begin{pmatrix} \sigma_+^{\mu\nu} & 0 \\ 0 & \sigma_-^{\mu\nu} \end{pmatrix} \text{ where the } \sigma_\pm^{\mu\nu} \text{ are } 2\times 2 \text{ matrices.} \tag{4.90}$$

The ij-components are rotations,

$$\sigma_+^{ij} = \sigma_-^{ij} = -\varepsilon^{ijk}\tau_k, \quad i,j,k \in \{1,2,3\}. \tag{4.91}$$

E.g. for a rotation around the z-axis we have

$$\begin{aligned} \varepsilon_3 T_3 &\equiv -\frac{1}{4}\left(\varepsilon_{12}\sigma^{12} + \varepsilon_{21}\sigma^{21}\right), \qquad\qquad (\varepsilon_{12} = -\varepsilon_{21} \equiv \varepsilon_3) \\ &= -\frac{1}{2}\varepsilon_3\sigma^{12} = -\frac{1}{2}\varepsilon_3(-\varepsilon^{123}\tau_3) = \varepsilon_3\frac{\tau_3}{2}. \end{aligned} \tag{4.92}$$

It follows that if we have

$$\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = \psi_L, \quad \begin{pmatrix} \psi_3 \\ \psi_4 \end{pmatrix} = \psi_R, \quad \psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix}, \tag{4.93}$$

then ψ_L and ψ_R transform as 2-component spinors with respect to rotations.

The σ^{ok}-components are boosts,

$$\sigma_+^{0k} = -\sigma_-^{0k} = i\tau_k. \tag{4.94}$$

The boost generators are *not* hermitian.
Commutation relations:

$$\begin{aligned} T_1 &= -\frac{1}{2}\sigma^{23}, \quad T_2 = -\frac{1}{2}\sigma^{31}, \quad T_3 = -\frac{1}{2}\sigma^{12}, \\ T_4 &= -\frac{1}{2}\sigma^{01}, \quad T_5 = -\frac{1}{2}\sigma^{02}, \quad T_6 = -\frac{1}{2}\sigma^{03}. \end{aligned} \tag{4.95}$$

$$\boxed{[\sigma^{\mu\nu}, \sigma^{\rho\tau}] = 2i\left(\eta^{\nu\rho}\sigma^{\mu\tau} - \eta^{\mu\rho}\sigma^{\nu\tau} - \eta^{\nu\tau}\sigma^{\mu\rho} + \eta^{\mu\tau}\sigma^{\nu\rho}\right)} \tag{4.96}$$

These are the commutation relations for the Lorentz algebra!
$\psi \equiv$ four dimensional *reducible* representation of the Lorentz group.

4.2.3 Weyl Spinors

As we have seen before, the matrices $\sigma^{\mu\nu}$ are block-diagonal, which means that they do not mix all components of a 4-spinor Ψ into each other, but only the first two and the last two. Mathematically speaking, there are two invariant subspaces, so the Dirac representation is called reducible. This is why we introduce now the Weyl representation, which will be a two-dimensional irreducible representation (irrep). We define

$$\Psi_L = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ 0 \\ 0 \end{pmatrix}, \qquad \Psi_R = \begin{pmatrix} 0 \\ 0 \\ \Psi_3 \\ \Psi_4 \end{pmatrix}. \tag{4.97}$$

From now on, we will surpress the 0's in the Weyl spinors and just write

$$\Psi_L = \begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}, \qquad \Psi_R = \begin{pmatrix} \Psi_3 \\ \Psi_4 \end{pmatrix}. \tag{4.98}$$

We will later usw Weyl spinors to describe neutrinos. For electrons we will need Dirac Spinors.

Projection Matrix

Now we introduce a matrix γ^5, such that we can make a projection from the Dirac to the Weyl representation by

$$\begin{aligned} \Psi_L &= \frac{1}{2}(1+\gamma^5)\Psi, \\ \Psi_R &= \frac{1}{2}(1-\gamma^5)\Psi. \end{aligned} \tag{4.99}$$

This is obviously fulfilled by

$$\gamma^5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{4.100}$$

where the 1 represents a 2×2-unit-matrix. One can check that

$$\begin{aligned} [\gamma^5, \sigma^{\mu\nu}] &= 0, \\ \left(\gamma^5\right)^2 &= 1. \end{aligned} \tag{4.101}$$

However, we want to treat the matrix γ^5 in a more general way and express it in terms of the other γ-matrices, so that we know it independently of the representation. First we show that for the relations (4.101) to hold, it is sufficient that

$$\left\{\gamma^\mu, \gamma^5\right\} = 0. \tag{4.102}$$

Proof:

$$\gamma^5\sigma^{\mu\nu} = \frac{i}{2}\gamma^5(\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu) = -\frac{i}{2}(\gamma^\mu\gamma^5\gamma^\nu - \gamma^\nu\gamma^5\gamma^\mu)$$
$$= \frac{i}{2}(\gamma^\mu\gamma^\nu - \gamma^\nu\gamma^\mu)\gamma^5 = \sigma^{\mu\nu}\gamma^5. \tag{4.103}$$

One can check as an exercise that this relation is indeed fulfilled when we define

$$\gamma^5 = -i\gamma^0\gamma^1\gamma^2\gamma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.104}$$

Now one can easily check that

$$\frac{1+\gamma^5}{2} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \frac{1-\gamma^5}{2} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{4.105}$$

Please also check that

$$\gamma^5\Psi_L = \Psi_L, \qquad \gamma^5\Psi_R = -\Psi_R \tag{4.106}$$

Parity Transformation

The parity transformation is defined by

$$\Psi(x) \to \gamma^0\Psi(Px), \qquad Px = (x^0, -\vec{x}). \tag{4.107}$$

So how transform the individual Weyl spinors? We observe that

$$\gamma^0 \begin{pmatrix} \Psi_L \\ \Psi_R \end{pmatrix} = -i \begin{pmatrix} \Psi_R \\ \Psi_L \end{pmatrix}. \tag{4.108}$$

So we note that

$$(\Psi')_L = -i\Psi_R, \qquad (\Psi')_R = -i\Psi_L, \tag{4.109}$$

i. e. parity exchanges left and right components. This is indeed one of the reasons why we will need a left-handed and a right-handed Weyl spinor to describe electrons. Neutrinos are described only by a left-handed Weyl spinor, so obviously they violate parity!

4.2.4 Dirac Matrices

Let's look in some more detail at the Dirac matrices we have used so far. Their defining property is given by

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}. \tag{4.110}$$

This is known as the Clifford algebra. For this relations one can derive all the commutator relations for the $\sigma^{\mu\nu}$ and γ^5! For instance one can obviously see that $(\gamma^i)^2 = 1, \quad i =$

$1, 2, 3$ and $(\gamma^0)^2 = -1$. This is quite useful, since different books will use different representations of the Clifford algebra (however, also take care for the signature of the metric in different books!). We can go from one representation to another using a similarity transformation

$$\gamma^\mu \to \gamma'^\mu = A\gamma^\mu A^{-1}. \tag{4.111}$$

We can easily check that such a transformation does not change the anticommutator relations:

$$\left\{\gamma'^\mu, \gamma'^\nu\right\} = A\left\{\gamma^\mu, \gamma^\nu\right\}A^{-1} = 2A\eta^{\mu\nu}A^{-1} = \eta^{\mu\nu} \tag{4.112}$$

4.3 Free Relativistic Fermions

4.3.1 Invariant Action

Now we want to use the spinor representation discussed in the previous section to write down Lorentz invariant actions for fermions. In fact, it is possible to write down a kinetic term with only one derivative:

$$S = \int d^4x\mathcal{L}, \qquad \mathcal{L} = -i\bar{\Psi}\gamma^\mu\partial_\mu\Psi. \tag{4.113}$$

Here $\Psi(x)$ and $\bar{\Psi}(x)$ are independent Grassmann variables. As usual, Ψ denotes a column vector, i. e. $\Psi = \begin{pmatrix} \Psi_1 \\ \Psi_2 \\ \Psi_3 \\ \Psi_4 \end{pmatrix}$, and $\bar{\Psi}$ is a line vector, i. e. $\bar{\Psi} = \begin{pmatrix} \bar{\Psi}_1, & \bar{\Psi}_2, & \bar{\Psi}_3, & \bar{\Psi}_4 \end{pmatrix}$. This is much simpler that the kinetic term for fermions, where we must use two derivatives in the kinetic term. Under a Lorentz transformation, Ψ and $\bar{\Psi}$ transform as

$$\begin{aligned} \delta\Psi &= -\frac{i}{4}\epsilon_{\mu\nu}\sigma^{\mu\nu}\Psi, \\ \delta\bar{\Psi} &= \frac{i}{4}\epsilon_{\mu\nu}\bar{\Psi}\sigma^{\mu\nu}. \end{aligned} \tag{4.114}$$

One can introduce a complex structure in the Grassmann algebra by

$$\bar{\Psi} = \Psi^\dagger\gamma^0. \tag{4.115}$$

This is indeed the defining relation for Ψ^* (since for any matrix A, $A^\dagger = A^{*T}$)! You can also check that accordingly,

$$\delta\bar{\Psi} = (\delta\Psi)^\dagger\gamma^0. \tag{4.116}$$

Having defined Ψ^*, one could define real and imaginary parts $\Psi_{Re} = \frac{1}{2}(\Psi + \Psi^*)$ and $\Psi_{Im} = -\frac{i}{2}(\Psi - \Psi^*)$ and use them as independent variables.

4.3.2 Transformation of Spinor Bilinears

Up to know, we can only write down a kinetic term for our Lagrangian. Now we want to consider more general bilinear forms of spinors and check their properties under Lorentz transformations. Then we can write down more general Lagrangians. We will only consider infinitesimal Lorentz transformations here, since we can build all actual Lorentz transformations from infinitesimal ones. The first relation we proof is that

$$\delta(\bar{\Psi}\Psi) = 0. \tag{4.117}$$

Indeed,

$$\delta(\bar{\Psi}\Psi) = \delta\bar{\Psi}\Psi + \bar{\Psi}\delta\Psi = \frac{i}{4}\left(\bar{\Psi}\sigma^{\mu\nu}\Psi - \bar{\Psi}\sigma^{\mu\nu}\Psi\right) = 0. \tag{4.118}$$

This means that $\bar{\Psi}\Psi$ transforms as a scalar under Lorentz transformations. Next we will show that

$$\delta(\bar{\Psi}\gamma^\mu\Psi) = \delta\Lambda^\mu{}_\nu(\bar{\Psi}\gamma^\nu\Psi) = \epsilon^\mu{}_\nu\bar{\Psi}\gamma^\nu\Psi, \tag{4.119}$$

i. e. it transforms as a vector under Lorentz transformations. This can be seen in three steps. First we note that

$$\delta(\bar{\Psi}\gamma^\rho\Psi) = \delta\bar{\Psi}\gamma^\rho\Psi + \bar{\Psi}\gamma^\rho\delta\Psi = \frac{i}{4}\epsilon_{\mu\nu}(\bar{\Psi}\sigma^{\mu\nu}\gamma^\rho\Psi - \bar{\Psi}\gamma^\rho\sigma^{\mu\nu}\Psi) = \frac{i}{4}\epsilon_{\mu\nu}\bar{\Psi}\left[\sigma^{\mu\nu},\gamma^\rho\right]\Psi. \tag{4.120}$$

Second, we see

$$\gamma^\mu\gamma^\nu\gamma^\rho = \gamma^\mu\left\{\gamma^\nu,\gamma^\rho\right\} - \gamma^\mu\gamma^\rho\gamma^\nu = 2\eta^{\nu\rho}\gamma^\mu - \gamma^\mu\gamma^\rho\gamma^\nu. \tag{4.121}$$

Using this, we find

$$\begin{aligned}
\left[\sigma^{\mu\nu},\gamma^\rho\right] &= \frac{i}{2}\left(\gamma^\mu\gamma^\nu\gamma^\rho - \gamma^\nu\gamma^\mu\gamma^\rho - \gamma^\rho\gamma^\mu\gamma^\nu + \gamma^\rho\gamma^\nu\gamma^\mu\right)\\
&= \frac{i}{2}\left(2\eta^{\nu\rho}\gamma^\mu - \gamma^\mu\gamma^\rho\gamma^\nu - 2\eta^{\mu\rho}\gamma^\nu + \gamma^\nu\gamma^\rho\gamma^\mu - 2\eta^{\mu\rho}\gamma^\nu\right.\\
&\quad\left. + \gamma^\mu\gamma^\rho\gamma^\nu + 2\eta^{\nu\rho}\gamma^\mu - \gamma^\nu\gamma^\rho\gamma^\mu\right) = 2i\left(\eta^{\nu\rho}\gamma^\mu - \eta^{\mu\rho}\gamma^\nu\right)
\end{aligned} \tag{4.122}$$

Since we also know the transformation properties of ∂_ρ, we can easily check that $\bar{\Psi}\gamma^\rho\partial_\rho\Psi$ transforms as a scalar:

$$\begin{aligned}
\delta(\bar{\Psi}\gamma^\rho\partial_\rho\Psi) &= \epsilon^\rho{}_\nu\bar{\Psi}\gamma^\nu\partial_\rho\Psi + \epsilon_\rho{}^\nu\bar{\Psi}\gamma^\rho\partial_\nu\Psi\\
&= \epsilon_{\rho\nu}\bar{\Psi}\gamma^\nu\partial^\rho\Psi + \epsilon_{\nu\rho}\bar{\Psi}\gamma^\nu\partial^\rho\Psi = 0.
\end{aligned} \tag{4.123}$$

Now that we have constructed a mighty formalism to describe fermions, the only thing we need to do from now on is to construct invariant Lagrange densities $\mathcal{L}$ appropriate for the given system.

4.3.3 Dirac Spinors with Mass

Dirac Equation

We would now like to look at a system of free electrons. Such a system is described by the the Lagrangian

$$-\mathcal{L} = i\bar{\Psi}\gamma^{\mu}\partial_{\mu}\Psi + im\bar{\Psi}\Psi \tag{4.124}$$

The minus sign comes from our convention of the metric. The functional variation of the associated action S with regard to $\bar{\Psi}$ leads to the famous **Dirac equation**

$$\frac{\delta S}{\delta\bar{\Psi}} = 0 \Rightarrow \left(\gamma^{\mu}\partial_{\mu} + m\right)\Psi = 0. \tag{4.125}$$

This equation is of course relativistic covariant, because (4.138) is. Due to the fact that (4.125) is the inverse to the propagator P of the particle,

$$\left(\gamma^{\mu}\partial_{\mu} + m\right)P = 1 \tag{4.126}$$

its solutions (eigenvectors with 0 eigenvalues) lead directly to the poles of P, which of course give us the needed dispersion relations!

Energy - Momentum Relation

To get to the energy momentum relation for a relativistic particle, we square the Dirac equation

$$\gamma^{\nu}\partial_{\nu}\gamma^{\mu}\partial_{\mu}\Psi = m^2\Psi. \tag{4.127}$$

To evaluate this ansatz, we make use of the anticommutator relation for the γ matrices

$$\frac{1}{2}\{\gamma^{\nu},\gamma^{\mu}\}\partial_{\nu}\partial_{\mu}\Psi = \eta^{\nu\mu}\partial_{\nu}\partial_{\mu}\Psi = \partial^{\mu}\partial_{\mu}\Psi = m^2\Psi \tag{4.128}$$

Now the last equation is exactly the Klein-Gordon equation $(\partial^{\mu}\partial_{\mu} - m^2)\Psi = 0$, so we see that solutions for (4.125) also solve this equation.

Plain waves of the form $\Psi = \Psi_0 e^{ip^{\mu}x_{\mu}} = \Psi_0 e^{-i(Et-\mathbf{px})}$ are the easiest solutions, they lead to

$$\left(E^2 - \mathbf{p}^2 - m^2\right)\Psi = 0 \Longrightarrow E^2 = \mathbf{p}^2 + m^2. \tag{4.129}$$

So $E = \pm\sqrt{\mathbf{p}^2 + m^2}$ are both solutions, but since we are handling with *free* particles, what does the solution with the negative energy describe? To answer this question, lets exploit the ...

Hamilton Formulation

We just multiply (4.125) with $-i\gamma^0$

$$-i\gamma^0\gamma^\mu\partial_\mu\Psi = -i\left(\gamma^0\right)^2\partial_0\Psi - i\gamma^0\gamma^k\partial_k\Psi = i\gamma^0 m\Psi \tag{4.130}$$

and introduce

$$\alpha^k = -\gamma^0\gamma^k = \gamma^k\gamma^0 \qquad \beta = i\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4.131}$$

which lead to

$$i\dot{\Psi} = -i\alpha^k\partial_k\Psi + m\beta\Psi \tag{4.132}$$

In the momentum basis, we get a kind of Schrödinger equation

$$i\dot{\Psi} = H\Psi \quad \textit{with} \quad H = \alpha^k p_k + m\beta \tag{4.133}$$

Let's switch to the rest frame of the particle ($\mathbf{p} = 0$). For the Hamiltonian we get

$$H = m\begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \tag{4.134}$$

This matrix mixes the Weyl spinors Ψ_L and Ψ_R

$$m\beta\begin{pmatrix} \Psi_L \\ \Psi_R \end{pmatrix} = m\begin{pmatrix} \Psi_R \\ \Psi_L \end{pmatrix} \tag{4.135}$$

We can verify that H has 2 eigenvectors with positive ($E = +m$), and 2 with negative energy ($E = -m$). So even in the rest system we have negative energy states!

Interpretation of Dirac Equation, Positrons

We construct linear combinations of Ψ_L and Ψ_R, which are mass eigenstates

$$\Psi_\pm = \frac{1}{\sqrt{2}}\left(\Psi_L \pm \Psi_R\right) \qquad \text{and} \qquad i\dot{\Psi}_\pm = \pm m\Psi_\pm \tag{4.136}$$

By conjugating the equation for Ψ_-

$$-i\dot{\Psi}_-^* = -m\Psi_-^* \Rightarrow i\dot{\Psi}_-^* = m\Psi_-^* \tag{4.137}$$

we see that Ψ_-^* is a mass eigenstate with positive eigenvalue $E = +m$. This field can be interpreted as a new particle field, called the positron field. The positron is the *antiparticle* to the electron. Essentially the consequence of Lorentz symmetry is the existence of antiparticles! We will see that Ψ_-^* has electric charge $+|e|$, while Ψ_+ has charge $-|e|$!

Electrons and Positrons in the Electromagnetic Field

We want to see, how electrons and positrons act in the electromagnetic field, that means why they have opposite charges. The electromagnetic field is given by $A_\mu = (-\phi, \mathbf{A})$, and the covariant Lagrangian by

$$-\mathcal{L} = i\bar{\Psi}\gamma^\mu \left(\partial_\mu - ieA_\mu\right)\Psi + im\bar{\Psi}\Psi. \tag{4.138}$$

We use here conventions where e is negative for electrons and positive for positrons. This leads via least action principle to the following modifications of the Dirac equation

$$\begin{aligned} \partial_t\Psi &\longrightarrow \left(\partial_0 + ie\phi\right)\Psi, \\ \partial_k\Psi &\longrightarrow \left(\partial_k - ieA_k\right)\Psi \end{aligned} \tag{4.139}$$

This gives us the equation of motion

$$i\dot{\Psi} = \left(\alpha^k\left(p_k - eA_k\right) + e\phi + \begin{pmatrix} 0 & m \\ m & 0 \end{pmatrix}\right)\Psi \tag{4.140}$$

with

$$\alpha^k \begin{pmatrix} \Psi_L \\ \Psi_R \end{pmatrix} = \begin{pmatrix} -\tau_k & 0 \\ 0 & \tau_k \end{pmatrix}\begin{pmatrix} \Psi_L \\ \Psi_R \end{pmatrix} = \begin{pmatrix} -\tau_k\Psi_L \\ \tau_k\Psi_R \end{pmatrix} \tag{4.141}$$

The action of α^k on the linear combinations (4.136) is as follows

$$\begin{aligned} \alpha^k\Psi_+ &= -\tau_k\Psi_-, \\ \alpha^k\Psi_- &= -\tau_k\Psi_+ \end{aligned} \tag{4.142}$$

Now we can insert Ψ_+, Ψ_- in to (4.140), and we get

$$\begin{aligned} i\dot{\Psi}_+ &= (m + e\phi)\Psi_+ + i(\partial_k - ieA_k)\tau_k\Psi_- \\ i\dot{\Psi}_- &= (-m + e\phi)\Psi_- + i(\partial_k - ieA_k)\tau_k\Psi_+ \end{aligned} \tag{4.143}$$

We have to complex conjugate (4.143) for the same reason as in (4.137)

$$i\dot{\Psi}_-^* = (m - e\phi)\Psi_-^* + i(\partial_k + ieA_k)\tau_k^*\Psi_+^* \tag{4.144}$$

Now we can see, that because of the need of conjugation, the positrons have a positive charge $+e$. This is why the positrons are the antiparticles of the electrons.

Comments

So what have we learnt up to now? Relativistic covariance leads directly to the existence of antiparticles. In the case of charged fermions, there is always an antiparticle with the opposite charge (e^-, e^+ or μ^-, μ^+). But what is about the neutrinos. They are neutral, but under charge conjugation, the righthanded neutrino turns into a lefthanded one, and vice versa. But the weak force breaks this symmetry, because it only couples to lefthanded neutrinos. Thus we cannot prove this existence righthanded ones. There is a possible solution, namely the Majorana representation, in which the particles are identical to the antiparticles, but we don't know which representation (Dirac or Majorana) is realized in nature. In recent research one searches for Majorana neutrinos in the so called double β decay. In this experiment one searches for double neutron decays of the following kind

$$2n \longrightarrow 2p^+ + 2e^- \tag{4.145}$$

because one neutron decays like

$$n \longrightarrow p^+ + e^- + \bar{\nu} \tag{4.146}$$

or

$$n + \nu \longrightarrow p^+ + e^-. \tag{4.147}$$

The combination of both processes leads to (4.145) if and only if the neutrino is a Majorana particle!

In the case of charged bosons antiparticles also exist, but not always. For example the gauge bosons of the weak force, $W^\pm$, or the pions $\pi^\pm$. There also exists Majorana bosons like the photon γ, neutral pion π^0 or the neutral weak gauge boson Z^0.

Nonrelativistic approximation

We want to make contact between the Dirac equation (4.125) and nonrelativistic equations, which also describe the spin, like the Pauli equation. For this, we exploit the squared Dirac equation

$$\gamma^\nu \left(\partial_\nu - ieA_\nu\right) \gamma^\mu \left(\partial_\mu - ieA_\mu\right) \Psi = m^2 \Psi. \tag{4.148}$$

Using the identity

$$\gamma^\nu \gamma^\mu = \frac{1}{2}\{\gamma^\nu, \gamma^\mu\} + \frac{1}{2}\left[\gamma^\nu, \gamma^\mu\right] = \eta^{\nu\mu} - i\sigma^{\nu\mu} \tag{4.149}$$

we can transform (4.148) to

$$\{\left(\partial^\mu - ieA^\mu\right)\left(\partial_\mu - ieA_\mu\right) - \frac{e}{2}\sigma^{\mu\nu} F_{\mu\nu} - m^2\}\Psi = 0 \tag{4.150}$$

where

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \tag{4.151}$$

Now what is $\frac{1}{2}\sigma^{\mu\nu}F_{\mu\nu}$. We use the fact that $F_{\mu\nu}$ is antisymmetric, and thus has vanishing diagonal elements. We then get

$$\begin{aligned}\frac{1}{2}\sigma^{\mu\nu}F_{\mu\nu} =&\frac{1}{2}\sigma^{kl}F_{kl} + \sigma^{0k}F_{0k} \\ =&\frac{1}{2}\left(-\epsilon^{klm}\hat{\tau}_m F_{kl}\right) + i\hat{\tau}_k F_{0k}\gamma^5 \\ =&-B_k\hat{\tau}_k - iE_k\hat{\tau}_k\gamma^5\end{aligned} \tag{4.152}$$

with

$$\hat{\tau}_k = \begin{pmatrix} \tau_m & 0 \\ 0 & \tau_m \end{pmatrix}, \qquad \frac{1}{2}\epsilon^{klm}F_{kl} = B_m \qquad , \qquad F_{0k} = -E_k \tag{4.153}$$

We will do the following calculations in the basis of mass eigenstates $\psi_\pm$ which we have already introduced with equation (4.136). Remind yourself of the relation to the helicity basis

$$\psi = \begin{pmatrix} \psi_L \\ \psi_R \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \psi_+ + \psi_- \\ \psi_+ - \psi_- \end{pmatrix}. \tag{4.154}$$

If we let γ^5 act on ψ from the left

$$\gamma^5\psi = \begin{pmatrix} \psi_L \\ -\psi_R \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} \psi_+ + \psi_- \\ -\psi_+ + \psi_- \end{pmatrix}. \tag{4.155}$$

we notice that γ^5 maps ψ_+ on ψ_- and vice versa

$$\gamma^5\psi_\pm = \psi_\mp. \tag{4.156}$$

Some books use the basis of mass eigenstates. In these books γ^5 has a different form than what we use. If one uses

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \tag{4.157}$$

one also has to use

$$\gamma^5 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4.158}$$

to suffice equation (4.156). But for us ψ will always be in the helicity basis and γ^5 will continue to be

$$\gamma^5 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.159}$$

If we use the mass basis we will explicitly write ψ_+ and ψ_-.

The effect of the Pauli-matrices does not change when switching to mass eigenstates. If the 4×4 matrix $\hat{\tau}_k$ acts on ψ we get

$$\hat{\tau}_k = \begin{pmatrix} \tau_k\psi_L \\ \tau_k\psi_R \end{pmatrix} = \begin{pmatrix} \tau_k\psi_+ + \tau_k\psi_- \\ \tau_k\psi_+ - \tau_k\psi_- \end{pmatrix} \tag{4.160}$$

and thus $\hat{\tau_k}$ acts on ψ by acting with τ_k on the two sub components $\psi_{L,R}$ in helicity base or $\psi_\pm$ if ψ is expressed in mass eigenstates.

In the following we will consider $\psi_\pm$ as two component spinors. To continue with our non-relativistic approximation of the Dirac equation we insert equation (4.152) in (4.150) to get

$$\left\{(\partial^\mu - ieA^\mu)(\partial_\mu - ieA_\mu) - m^2 + eB_k\tau_k\right\}\psi_\pm = -ieE_k\tau_k\psi_\mp \tag{4.161}$$

To simplify this equation we make the approach that there are no positrons, i.e. $\psi_- = 0$. This approximation is exact for zero energy. For non zero energies there is always the possibility of fluctuations that involve positrons but for non-relativistic systems the energy will be much less then the rest mass of the electron and therefore positrons should be negligible. One could proof this to be a good approximation by an iterative approach which we will skip here. Note that the approximation $\psi_- = 0$ destroys Lorentz invariance.

First we factor out the phase from the rest mass and write

$$\begin{aligned}
\psi_+ &= e^{-imt}\chi, \\
\partial_t\psi_+ &= -im\psi_+ + e^{-imt}\partial_t\chi, \\
\partial_t^2\psi_+ &= -m^2\psi_+ - 2ime^{-imt}\partial_t\chi + e^{-imt}\partial_t^2\chi, \\
(-\partial_t^2 - m^2)\psi_+ &= e^{-imt}(2im\partial_t\chi - \partial_t^2\chi).
\end{aligned} \tag{4.162}$$

Now, we take equation (4.161) with our no positron approximation, divide it by $2me^{-imt}$ and insert equation (4.162) to get

$$\begin{aligned}
&\{(\partial^k - ieA^k)(\partial_k - ieA_k) + (-\partial_t^2 - m^2) \\
&-ie(\partial^0 A_0) - ieA_0\partial^0 - ieA^0\partial_0 - e^2A^0A_0 + eB_k\tau_k\}\psi_+ = 0 \quad (4.163) \\
\Leftrightarrow \quad & i\partial_t\chi - \frac{1}{2m}\partial_t^2\chi + \frac{1}{2m}(\partial^k - ieA^k)(\partial_k - ieA_k)\chi \\
&+i\frac{e}{2m}(\partial_t A_0)\chi + eA_0\chi + \frac{ie}{m}A_0\partial_t\chi + \frac{e^2}{2m}A_0^2\chi + \frac{e}{2m}B_k\tau_k\chi = 0.
\end{aligned}$$

We are already very close to a Schrödinger equation which is of the form $i\partial_t\chi = H_{NR}\chi$ where $H_{NR} \mathrel{\hat{=}} E - m$. We reach our goal when we do one more non-relativistic approximation. We assume $|H_{NR}| \ll m$ and thus neglect all terms containing $\frac{\partial_t^2}{m}$, $\frac{A_0\partial_t}{m}$, $\frac{\partial_t A_0}{m}$ or $\frac{A_0^2}{m}$. What remains is the Hamilton operator

$$\begin{aligned}
H_{NR} &= \frac{1}{2m}(p_k - eA_k)(p_k - eA_k) - eA_0 - \frac{e}{2m}B_k\tau_k \\
&= \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi - \frac{e}{m}\mathbf{SB}
\end{aligned} \tag{4.164}$$

which we already know from other lectures. The noteworthy part is not only that the coupling to the electric field and the coupling of spin to the magnetic field automatically drop out of the calculation but also the correct coupling constant for the spin magnetic moment. This factor of two just fall out of the sky in our previous lectures. Of cause we know that the coupling constant is not exactly equal to 2. We would get these corrections if we would include vacuum fluctuations in the Dirac equation and then proceed the same way we did here.

We will now work a little with the Hamiltonian for non-relativistic atoms that we just derived. This Hamiltonian is the basis of quantum mechanics of atoms.

$$\boxed{H = \frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2 + e\phi - \frac{e}{m}\mathbf{SB}} \tag{4.165}$$

If only weak and constant electromagnetic fields are involved, we can neglect all higher order terms in $\mathbf{A}$. The term $\frac{1}{2m}(\mathbf{p} - e\mathbf{A})^2$ then becomes $\frac{\mathbf{p}^2}{2m} - \frac{e}{2m}\mathbf{LB}$. We arrive at the well known weak field approximation of the Hamiltonian for non-relativistic atoms

$$\boxed{H = \frac{1}{2m}\mathbf{p}^2 + e\phi - \frac{e}{2m}\mathbf{LB} - \frac{e}{m}\mathbf{SB}.} \tag{4.166}$$

4.3.4 Dirac Propagator

We now take a look at the propagator of a Dirac spinor in an electromagnetic background field

$$\begin{aligned} G(p', p) &= \langle \psi(p')\bar{\psi}(p)\rangle \\ &= Z^{-1} \int \mathcal{D}\psi \psi(p')\bar{\psi}(p) e^{iS} \end{aligned} \tag{4.167}$$

with

$$Z = \int \mathcal{D}\psi e^{iS}. \tag{4.168}$$

The action is given by

$$S = \int \mathrm{d}^4 x \left\{ -i\bar{\psi}\gamma^\mu(\partial_\mu - ieA_\mu)\psi - im\bar{\psi}\psi) \right\} \tag{4.169}$$

or in momentum space by

$$S = \int_p \bar{\psi}(p)(\gamma^\mu p_\mu - im)\psi(p) - e\int_p \int_q \bar{\psi}(p)\gamma^\mu A_\mu(q)\psi(p-q) \tag{4.170}$$

where $\psi(x) = \int_p e^{ip_\mu x^\mu}\psi(p)$ and $-i\partial_\mu\psi$ becomes $p_\mu\psi$. Due to the double momentum integral in the interaction the coefficient of the term quadratic in ψ is no more diagonal in momentum space. As a consequence, the propagator is quite complicated, especially for strong, space dependent electromagnetic fields. There is still research going on in this area. At this point we will simplify the setting for us.

We will only consider the free propagator

$$G_0 = i(\gamma^\mu p_\mu - im)^{-1}\delta(p - p') = \bar{G}(p)\delta(p - p'). \tag{4.171}$$

In this case the action is diagonal which makes it easy to form the inverse. Using the abbreviation $\not{p} = \gamma^\mu p_\mu$ we get

$$\boxed{\bar{G}(p) = i(\not{p} - im)^{-1} = i\frac{\not{p} + im}{p^2 + m^2}.} \tag{4.172}$$

We can check this result by the explicitly calculating

$$\frac{\not{p} + im}{p^2 + m^2} \cdot (\not{p} - im) = \frac{\not{p}^2 + m^2}{p^2 + m^2} = 1. \tag{4.173}$$

using

$$\not{p}^2 = \gamma^\mu \gamma^\nu p_\mu p_\nu = \frac{1}{2}\{\gamma^\mu, \gamma^\nu\} p_\mu p_\nu = \eta^{\mu\nu} p_\mu p_\nu = p^2. \tag{4.174}$$

The propagator has two poles at $\omega = p^0 = \pm\sqrt{p^2 + m^2} = \pm E(p)$. For the Fourier transformation

$$\bar{G}(t' - t, \mathbf{p}) = \int \frac{\mathrm{d}\omega}{2\pi} \bar{G}(\omega, \mathbf{p}) e_e^{-i\omega(t'-t)} \tag{4.175}$$

we add an infinitesimal imaginary displacement $E(p) \to E(p) - i\epsilon, \epsilon > 0$. Then we can integrate around the the poles and find the residua as we have done before. We stop our calculation here and will resume with this situation later. We see already that we will get two particles one with positive ω, the electron, and one with negative ω, the positron. Due to Lorentz invariance we always get two solutions from the propagator. So anti-particles for every particle automatically arise naturally in a relativistic theory.

4.4 Scalar Field Theory

4.4.1 Charged Scalar Fields

Charged scalar fields, e.g. pions $\pi^\pm$, are described by a complex scalar field $\phi(x)$. The Lagrangian density is given by

$$-\mathcal{L} = \partial^\mu \phi^* \partial_\mu \phi + V(\phi^* \phi) \tag{4.176}$$

with the potential $V(\phi^*\phi)$ which is $V(\phi^*\phi) = m^2\phi^*\phi$ for a free field with mass m. The action is

$$S = \int_p \phi^*(\omega, \mathbf{p})(\omega^2 - \mathbf{p}^2 - m^2)\phi(\omega, \mathbf{p}) \tag{4.177}$$

and the free correlation function

$$\begin{aligned} G_0(p', p) &= \langle \phi(p') \phi^*(p) \rangle \\ &= \bar{G}(p) \delta(p' - p) \\ &= \bar{G}(\omega, \mathbf{p}) \delta(p' - p) \\ &= \frac{i}{\omega^2 - E^2(\mathbf{p})} \delta(p' - p). \end{aligned} \tag{4.178}$$

Obviously, we have two poles with energies $E(\mathbf{p}) = \pm\sqrt{m^2+\mathbf{p}^2}$. These two poles are associated with the pions π^+ and π^-. In scalar theory particle and anti-particle arise from the fact that the propagator has two poles. Conceptually this might be a little harder to understand than for fermions where we got an extra field that the anti-particles where coming from. That is why we did fermions first.

4.4.2 Feynman Propagator

The Feynman propagator is given by

$$\boxed{G_0(x-y) = \int \frac{\mathrm{d}^4 p}{(2\pi)^4} \frac{-i}{p^2+m^2-i\epsilon} e^{ip(x-y)}.} \tag{4.179}$$

We separate the time component in p and $(x-z)$ which leaves us with

$$\begin{aligned} p(x-y) &= p_\mu(x^\mu - y^\mu) = -\omega(t'-t) + \mathbf{p}(\mathbf{x}-\mathbf{y}), \\ p^2+m^2 &= -\omega^2 + \mathbf{p}^2 + m^2 = -\omega^2 + E^2(\mathbf{p}) \end{aligned} \tag{4.180}$$

and

$$G(x-y) = \int \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{d}^3 p}{(2\pi)^3} \frac{i}{\omega^2 - E^2(\mathbf{p}) + i\epsilon} e^{-i\omega(t'-t)} e^{i\mathbf{p}(\mathbf{x}-\mathbf{y})}. \tag{4.181}$$

We see poles at $\omega = \pm\tilde{E}(p)$ where $\tilde{E}(p) = \sqrt{\mathbf{p}^2+m^2-i\epsilon} = E(p) - i\epsilon'$. Using this abbreviation we arrive at

$$\begin{aligned} \frac{i}{\omega^2 - \tilde{E}^2(p)} &= \frac{i}{(\omega - \tilde{E}(p))(\omega + \tilde{E}(p)} \\ &= \frac{i}{2\tilde{E}} \left(\frac{1}{\omega - \tilde{E}} - \frac{1}{\omega + \tilde{E}} \right) \\ &= \frac{1}{2E} \left(\frac{i}{\omega - E(p) + i\epsilon'} + \frac{i}{-\omega - E(p) + i\epsilon'} \right) \end{aligned} \tag{4.182}$$

which has a very close analogy to Dirac fields.

`Insert figures of integral paths.`

$$G_0(x-y) = \int \frac{d^3 p}{(2\pi)^3} \frac{1}{2E(\mathbf{p})} e^{i\mathbf{px}} \left(e^{-iE(p)(t'-t)} \Theta(t'-t) + e^{-iE(p)(t-t')} \Theta(t-t') \right). \tag{4.183}$$

4.4.3 Particles and Antiparticles

Compare the Feynman propagator with the non-relativistic propagator

$$G_0(t', \mathbf{p}', t, \mathbf{p}) = e^{-iE(\mathbf{p})(t'-t)}\Theta(t'-t)\delta(\mathbf{p}'-\mathbf{p}) \text{ with } E(\mathbf{p}) = \frac{\mathbf{p}^2}{2m}. \tag{4.184}$$

The differences are

(i) The relativistic energy-momentum relation

$$E(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2} = m + \frac{\mathbf{p}^2}{2m} + O\left(\frac{\mathbf{p}^4}{m^2}\right). \tag{4.185}$$

(ii) The normalization factor $\frac{1}{2E(\mathbf{p})}$ in the relativistic propagator. It can be absorbed via a rescaling of the fields:

$$\varphi(\mathbf{p}) \sim \frac{1}{\sqrt{2E(\mathbf{p})}}\, a(\mathbf{p}) \tag{4.186}$$

with

$$\langle a(\mathbf{p}')a^*(\mathbf{p})\rangle = 2E(\mathbf{p})\langle\varphi(\mathbf{p}')\varphi^*(\mathbf{p})\rangle \quad (\text{for } \omega > 0). \tag{4.187}$$

The associated operators fulfill the standard commutation relations at equal times,

$$[\hat{a}(\mathbf{p}'), \hat{a}^\dagger(\mathbf{p})] = \delta(\mathbf{p}'-\mathbf{p}). \tag{4.188}$$

(iii) There are contributions for $t' > t$ and $t' < t$. This corresponds to the presence of particles and antiparticles.

$$\begin{aligned} \langle\varphi_{NR}(t', \mathbf{p}')\varphi^*_{NR}(t, \mathbf{p})\rangle &= e^{-iE(\mathbf{p})(t'-t)}\Theta(t'-t)\delta(\mathbf{p}'-\mathbf{p}), \\ \langle\varphi^*_{NR}(t', \mathbf{p}')\varphi_{NR}(t, \mathbf{p})\rangle &= e^{-iE(\mathbf{p})(t-t')}\Theta(t-t')\delta(\mathbf{p}'-\mathbf{p}) \end{aligned} \tag{4.189}$$

$$\begin{aligned} \omega > 0 &: \varphi(t, \mathbf{p}) \text{ corresponds to } \varphi_{NR}(t, \mathbf{p}), \\ \omega < 0 &: \varphi(t, \mathbf{p}) \text{ corresponds to } \varphi^*_{NR}(t, \mathbf{p}). \end{aligned} \tag{4.190}$$

Only $\omega > 0$ describes particles

$$\varphi_+(t, \mathbf{p}) \sim \frac{a(t, \mathbf{p})}{\sqrt{2E(\mathbf{p})}}, \tag{4.191}$$

$\omega < 0$ describes antiparticles

$$\varphi_-(t, \mathbf{p}) \sim \frac{b^\dagger(t, -\mathbf{p})}{\sqrt{2E(\mathbf{p})}}. \tag{4.192}$$

$$\varphi(\omega, \mathbf{p}) = \frac{1}{\sqrt{2E(\mathbf{p})}}[a(\omega, \mathbf{p})\Theta(\omega) + b^*(-\omega, -\mathbf{p})\Theta(-\omega)] \tag{4.193}$$

Define

$$\varphi(\omega, \mathbf{p}) = \varphi_+(\omega, \mathbf{p})\Theta(\omega) + \varphi_-(\omega, \mathbf{p})\Theta(-\omega). \tag{4.194}$$

Then $\varphi_+(\omega, \mathbf{p})$ will describe particles with positive energy, $\varphi_+(-|\omega|, \mathbf{p}) = 0$.
And $\varphi_-^*(\omega, \mathbf{p}) = \varphi^{C*}(-\omega, -\mathbf{p})$ will describe antiparticles with positive energy, $\varphi_-(|\omega|, \mathbf{p}) = 0$.
Both $\varphi_+(\omega, \mathbf{p})$ and $\varphi^C(\omega, \mathbf{p})$ have only positive frequency parts. In coordinate space one has

$$\varphi(t, \mathbf{x}) = \varphi_+(t, \mathbf{x}) + \varphi_-(t, \mathbf{x}), \tag{4.195}$$

with

$$\begin{aligned}
\varphi_+(t, \mathbf{x}) &= \int \frac{d\omega}{2\pi} \frac{d^3\mathbf{p}}{(2\pi)^3} e^{-i(\omega t - \mathbf{p}\mathbf{x})} \frac{1}{\sqrt{2E(\mathbf{p})}}\, a(\omega, \mathbf{p})\Theta(\omega), \\
\varphi_-(t, \mathbf{x}) &= \int \frac{d\omega}{2\pi} \frac{d^3\mathbf{p}}{(2\pi)^3} e^{-i(\omega t - \mathbf{p}\mathbf{x})} \frac{1}{\sqrt{2E(\mathbf{p})}}\, b^*(-\omega, -\mathbf{p})\Theta(-\omega) \\
&= \int \frac{d\tilde{\omega}}{2\pi} \frac{d^3\mathbf{p}}{(2\pi)^3} e^{i(\tilde{\omega} t - \mathbf{p}\mathbf{x})} \frac{1}{\sqrt{2E(\mathbf{p})}}\, b^*(\tilde{\omega}, \mathbf{p})\Theta(\tilde{\omega}).
\end{aligned} \tag{4.196}$$

The relation to the operator picture is

$$\begin{aligned}
a(t, \mathbf{p}),\ a^*(t, \mathbf{p}) \quad &\leftrightarrow \quad \hat{a}(t, \mathbf{p}),\ \hat{a}^\dagger(t, \mathbf{p}), \\
b(t, \mathbf{p}),\ b^*(t, \mathbf{p}) \quad &\leftrightarrow \quad \hat{b}(t, \mathbf{p}),\ \hat{b}^\dagger(t, \mathbf{p}).
\end{aligned} \tag{4.197}$$

4.4.4 In- and Out Fields

Transition amplitudes for $t' \to \infty$ and $t \to -\infty$:

(i) Incoming $\pi^+, \mathbf{p}$; outgoing $\pi^+, \mathbf{p}'$:

$$\langle a(t', \mathbf{p}')a^*(t, \mathbf{p})\rangle = \sqrt{4E(\mathbf{p}')E(\mathbf{p})}\langle\varphi_+(t', \mathbf{p}')\varphi_+^*(t, \mathbf{p})\rangle. \tag{4.198}$$

(ii) Incoming $\pi^-, \mathbf{p}$; outgoing $\pi^+, \mathbf{p}'$:

$$\langle b(t', \mathbf{p}')b^*(t, \mathbf{p})\rangle = \sqrt{4E(\mathbf{p}')E(\mathbf{p})}\langle\varphi_-^*(t', -\mathbf{p}')\varphi_-(t, -\mathbf{p})\rangle. \tag{4.199}$$

(iii) Incoming $\pi^+(\mathbf{p}_1),\ \pi^-(\mathbf{p}_2)$; outgoing $\pi^+(\mathbf{p}_3),\ \pi^-(\mathbf{p}_4)$:

$$\begin{aligned}
\langle a(t', \mathbf{p}_3)b(t', \mathbf{p}_4)a^*(t, \mathbf{p}_1)b^*(t, \mathbf{p}_2)\rangle =& 4\sqrt{E(\mathbf{p}_1)E(\mathbf{p}_2)E(\mathbf{p}_3)E(\mathbf{p}_4)} \\
&\langle\varphi_+(t', \mathbf{p}_3)\varphi_-^*(t', -\mathbf{p}_4)\varphi_+^*(t, \mathbf{p}_1)\varphi_-(t, -\mathbf{p}_2)\rangle.
\end{aligned} \tag{4.200}$$

Summary

- Particles and antiparticles are determined by the location of the poles of $G_0(\omega, \mathbf{p})$.
- The normalization is uniquely fixed by the residua of the poles.

5 Scattering and decay

5.1 S-Matrix and Greens-Functions

5.1.1 Scattering amplitude for relativistic charged scalar field

5.1.2 The LSZ Formalism

In 1955, the three German physicists Harry **L**ehmann, Kurt **S**ymanzik and Wolfhart **Z**immermann invented the following method to compute S-matrix elements

$$\langle \mathbf{p}_3\mathbf{p}_4|S|\mathbf{p}_1\mathbf{p}_2\rangle \tag{5.1}$$

for $t' \to \infty$ and $t \to -\infty$.

$$\prod_{i=1}^{4}\int d^4x_i e^{-ix_ip_i}\langle\varphi_-^*(x_4)\varphi_+(x_3)\varphi_-(x_2)\varphi_+(x_1)\rangle\bigg|_{p_{0i}=E(\mathbf{p}_i)} \sim \tag{5.2}$$

$$\prod_{i=1}^{4}\frac{i\sqrt{Z}}{p_i^2+m^2-i\varepsilon}\langle \mathbf{p}_3\mathbf{p}_4|S|\mathbf{p}_1\mathbf{p}_2\rangle \tag{5.3}$$

Take successively $x_{40} \to -\infty$, $x_{30} \to \infty$, ... and use

$$\mathbf{1} = \sum_\lambda\int\frac{d^3q}{(2\pi)^3}\frac{1}{2E_\lambda(\mathbf{q})}|\lambda\mathbf{q}\rangle\langle\lambda\mathbf{q}|, \tag{5.4}$$

with $|\lambda_q\rangle$ being the eigenstates and $E_\lambda(\mathbf{q})$ being the eigenvalues of the Hamiltonian.

$$\langle\varphi_-^*(x_4)\varphi_+(x_3)\ldots\rangle = \sum_\lambda\int\frac{d^3q}{(2\pi)^3}\frac{1}{2E_\lambda(\mathbf{q})}\overbrace{\langle\varphi_-^*(x_4)|\lambda\mathbf{q}\rangle}^{\langle\Omega|\varphi_-^*(x_4)|\lambda\mathbf{q}\rangle}\langle\lambda\mathbf{q}|\varphi_+(x_3)\ldots\rangle \tag{5.5}$$

Use the invariance of Ω under translations, i.e.

$$\langle\Omega|\varphi_-^*(x_4)|\lambda\mathbf{q}\rangle = \langle\Omega|\varphi_-^*(0)|\lambda_0\rangle e^{-iqx}\big|_{q_0=E_q(\lambda)}, \tag{5.6}$$

and furthermore

$$\delta^3(\mathbf{p}-\mathbf{q})\int_{T_>}^{\infty} e^{-ip^0x^0}e^{+iq^0x^0}\bigg|_{q_0=E(\mathbf{q})} e^{-\varepsilon x^0} = \frac{i}{p^0-E(\mathbf{q})-i\varepsilon} \to \infty. \tag{5.7}$$

...

5.2 Scattering and decay

5.2.1 Differential cross section

5.2.2 Lorentz covariant building blocks

5.2.3 Tree scattering in scalar theory

5.2.4 Generalizations

After we worked through the theory of point like interactions, we will now look at momentum dependent interactions.

The interaction part of the vertex is

$$-S_{int} = \frac{1}{2}\int_{q_1,\ldots,q_4} \delta(q_1+q_2-q_3-q_4)\lambda(s)\phi^*(q_1)\phi(-q_2)\phi^*(-q_4)\phi(q_3). \tag{5.8}$$

The difference to our previous calculation lies in the s dependence of λ. But $s = (q_1+q_2)^2 = (q_3+q_4)^2$ can be expressed in terms of incoming momenta which are fixed quantities and do not influence phase space integration. Hence we still get the simple s dependence

$$\boxed{\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\lambda^2(s)}{16\pi^2 s}.} \tag{5.9}$$

The total scattering cross section is

$$\sigma_{tot} = \frac{\lambda^2(s)}{4\pi s}. \tag{5.10}$$

Scattering $s_+s_+ \to s_+s_+$

The interaction of $s_+s_+ \to s_+s_+$ scattering differs from the interaction of $s_+s_- \to s_+s_-$.

Firstly, we take a look at the point like interaction of $s_+s_+ \to s_+s_+$. The relevant four point function is

$$\langle \phi_+(t',\mathbf{p}_3)\phi_+(t',\mathbf{p}_4)\phi_+^*(t,\mathbf{p}_1)\phi_+^*(t,\mathbf{p}_2)\rangle. \tag{5.11}$$

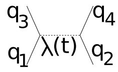
To first order in perturbation theory this becomes

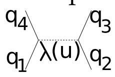
$$-\frac{i\lambda}{2}\langle \phi(p_3)\phi(p_4)\phi^*(p_1)\phi^*(p_2)\phi^*(q_3)\phi^*(q_4)\phi(q_1)\phi(q_2)\rangle_0 \delta(q_1+q_2-q_3-q_4). \tag{5.12}$$

There are four possibilities for combining p's and q's resulting in a scattering matrix

$$|\mathcal{M}|^2 = 4\lambda^2. \tag{5.13}$$

For point like interactions the cross sections for $s^+s^+ \to s^+s^+$ and $s^+s^- \to s^+s^-$ are the same. This symmetry is called *crossing symmetry*.

For the momentum dependent vertex λ is not constant but depends on $t = (q_1 - q_3)^2$ or $u = (q_1 - q_4)^2$. We have the two diagrams 

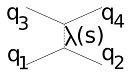
and 

resulting in

$$\mathcal{M} \sim \lambda(t) + \lambda(u). \tag{5.14}$$

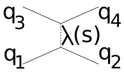
This results in

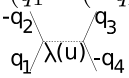
$$\mathcal{M} = \lambda^2(t) + \lambda^2(u) + 2\lambda(t)\lambda(u). \tag{5.15}$$

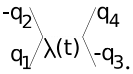
The last term describes the interference of two identical particles. The interference term would have a minus sign if we had considered fermions. This comes from the exchange of $\phi^*(q_3)$ and $\phi^*(q_4)$ in (5.12). The additional interference term does not occur in $s_+s_- \rightarrow s_+s_-$ scattering which has only the one diagram 

and $\mathcal{M} \sim 2\lambda(s)$.

Properties of a Momentum Dependent Vertex

The crossing symmetry can be useful to facilitate calculations. We can identify an incoming antiparticle with momentum q with an outgoing particle with momentum $-q$ because $s = (q_1 + q_2)^2 = (q_1 - (-q_2))^2$.


is the same as 

or 

.
Of cause, in reality all particles have positive energy but for mathematical purposes this symmetry is useful.

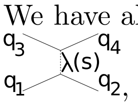
The spacial distribution of outgoing particles depends on t and u therefore the phase space integration of the momentum dependent scattering cross section for $s^+s^+ \rightarrow s^+s^+$ scattering depends on $\lambda(t)$ and $\lambda(u)$ and $\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega}$ depends on the angle.

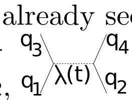
The variables s, t and u are called Mandelstam variables. The relativistic kinematic of $2 \rightarrow 2$ scattering can be expressed in terms of these variables. Such an interaction has three independent four momenta, p_1, p_2 and p_3. The fourth four momentum $p_4 = p_1 + p_2 - p_3$ is a linear combination of these three. The independent four momenta combine to several Lorentz invariant scalars

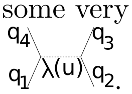
$$\begin{gathered} p_1^2 = m_1^2, \quad p_2^2 = m_2^2, \quad p_3^2 = m_3^2, \quad (p_1 + p_2 - p_3)^2 = p_4^2 = m_4^2, \\ (p_1 + p_2)^2 = s \ , \ (p_1 - p_3)^2 = t \\ (p_1 - p_4)^2 = (p_3 - p_2)^2 = u \end{gathered} \tag{5.16}$$

which makes the Mandelstam variables the logical choice for relativistic calculations.

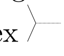
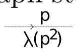
Feynman Graphs

We have already seen some very simple Feynman graphs like


, 

or 

.

Feynman graphs are nothing more than a simple way to remember what goes into the calculation. Each part of a graph stands for a part of the formula. A vertex  adds the factor 1 and an internal path 

inserts a factor $\lambda(p^2)$.

To compute $\mathcal{M}$ one just has to

1. throw in all different graphs and

2. evaluate the resulting formula.

But *be careful with relative weight and with* $\pm$ *for fermions.* There can be "statistical factors". For example, we have seen that the vertex of s_+s_- scattering gives 2λ but has only one Feynman diagram while s_+s_+ scattering has two diagrams which vertices contribute with a factor of λ each. These "statistical factors" can be cast into relatively simple rules or (better) can be figured out from the functional integral and perturbation theory.

5.2.5 Point like Interaction of Non-relativistic Spinless Atoms

The only differences to our relativistic calculation are that the factors of $\frac{1}{2E_j}$ are absent and that $|\mathbf{v}_1 - \mathbf{v}_2| = \frac{2p}{m}$ in the rest frame. The action is

$$-S = \int_x \frac{\lambda_{NR}}{2} (\phi^* \phi)^2 \tag{5.17}$$

and the reduced transition matrix reads in the classical approximation

$$\mathcal{M} = 2\lambda_{NR}. \tag{5.18}$$

The propagator has only one pole at $\frac{i}{\omega - E(p)}$, there are no anti-particles. The differential cross section is

$$\begin{aligned} \mathrm{d}\sigma &= \frac{\mathrm{d}^3 q}{(2\pi)^3} 2\pi\delta(2E(\mathbf{q}) - 2E(\mathbf{p}))(2\lambda)^2 \frac{m}{2p} \\ \Rightarrow \qquad \frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} &= \frac{\lambda_{NR}^2}{\pi^2} \int_0^\infty \mathrm{d}q\, q^2 \underbrace{\delta\left(\frac{q^2}{m} - \frac{p^2}{m}\right)}_{=\frac{m}{2q}\delta(p-q)} \frac{m}{2p} \end{aligned} \tag{5.19}$$

such that

$$\boxed{\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\lambda_{NR}^2}{4\pi^2} m^2.} \tag{5.20}$$

This cross section can also be computed by quantum mechanics for two particle states. Note that λ_{NR} is *not* the non-relativistic limit of the relativistic scalar interaction. It is useful to check the dimensions for the relativistic and non-relativistic interaction. The term $\int_x \partial_\mu \phi \partial^\mu \phi$ of the action gives the dimension of $\phi(x)$ and the $\int_x \lambda\phi^4$ term gives the dimension of λ. We discover

$$\begin{aligned}
&\text{relativistic} && [\phi(x)] = M && [\lambda] = M^0 && \Rightarrow && [\sigma] = M^{-2} = \text{area} \\
&\text{non-relativistic} && [\phi(x)] = M^{3/2} && [\lambda] = M^{-2} && \Rightarrow && [\sigma] = M^{-2} = \text{area}.
\end{aligned} \tag{5.21}$$

These differences in dimensions are directly related to the $\frac{1}{2E_j}$ factors. We find

$$\phi_{NR} = \sqrt{2E}\phi \tag{5.22}$$

and from $\lambda_{NR}\phi_{NR}^4 = \lambda\phi^4$

$$\lambda_{NR} = \frac{1}{4E^2}\lambda = \frac{\lambda}{s}. \tag{5.23}$$

Knowing these relations we can write down the non-relativistic limit of the relativistic cross section

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\lambda^2}{16\pi^2 s} = \frac{\lambda_{NR}^2 s}{16\pi^2} \approx \frac{\lambda_{NR}^2}{4\pi^2} m^2 \tag{5.24}$$

which proves to be the same as the non-relativistic cross section we calculated above.

5.2.6 Point like Interaction of Non-relativistic Atoms with Spin 1/2

When considering particles with spin 1/2 we have to use Grassmann fields. The interaction part of the action is

$$-S_{int} = \frac{\lambda_\psi}{2}\int_x (\psi^\dagger\psi)^2. \tag{5.25}$$

We decompose the interaction in different spin states which gives

$$\begin{aligned}
\psi^\dagger\psi &= \psi_\uparrow^*\psi_\uparrow + \psi_\downarrow^*\psi_\downarrow, \\
(\psi^\dagger\psi)^2 &= 2\psi_\uparrow^*\psi_\uparrow\psi_\downarrow^*\psi_\downarrow, \\
\bar{S}^{(4)} &= -\lambda_\psi
\end{aligned} \tag{5.26}$$

and

$$|\mathcal{M}|^2 = \lambda_\psi^2. \tag{5.27}$$

The rest of the calculations are the same as for bosons. We arrive at the cross sections

$$\boxed{\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} = \frac{\lambda_\psi^2 m^2}{16\pi^2}} \qquad \boxed{\sigma_{tot} = \frac{\lambda_\psi^2 m^2}{4\pi}}. \tag{5.28}$$

These cross sections only apply for scattering of particles with opposite spin. In the limit of point like interaction the cross section for equal particles with equal spin is zero.

They cannot interact because the Pauli principle forbids them to be at the same place. The interaction term would be proportional to $\psi_\uparrow\psi_\uparrow\psi_\uparrow^*\psi_\uparrow^*$.

Bosons have a relative factor of 2 in the amplitude compared to fermions. When we apply perturbation theory, the term $\langle\psi_\downarrow\psi_\uparrow\psi_\downarrow^*\psi_\uparrow^*\rangle$ in the interaction part of the action becomes

$$-i\frac{\lambda}{2}\langle\psi_\downarrow\psi_\uparrow\psi_\downarrow^*\psi_\uparrow^*(\psi^\dagger\psi)^2\rangle = -i\lambda\langle\psi_\downarrow\psi_\uparrow\psi_\downarrow^*\psi_\uparrow^*\psi_\uparrow^*\psi_\uparrow\psi_\downarrow^*\psi_\downarrow\rangle_0. \tag{5.29}$$

With the relations

$$\langle\psi_\downarrow\psi_\downarrow^*\rangle_0 \sim G_0\ ,\ \langle\psi_\uparrow\psi_\uparrow^*\rangle_0 \sim G_0, \langle\psi_\downarrow\psi_\uparrow^*\rangle_0 = 0. \tag{5.30}$$

only one combination remains. So the definition of the vertex by $\bar{S}^{(4)}$ takes care of these combinatoric factors.

5.2.7 Relativistic Dirac Particles: Normalization and On Shell Condition

Basis States

The interaction term of the action is

$$-S_{int} = \int_x \frac{\lambda_F}{2}(\bar{\psi}\psi)^2 = \int_x \frac{\lambda_f}{2}\bar{\psi}_\alpha\psi_\alpha\bar{\psi}_\beta\psi_\beta. \tag{5.31}$$

The lesson that we have learned from non-relativistic atoms is that scattering depends on quantum numbers of incoming and outgoing particles. Our first guesses for good basis states are

- helicity eigenstates

$$\begin{aligned}\psi &= \psi_L + \psi_R,\\ \psi_L &= \frac{1+\gamma^5}{2}\psi, \quad \psi_R = \frac{1-\gamma^5}{2}\psi,\end{aligned} \tag{5.32}$$

- mass eigenstates in the rest frame

$$\begin{aligned}\psi &= \psi_+ + \psi_-\\ \psi_+ &= \frac{1+i\gamma^0}{2}\psi, \quad \psi_- = \frac{1-i\gamma^0}{2}\psi,\end{aligned} \tag{5.33}$$

  In the rest frame the fields $\psi_\pm$ are eigenstates of the mass operator $M = mi\gamma^0$ with eigenvalues $\pm m$. ψ_+ has an eigenvalue with positive energy and describes the electron field, ψ_- describes the complex conjugate of the positron field. Unfortunately, these states are only eigenstates in their rest frame.

In principle our choice of basis is free but it is crucial for calculation where we need to be able to diagonalize the propagator. The bases we know up to now are useful for calculations in both limiting cases: helicity eigenstates for highly relativistic particles, mass eigenstates for non-relativistic particles. But we do not have a basis of eigenstates for the whole energy range.

Bilinears expressed in basic states

For the calculation of bilenears, we first remind the definition of the complex conjugate of Grassmann fields $\bar{\psi}$:

$$\bar{\psi} = \psi^\dagger \gamma^0. \tag{5.34}$$

This we will need several times down below.

- helicity eigenstates

  In the last small subsection we already mentioned the projection operator of ψ_L and ψ_R. But what are the projection operators for $\bar{\psi}_L$ and $\bar{\psi}_R$? Let's do it step by step:

  $$\bar{\psi}_L = \psi_L^\dagger \gamma^0 = \left(\frac{\mathbf{1} + \gamma^5}{2} \psi \right)^\dagger \gamma^0 = \psi^\dagger \left(\frac{\mathbf{1} + \gamma^5}{2} \right) \gamma^0. \tag{5.35}$$

  As the γ-matrices anticommute, we can go on and write

  $$\bar{\psi}_L = \psi^\dagger \gamma^0 \frac{\mathbf{1} - \gamma^5}{2} = \bar{\psi} \frac{\mathbf{1} - \gamma^5}{2} \tag{5.36}$$

  This is now a direct relation between $\bar{\psi}_L$ and $\bar{\psi}$, just as we wanted. An analogue calculation for $\bar{\psi}_R$ yields

  $$\bar{\psi}_R = \bar{\psi} \left(\frac{1 + \gamma^5}{2} \right) \tag{5.37}$$

  Now let's recall the Lagrangian for free Dirac particles with mass m

  $$-\mathcal{L} = i\bar{\psi}\gamma^\mu \partial_\mu \psi + im\bar{\psi}\psi \tag{5.38}$$

  and have a look at the very simple bilinear $\bar{\psi}\psi$. How does it look like when we use the decomposition into helicity eigenstates?

  $$\begin{aligned} \bar{\psi}\psi &= (\bar{\psi}_L + \bar{\psi}_R)(\psi_L + \psi_R) \\ &= \bar{\psi}_L \psi_R + \bar{\psi}_R \psi_L \end{aligned} \tag{5.39}$$

  The last equation holds, because $\bar{\psi}_L\psi_L = \bar{\psi}_R\psi_R = 0$. Proof (for $\bar{\psi}_L\psi_L$):

  $$\begin{aligned} \bar{\psi}_L \psi_L &= \bar{\psi} \left(\frac{\mathbf{1} - \gamma^5}{2} \right) \left(\frac{\mathbf{1} + \gamma^5}{2} \right) \psi \\ &= \frac{1}{4} \bar{\psi} \left(\mathbf{1} - (\gamma^5)^2 \right) \psi = 0 \end{aligned} \tag{5.40}$$

  because $(\gamma^5)^2 = \mathbf{1}$.

  Well, what does equation (5.39) tell us? Obviously, that the mass term is not diagonal in the helicity eigenstates, but mixes them. In particular, if we consider neutrinos, this has consequences: We know, that neutrinos are particles which only couple through weak interaction, and the weak interaction only couples to left-handed particles (fields ψ_L) and right-handed antiparticles ($\bar{\psi}_R$). Now there are two possibilities: Either there are right-handed neutrinos and left-handed antineutrinos that we don't see, or they aren't there at all. But if the last case is true, meaning $\psi_R = \bar{\psi}_L = 0$, we will never have a mass-term.

We can also argue another way: If neutrinos have a mass, they travel slower than light, and thus we will always find a system of inertia that travels with higher speed than the neutrinos. But in this case, the direction of the relative motion between neutrinos and different systems of inertia will change, and thus helicity will also change. So we essentially need fields ψ_R and $\bar{\psi}_L$ to describe neutrinos (and anti-neutrinos) in those systems of inertia.

However, what about the kinetic term of the Lagrangian? Here the situation as different from the mass term. If we consider $\bar{\psi}\gamma^\mu\psi$, we observe that

$$\begin{aligned}\bar{\psi}\gamma^\mu\psi &= (\bar{\psi}_L + \bar{\psi}_R)\gamma^\mu(\psi_L + \psi_R)\\ &= \bar{\psi}_L\gamma^\mu\psi_L + \bar{\psi}_R\gamma^\mu\psi_L + \bar{\psi}_L\gamma^\mu\psi_R + \bar{\psi}_R\gamma^\mu\psi_R\\ &= \bar{\psi}_L\gamma^\mu\psi_L + \bar{\psi}_R\gamma^\mu\psi_R \end{aligned}\tag{5.41}$$

The mixed terms vanish, because of

$$\begin{aligned}\bar{\psi}_R\gamma^\mu\psi_L &= \bar{\psi}\left(\frac{1+\gamma^5}{2}\right)\gamma^\mu\left(\frac{1+\gamma^5}{2}\right)\psi\\ &= \bar{\psi}\gamma^\mu\left(\frac{1-\gamma^5}{2}\right)\left(\frac{1+\gamma^5}{2}\right)\psi = 0. \end{aligned}\tag{5.42}$$

So in contrast to the mass term, the kinetic term *is* diagonal in helicity eigenstates (the ∂_μ in the Lagrangian doesn't change the fact, that $\bar{\psi}_R\gamma^\mu\psi_L$ and $\bar{\psi}_L\gamma^\mu\psi_R$ vanish).

- mass eigenstates
  Let us now have a look at the same bilinears in another basis system, the mass eigenstates. First we again derive the relation between $\bar{\psi}_+$ and $\bar{\psi}$:

$$\begin{aligned}\bar{\psi}_+ &= \psi_+^\dagger\gamma^0 = \left(\frac{\mathbf{1}+i\gamma^0}{2}\psi\right)^\dagger\gamma^0\\ &= \psi^\dagger\left(\frac{\mathbf{1}-i(\gamma^0)^\dagger}{2}\right)\gamma^0 = \bar{\psi}\left(\frac{\mathbf{1}+i\gamma^0}{2}\right) \end{aligned}\tag{5.43}$$

where we used $(\gamma^0)^\dagger = -\gamma^0$ in the last equation. Similarly, one can derive

$$\bar{\psi}_- = \bar{\psi}\left(\frac{\mathbf{1}-i\gamma^0}{2}\right).\tag{5.44}$$

Having this, we can start to compute bilinears. We begin again with the mass term:

$$\bar{\psi}\psi = (\bar{\psi}_+ + \bar{\psi}_-)(\psi_+ + \psi_-) = \bar{\psi}_+\bar{\psi}_+ + \bar{\psi}_-\bar{\psi}_- \tag{5.45}$$

This is true, because $\bar{\psi}_-\psi_+ = \bar{\psi}_+\psi_- = 0$. Let's make a short proof for this:

$$\begin{aligned}\bar{\psi}_-\psi_+ &= \bar{\psi}\left(\frac{\mathbf{1} - i\gamma^0}{2}\right)\left(\frac{\mathbf{1} + i\gamma^0}{2}\right)\psi \\ &= \frac{1}{4}\bar{\psi}\left(\mathbf{1} - i\gamma^0 + i\gamma^0 + (\gamma_0)^2\right)\psi = 0,\end{aligned} \tag{5.46}$$

because $(\gamma^0)^2 = -\mathbf{1}$.

The result in (5.45) tells us, that in the basis of mass eigenstates the mass term is diagonal. But this time, the kinetic isn't diagonal. A little bit longer, but in principle easy calculation shows

$$\begin{aligned}\bar{\psi}\gamma^\mu p_\mu \psi &= (\bar{\psi}_+ + \bar{\psi}_-)\gamma^\mu(i\partial_\mu)(\psi_+ + \psi_-) \\ &= \bar{\psi}_+\gamma^0 p_0\psi_+ + \bar{\psi}_-\gamma^0 p_0\psi_- + \bar{\psi}_+\gamma^i p_i\psi_- + \bar{\psi}_-\gamma^i p_i\psi_+.\end{aligned} \tag{5.47}$$

This is only diagonal when we work in the rest frame with momentum $\mathbf{p} = 0$.

What do all these calculations tell us? Well, to solve a problem in the path-integral formulation, it is convenient to have the free part of the action diagonal in the fields. But neither the helicity nor the mass eigenstates are diagonal, they always contain both diagonal and off-diagonal terms. Only in limiting cases they are convenient basis states: helicity eigenstates for ultrarelativistic and mass eigenstates for non relativistic problems.

Let's now come to the solution for this problem: We will show now that the eigenstates to the operator $\not{p} = p_\mu\gamma^\mu$ lead to diagonal expressions for mass *and* kinetic term:

- $\not{p}$-eigenstates

  Let us remind the simple relation $\not{p}^2 = p^2\mathbf{1} = (-\omega^2 + \mathbf{p}^2)\mathbf{1}$. This already tells us, that $\not{p}^2$ has just one eigenvalue, namely p^2. From this it follows that the operator $\not{p}$ has two different eigenvalues, $\pm\sqrt{p^2} = \pm\sqrt{-\omega^2 + \mathbf{p}^2}$.

  We define now the eigenstate corresponding to the "+"-solution as $\psi_>$ and the eigenstate corresponding to "−"-solution as $\psi_<$, so we have

$$\not{p}\psi_> = +\sqrt{p^2}\psi_> \ , \ \not{p}\psi_< = -\sqrt{p^2}\psi_<. \tag{5.48}$$

  Depending on the choice of the four components of p, the $p^2 = -\omega^2 + \mathbf{p}^2$ can be either positive or negative. So if we replace $\sqrt{p^2}$ by $\sqrt{|p^2|}$ for $p^2 > 0$ and $\sqrt{p^2}$ by $i\sqrt{|p^2|}$, we observe the following behaviour of $\not{p}$-eigenstates:

$$\begin{aligned}\not{p}\psi_> &= +\sqrt{|p^2|}\psi_> \quad for \quad p^2 \geq 0 \\ \not{p}\psi_> &= +i\sqrt{|p^2|}\psi_> \quad for \quad p^2 < 0 \\ \not{p}\psi_< &= -\sqrt{|p^2|}\psi_< \quad for \quad p^2 \geq 0 \\ \not{p}\psi_< &= -i\sqrt{|p^2|}\psi_< \quad for \quad p^2 < 0.\end{aligned} \tag{5.49}$$

Now we define a new operator:

$$A(p) = (-i)^{\Theta(-p^2)} \frac{\not{p}}{\sqrt{|p^2|}} \tag{5.50}$$

This operator acts on the $\psi_>$ and $\psi_<$ states as follows:

$$A(p)\psi_> = +\psi_> \ , \ A(p)\psi_< = -\psi_< \tag{5.51}$$

Obviously $1 \pm A(p)$ are projectors, as the squared of $A(p)$ is the unit matrix:

$$A(p)^2 = (-1)^{\Theta(-p^2)} \frac{p^2 \mathbf{1}}{|p^2|} = \mathbf{1}. \tag{5.52}$$

For the projection of an arbitrary state ψ onto the two $\not{p}$-eigenstates, we employ

$$\begin{aligned} \psi &= \psi_> + \psi_<, \\ \psi_> &= \frac{1}{2}(\mathbf{1} + A(p))\psi_> \ , \ \psi_< = \frac{1}{2}(\mathbf{1} - A(p))\psi_< \end{aligned} \tag{5.53}$$

The next step is to define the complex conjugate Grassmann fields $\bar{\psi}_>$ and $\bar{\psi}_<$:

$$\bar{\psi}_> = \bar{\psi} \left(\frac{1}{2}(\mathbf{1} + A(p)) \right) \ , \ \psi_< = \bar{\psi} \left(\frac{1}{2}(\mathbf{1} - A(p)) \right) \tag{5.54}$$

Now we can return to the calculation of bilinears:
Let us start with the mass term. It is

$$\begin{aligned} \bar{\psi}\psi &= \bar{\psi}_>\psi_> + \bar{\psi}_>\psi_< + \bar{\psi}_<\psi_> + \bar{\psi}_<\psi_< \\ &= \bar{\psi}_>\psi_> + \bar{\psi}_<\psi_<, \end{aligned} \tag{5.55}$$

as the mixed terms are zero because of

$$\bar{\psi}_<\psi_> = \bar{\psi} \left(\frac{1}{2}(\mathbf{1} - A(p)) \right) \psi_> = 0. \tag{5.56}$$

We used here the definition of $\bar{\psi}_<$ and the fact, that $A(p)\psi_> = \psi_>$.
So far, so good. But this time, also the kinetic term is diagonal:

$$\begin{aligned} \bar{\psi} p_\mu \gamma^\mu \psi &= \bar{\psi} \not{p} \psi \\ &= i^{\Theta(-p^2)} \sqrt{|p^2|} \bar{\psi}(\psi_> - \psi_<) \\ &= i^{\Theta(-p^2)} \sqrt{|p^2|} (\bar{\psi}_>\psi_> - \bar{\psi}_<\psi_<) \\ &= \bar{\psi}_> \not{p} \psi_> + \bar{\psi}_< \not{p} \psi_< \end{aligned} \tag{5.57}$$

So finally we reached our aim to find a basis in which both terms of the Lagrangian are block-diagonal, and thus is the free action S.

Residua at poles of the Dirac-propagator

Let us recall the Dirac-propagator:

$$\begin{aligned} G_0(p) &= \bar{G}(p)\delta(p-p'), \\ \bar{G}(p) &= i\frac{\not{p}+im}{p^2+m^2}. \end{aligned} \tag{5.58}$$

Here in, m is the mass of the particle, and thus of course real and positive.

Obviously, the propagator has poles at

$$p^2 = -m^2. \tag{5.59}$$

This equation has no solutions for $p^2 > 0$. For $p^2 < 0$ we get

$$\sqrt{|p^2|} = m. \tag{5.60}$$

This may now look as we have just one pole, in contrast to what we had in previous chapters. But this is not true: Remind that $\sqrt{|p^2|} = \sqrt{|-\omega^2 + \mathbf{p}^2|} = m$ still has two solutions, namely $\omega = \sqrt{\mathbf{p}^2 + m^2}$ and $\omega = -\sqrt{\mathbf{p}^2 + m^2}$

Anyhow, since we know that $p^2 < 0$, we can compute the action of $\not{p}$ on $\psi_>$ and $\psi_<$, if we combine equations (5.49) and (5.60):

$$\not{p}\psi_> = im\psi_> \ , \ \not{p}\psi_< = -im\psi_<, \tag{5.61}$$

and thus

$$\begin{aligned} (\not{p}+im)\psi_> &= 2im\psi_>, \\ (\not{p}+im)\psi_< &= 0. \end{aligned} \tag{5.62}$$

But from this it follows directly, that

$$lim_{p^2\to -m^2}\bar{G}(p) < \infty \tag{5.63}$$

if (and only if!) we consider the propagation of the $\psi_<$-field. So $\psi_<$ does *not* describe a particle! And this makes really sense: The Dirac Spinor has four complex components, and thus eight real degrees of freedom. But we can only have four different physical situations: The spin of the particle may be up or down, and the same is valid for the spin of the antiparticle. When we considered mass or helicity eigenstates, the two spinors ψ_L and ψ_R (or ψ_+ and ψ_-) "lost" four degrees of freedom, because the helicity eigenstates had two zero-entries and in the mass eigenstates we only had two independent entries. But here, we have really eight degrees of freedom. In somehow we can understand this as a price we have to pay for simplifying our action. For making it block-diagonal, we needed to introduce a field ψ_-, which does not correspond to a propagating particle.

Similar as we already did it for the bosons, we are now able to formulate a "mass shell condition" (or "on-shell condition") for fermions. Actually, first one would think that the identical denominator $p^2 + m^2$ leads to an identical mass shell condition. But as we just showed, this is not restrictive enough for fermions. We need to demand $p^2 + m^2 = 0$ and that the incoming and outgoing field is $\psi_>$. But we can also formulate this in *one* equation:

$$\not{p}\psi = im\psi. \tag{5.64}$$

Or, for the complex conjugate field:

$$\bar{\psi}\not{p} = im\bar{\psi}. \tag{5.65}$$

We wrote this equation down for an arbitrary field ψ, because now that we found out the necessary condition with the help of the $\not{p}$-eigenstates, we can now again forget about them and consider general Dirac spinors.

However, knowing that a field ψ obtains the condition is not yet enough for being a physical relevant field. A second necessary condition is the correct normalization. We must find out which fields have a residuum equal to one at the pole, and it will be those fields which stand for the particles (and antiparticles).

So let's see what the residuum of the propagator of $\psi_>$ is:

$$\begin{aligned} \bar{G}(p) &= -i\frac{\not{p} + im}{\omega^2 - E^2(\mathbf{p})} \\ \hookrightarrow \bar{G}(p) &= \frac{2m}{\omega^2 - E^2(\mathbf{p})} \\ &= \frac{m}{E}\left(\frac{1}{\omega - E(\mathbf{p})} - \frac{1}{\omega + E(\mathbf{p})}\right) \end{aligned} \tag{5.66}$$

So we have two poles, with residua $\frac{m}{E}$ for $\omega = E$ and $-\frac{m}{E}$ for $\omega = -E$. This gives us two important informations: First, the existence of two poles tells us that again we encounter particles and antiparticles. We can "split up" our field into a positive and negative frequency part, each describing *one* particle. We could write this down in a equation like

$$\psi(\omega, \mathbf{p}) = \psi_a(\omega, \mathbf{p})\Theta(\omega) + \psi_b(\omega, \mathbf{p})\Theta(-\omega). \tag{5.67}$$

In the next step we identify the positive frequency part with a particle and the negative frequency part with the antiparticle. For writing down the physical relevant fields of these particles, we extract the second information of (5.66): The fields a and b^* that describe the particles, should be $\sqrt{\frac{E}{m}}$ times the ψ-fields:

$$\begin{aligned} a(\omega, \mathbf{p}) &= \sqrt{\frac{E}{m}}\psi(\omega, \mathbf{p}) \quad for \quad \omega \geq 0, \\ b^*(-\omega, -\mathbf{p}) &= \sqrt{\frac{E}{m}}\psi(\omega, \mathbf{p}) \quad for \quad \omega < 0 \end{aligned} \tag{5.68}$$

The propagators of the fields a, b will have a residuum $= 1$, so a and b are properly normalized.

Finally we can write down the decomposition of the ψ field:

$$\psi(\omega, \mathbf{p}) = \sqrt{\frac{m}{E}}\left(a(\omega, \mathbf{p})\Theta(\omega) + b^*(-\omega, -\mathbf{p})\Theta(-\omega)\right). \tag{5.69}$$

What we are of course always interested in, is not just the propagator and the reduced matrix element $\mathcal{M}$, but in the cross-section $d\sigma$ and/or the decay width $d\Gamma$.

$$\begin{aligned} d\sigma &= d\phi_N I_{scatter}|M|^2, \\ d\Gamma &= d\phi_N I_{decay}|M|^2, \end{aligned} \tag{5.70}$$

As everything else are just intermediate results (and not measurable quantities), we have some freedom to distribute normalization factors between the phase space $d\phi_N$ and the matrix element M. We use here the same phase space factor $d\phi_N$ and the same initial factor I for fermions and bosons. Comparing eqs. (4.193) a factor $1/\sqrt{2E}$ is absorbed in $d\phi_N$ and I, whereas the remaining factor $\sqrt{2m}$ needs to be incorporated into the computation of M, as explained later.

For the calculation of $d\sigma$ and $d\Gamma$ we have then exactly the same rules as for scalars, plus one additional rule, the on-shell condition for all incoming/outgoing fermions:

$$\not{p} \to im\mathbf{1}. \tag{5.71}$$

5.3 Solutions of free Dirac equation

So far we only discussed the kinematics of the scattering process. We saw, that all fermions have to obey the on-shell condition, which is (in this case!) absolutely identical to the free Dirac equation:

$$\not{p}\psi = im\psi. \tag{5.72}$$

The identity of both equations in the free theory should not hide that the residuum condition, which is dictated by the pole structure, is the more general one. In an interacting theory, where we have to deal with wave function renormalization factors Z_ψ, it would look like

$$\begin{aligned} Z_\psi \not{p}\psi &= im\psi \\ \Rightarrow \not{p}\psi &= i\frac{m}{Z_\psi}\psi. \end{aligned} \tag{5.73}$$

The quantity $\frac{m}{Z_\psi}$ is called the renormalized mass.

What we have also done is that we found out that the correct normalization factor is $\frac{m}{E}$. But we did not yet say a word about how we introduce the spin of a particle, but this is of course absolutely necessary, because quantum numbers like the spin specify our incoming and outgoing states, and without them we can't compute matrix elements. Furthermore, since we have two Dirac spinors with four components, we have again two many degrees of freedom, because each of the four component Dirac spinors a and b should only describe two spin degrees of freedom.

5.3.1 Basis spinors in rest frame

To find out how we have to define a and b in such a way, that they describe "spin up" or "spin down", we have a look at the

- Rest frame

  In the rest frame we of course have $\mathbf{p} = 0$. We can generalize the setting later by a Lorentz boost.

  As only the zero component of a (and b) are different from zero, the mass-shell condition for fermions simplifies to

  $$p_0 \gamma^0 \psi = im\psi. \tag{5.74}$$

  Herein, p_0 is given by $p_0 = -\omega = -E$. Multiplying this equation with γ^0 and using $(\gamma_0)^2 = -\mathbf{1}$ we yield

  $$\begin{aligned} E\psi &= im\gamma^0\psi \\ \Leftrightarrow \left(E\mathbf{1} - \begin{pmatrix} 0 m\mathbf{1} & \\ m\mathbf{1} & 0 \end{pmatrix}\right)\psi & \qquad\qquad = 0. \end{aligned} \tag{5.75}$$

  Going into the basis of mass eigenstates (convenient for rest frame), and remembering the equation

  $$\begin{pmatrix} 0 & m\mathbf{1} \\ m\mathbf{1} & 0 \end{pmatrix} \psi_\pm = \pm m\psi_\pm \tag{5.76}$$

  we get

  $$\begin{aligned} (E - m)\psi_+ &= 0 \\ (E + m)\psi_- &= 0. \end{aligned} \tag{5.77}$$

  So obviously we have $\omega > 0$ for ψ_+ - and this was also a property for the field a (or, to be more precise: $a(p) \neq 0$ only for $\omega > 0$). On the opposite site, we have $\omega < 0$ for ψ_- and a field $\bar{b}$ which was non-zero at the negative frequency part. So we conclude:

  $a(p)$ has only ψ_+ components and describes the electron ($p^0 > 0$),

  $\bar{b}(-p)$ has only ψ_- components and describes the positron, ($-p^0 > 0$).

  Remember that the ψ_+ field obeys

  $$\left(\begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix} - \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix}\right)\psi_+ = 0, \tag{5.78}$$

  because it is an eigenstate to both matrices to eigenvalue 1. From this it follows

  $$\begin{pmatrix} \psi_L - \psi_R \\ \psi_R - \psi_L \end{pmatrix} = 0\ ,\ \ \psi_L = \psi_R. \tag{5.79}$$

Explicitly we can write for the four components

$$\begin{pmatrix} (\psi_+)_1 - (\psi_+)_3 \\ (\psi_+)_2 - (\psi_+)_4 \\ -(\psi_+)_1 + (\psi_+)_3 \\ -(\psi_+)_2 + (\psi_+)_4 \end{pmatrix} = 0. \tag{5.80}$$

So we choose $(\psi_+)_1 = (\psi_+)_3$, $(\psi_+)_2 = (\psi_+)_4$ and thus loose two degrees of freedom (just as we wanted!). The a field, which has only ψ_+ components, must therefore have identical entries in zero and second component, and also in first and third component:

$$a(p) = \begin{pmatrix} a_\uparrow \\ a_\downarrow \\ a_\uparrow \\ a_\downarrow \end{pmatrix} = \frac{1}{\sqrt{2m}}\big(a_1(p)u_1(p) + a_2(p)u_2(p)\big). \tag{5.81}$$

The $a_1(p)$ and $a_2(p)$ are scalar prefactors which specify a give field $a(p)$ while the u_1 and u_2 are fixed basis spinors. But how exactly do we have to choose them? In the rest frame we normalize the u-vectors

$$u_1 = \frac{\sqrt{2m}}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, u_2 = \frac{\sqrt{2m}}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}. \tag{5.82}$$

Therefore the normalization condition in the rest frame is

$$u_1^\dagger u_1 = u_2^\dagger u_2 = 2m. \tag{5.83}$$

In this way, we ensure that the propagator of the a fields in eq. (5.69) as well as the a_i fields have residua 1.

As the spin-operator in the rest frame is defined by

$$\vec{S} = \frac{1}{2}\begin{pmatrix} \vec{\tau} & 0 \\ 0 & \vec{\tau} \end{pmatrix} \tag{5.84}$$

we identify u_1 with spin $s_z = +\frac{1}{2}$ and u_2 with spin $s_z = -\frac{1}{2}$.

Similarly as we did it here for a, the relation

$$\begin{pmatrix} \mathbf{1} & \mathbf{1} \\ \mathbf{1} & \mathbf{1} \end{pmatrix}\psi_- = 0, \tag{5.85}$$

leads to the following decomposition of the field $\bar{b}$:

$$b^*(-p) = \frac{1}{\sqrt{2m}}\big(b_1^*(-p)v_1(-p) + b_2^*(-p)v_2(-p)\big). \tag{5.86}$$

If you would have expected a $\bar{v}$, think again of the decomposition of ψ: ψ is a column spinor and so v should be. The basis spinors are here:

$$v_1 = \frac{\sqrt{2m}}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix}, v_2 = \frac{\sqrt{2m}}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1 \end{pmatrix} \tag{5.87}$$

We identify v_1 describing the spin up state and v_2 describing the spin down state.

5.3.2 General decomposition of Dirac Spinor

Summary

The field a describes the two spin states of the electron in the basis $u_s, s = 1, 2$, the field $\bar{b}$ describes the two spin states of the positron in basis v_s.

- Decomposition of Dirac Spinor

  Lets us now write down the final decomposition of the Dirac Spinor (cf. eq. (5.69)):

$$\psi(p) = \frac{1}{\sqrt{2E(\mathbf{p})}} \left(a_s(p) u_s(p) \Theta(\omega) + b_s^*(-p) v_s(-p) \Theta(-\omega) \right) \tag{5.88}$$

  The index s is a summation index.

  This equation is valid for arbitrary $\mathbf{p}$. Furthermore, the a_s and b_s^* fields have the correct normalization, because the u_s and v_s contain a factor $\sqrt{2m}$, and thus the overall normalization is $\sqrt{\frac{E}{m}}$ as demanded in (5.69).

  The step to the operator formalism can now easily be done. We link

  - $a_s(p)$ to the annihilation operator $\hat{a}_s(p)$ for electrons.
  - $b_s^*(-p)$ to the creation operator $\hat{b}_s^\dagger(-p)$. $\hat{b}_s^\dagger(p)$ is the creation operator for positrons.

  As a and b are normalized correctly, they obey the standard anti-commutations relations at equal time:

$$\{\hat{a}_s(\mathbf{p}), \hat{a}_t^\dagger(\mathbf{q})\} = \{\hat{b}_s(\mathbf{p}), \hat{b}_t^\dagger(\mathbf{q})\} = (2\pi)^3 \delta^3(\mathbf{p} - \mathbf{q}) \delta_{st} \tag{5.89}$$

  Of course we still have to respect the on shell condition for the spinors:

$$\begin{aligned} \not{p} u_s(p) &= im u_s(p), \\ \not{p} v_s(-p) &= im v_s(-p) \quad \text{or} \quad \not{p} v_s(p) = -im v_s(p) \end{aligned} \tag{5.90}$$

  Furthermore we have

$$\Theta(p^0) u_s(p) = u_s(p), \quad \Theta(p^0) v_s(p) = v_s(p). \tag{5.91}$$

For u_s and v_s we have positive energies:

$$p^0 = \omega = E = \sqrt{\mathbf{p}^2 + m^2} \tag{5.92}$$

The normalization in the rest frame is

$$u_s^\dagger u_s = v_s^\dagger v_s = 2m. \tag{5.93}$$

In the last equation, note that we do not mean a summation over s, but that the equation is valid for $s = 1, 2$.

Finally, we write down the decomposition of $\bar{\psi}$

$$\bar{\Psi}(p) = \frac{1}{\sqrt{2E(\mathbf{p})}} \left(a_s^*(p)\bar{u}_s(p)\Theta(\omega) + b_s(-p)\bar{v}_s(-p)\Theta(-\omega)\right) \tag{5.94}$$

where $\bar{u}_s(p) = u_s^\dagger \gamma^0$ and $\bar{v}_s(p) = v_s^\dagger \gamma^0$.

5.3.3 Reduced matrix element and scattering

5.3.4 Basis spinors for arbitrary momentum