Theoretical Physics V
ADVANCED QUANTUM MECHANICS

Lecture Script SS 2021
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Chapter 1

Second quantization

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

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

We start with some preliminary remarks.

1.1 Identical particles and many particle states

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

- Hamilton-Operator: \( \hat{H} = \hat{H}(r_1\sigma_1, r_2\sigma_2, \ldots, r_N\sigma_N) \) abbreviated as: \( \hat{H}(1, 2, \ldots, N) \)
- Wave function: \( \psi = \psi(r_1\sigma_1, r_2\sigma_2, \ldots, r_N\sigma_N) \) abbreviated as: \( \psi(1, 2, \ldots, N) \).

Definition: permutation operator \( P_{ij} \):

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

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

\[
\forall \ ij: \quad P_{ij} \hat{H} = \hat{H} P_{ij}
\]

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

\[
\hat{H}(r_1, r_2, \ldots, r_N) = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \sum_{i=1}^{N} U(r_i) + \sum_{\{i,j\}} W(|r_i - r_j|)
\]

\[
\Rightarrow \quad \hat{H}(\ldots, r_i, \ldots, r_j, \ldots) = \hat{H}(\ldots, r_j, \ldots, r_i, \ldots)
\]

\( S_N := \text{Group of all permutations of } N \text{ objects. } \#S_N = N! \).
Each \( P \in S_N \) can be represented as a product of transpositions \( P_{ij} \). \( P \) is said to be even (odd) when the number of transpositions \( P_{ij} \) composing it is even (odd).

Properties:

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

\[
\implies P\psi(1, \cdots, N) \text{ also eigenfunction with eigenvalue } E
\]

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

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

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

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

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

\[
\forall ij, \quad P_{ij}\psi_S = +\psi_S; \quad P_{ij}\psi_A = -\psi_A
\]

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

<table>
<thead>
<tr>
<th>Bosons</th>
<th>Fermions</th>
</tr>
</thead>
<tbody>
<tr>
<td>totally symmetric</td>
<td>totally antisymmetric</td>
</tr>
<tr>
<td>integer spin</td>
<td>half-integer spin</td>
</tr>
</tbody>
</table>

Remarks:

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

\[
\psi(t) = e^{-i\hat{H}t/\hbar}\psi(0) \implies P\psi(t) = e^{-i\hat{H}t/\hbar}P\psi(0)
\]

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

\[
\begin{align*}
P\psi_S &= \psi_S \\
P\psi_A &= (-1)^{\text{sgn}(P)}\psi_A \\
\text{with} (-1)^{\text{sgn}(P)} &= \begin{cases} 
+1 & \text{for even permutations } P \\
-1 & \text{for odd permutations } P
\end{cases}
\end{align*}
\]

Thus, the states \( \psi_S \) and \( \psi_A \) form the basis of two one-dimensional representations of the permutation group \( S_N \).

Example:

\[
N = 2 : \quad \psi_S(1, 2) = \psi(1, 2) + \psi(2, 1) \\
\psi_A(1, 2) = \psi(1, 2) - \psi(2, 1)
\]
\[ N = 3 : \quad \psi_S(1, 2, 3) = \psi(1, 2, 3) + \psi(2, 1, 3) + \psi(1, 3, 2) + \psi(3, 2, 1) + \psi(3, 1, 2) + \psi(2, 3, 1) \]
\[ \psi_A(1, 2, 3) = \psi(1, 2, 3) - \psi(2, 1, 3) - \psi(1, 3, 2) - \psi(3, 2, 1) + \psi(3, 1, 2) + \psi(2, 3, 1) \]

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

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

### 1.2 Totally symmetric and anti-symmetric states

Now let \( \{ |i\rangle \} = \{ |1\rangle, |2\rangle, \ldots \} \) be a complete orthonormal system basis of one-particle states. We denote a one-particle state of particle \( \alpha \) as \( |i\rangle_\alpha \).

\( \sim \) basis states of the \( N \)-particle system:

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

where \( |i_\alpha\rangle_\alpha \) means that particle \( \alpha \) is in state \( i_\alpha \).

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

The symmetrized and antisymmetrized basis states (i.e. the basis of \( \mathcal{H}_S^N \) and \( \mathcal{H}_A^N \)) are defined by

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

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

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

\( \sim \) The normalized Boson basis functions are

\[
\frac{S_+}{\sqrt{n_1!n_2! \cdots}} |i_1, \cdots, i_N\rangle = \frac{1}{\sqrt{N!n_1!n_2! \cdots}} \sum_{P \in S_N} P |i_1, \cdots, i_N\rangle
\]

\( [ \text{n.b. It is } S_- |i_1, \cdots, i_N\rangle = 0 \text{ if in } |i_1, \cdots, i_N\rangle \text{ one-particle states occur more than once.} ] \)
1.3 Bosons

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

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

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

\[
N = \sum_{i=1}^{\infty} n_i
\]

Apart from this constraint the \(n_i\) can take any of the values 0, 1, 2,.... These states form a complete orthonormal system of completely symmetric \(N\)-particle states. By linear superposition, one can construct from these any desired symmetric \(N\)-particle state.

We now combine the states for \(N = 0, 1, 2, \ldots\) and obtain a complete orthonormal system of states for arbitrary particle number, which form the basis of the Fock-space:

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

\(\mathcal{H}^0 = \{|0\rangle\}\) or vacuum (zero particles)

Complete orthonormal system: \(\{|n_1, n_2, \cdots\rangle\}_{n_i=0,1,\ldots}\)

- Orthogonality relation \(\langle n_1, n_2, \cdots | n'_1, n'_2, \cdots \rangle = \delta_{n_1,n'_1} \delta_{n_2,n'_2} \cdots\)
- Completeness relation: \(\sum_{n_1,n_2,\cdots} |n_1, n_2, \cdots \rangle \langle n_1, n_2, \cdots | = 1\)

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

\[
\hat{a}_i^\dagger |\cdots, n_i, \cdots\rangle = \sqrt{n_i + 1} |\cdots, n_i + 1, \cdots\rangle
\]

\[
\hat{a}_i |\cdots, n_i, \cdots\rangle = \sqrt{n_i} |\cdots, n_i - 1, \cdots\rangle
\]

(\(\ast\ast\))

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

\[
(\ast\ast) \implies \langle n_i | \hat{a}_i = \sqrt{n_i + 1} \langle n_i + 1 | = \langle n_i | \hat{a}_i \rangle \langle n_i | n'_i \rangle = \sqrt{n_i + 1} \delta_{n_i+1,n'_i}
\]

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

\[
[\hat{a}_i, \hat{a}_j] = 0; \quad [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0; \quad [\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}
\]
\[
\left( \hat{a}_i^\dagger \hat{a}_i | n_i \rangle = \hat{a}_i^\dagger \sqrt{n_i} | n_i - 1 \rangle = n_i | n_i \rangle ; \quad \hat{a}_i \hat{a}_i^\dagger | n_i \rangle = \sqrt{n_i + 1} \hat{a}_i | n_i + 1 \rangle = (n_i + 1) | n_i \rangle \right)
\]

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

\[
\hat{a}_i^\dagger | 0 \rangle = | 0, \cdots, n_i = 1, \cdots \rangle
\]

\[
\hat{a}_i^\dagger \hat{a}_j^\dagger | 0 \rangle = | 0, \cdots, n_i = 1, \cdots, n_j = 1, \cdots \rangle \quad i \neq j
\]

Generally:

\[
| n_1, n_2, \cdots \rangle = \prod_{i=1}^{\infty} (\hat{a}_i^\dagger)^{n_i} / \sqrt{n_i} ! | 0 \rangle
\]

Definition:

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

\[
\hat{n}_i | \cdots, n_i, \cdots \rangle = n_i | \cdots, n_i, \cdots \rangle
\]

\[ \hat{N} := \sum_i \hat{n}_i \] is the operator for the total number of particles

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

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

\[
T = \sum_{\alpha=1}^{N} t_\alpha
\]

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

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

Proof:

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

\[
\begin{align*}
n_j &= 1, \text{ wlog} \quad k_1 = j \quad \quad | i \rangle_1 \langle j |_1 k_1, k_2, \cdots, k_N \rangle &= | i, k_2, \cdots, k_N \rangle \\
n_j &= 2, \text{ wlog} \quad k_1 = k_2 = j \quad \quad | i \rangle_1 \langle j |_1 k_1, k_2, \cdots, k_N \rangle &= | i, k_2, k_3, \cdots, k_N \rangle \\
& \quad \quad | i \rangle_2 \langle j |_2 k_1, k_2, \cdots, k_N \rangle &= | k_1, i, k_3, \cdots, k_N \rangle
\end{align*}
\]

etc.

This means \( \hat{A}_{ij} \) decreases \( n_j \) by 1 and increases \( n_i \) by 1, in \( n_j \) summands.
CHAPTER 1. SECOND QUANTIZATION

\[ \sim \hat{A}_{ij} |n_1, n_2, \ldots \rangle = \hat{A}_{ij} \frac{S_+}{\sqrt{n_1!n_2!\ldots}} |k_1, k_2, \ldots, k_N\rangle \]
\[ = \frac{S_+}{\sqrt{n_1!n_2!\ldots}} \hat{A}_{ij} |k_1, k_2, \ldots, k_N\rangle \]
\[ = \frac{S_+}{\sqrt{n_1!n_2!\ldots}} (|i, k_2, \ldots, k_N\rangle + |k_1, i, k_3, \ldots\rangle + \cdots + \cdots + |k_{j-1}, i, k_{j+1}, \ldots\rangle) \]
\[ = n_j \cdot \frac{S_+}{\sqrt{\cdots (n_i + 1)!/(n_i + 1) \cdots (n_j - 1)!n_j \cdots}} |i, k_2, \ldots, k_N\rangle \]
\[ = n_j \cdot \frac{n_i + 1}{n_j} |\cdots, n_i + 1, \ldots, n_j - 1, \ldots\rangle \]
\[ = \sqrt{n_j (n_i + 1) |\cdots, n_i + 1, \ldots, n_j - 1, \ldots\rangle} \]
\[ = \hat{a}_i^\dagger \hat{a}_j |\cdots, n_i, \ldots, n_j, \ldots\rangle \]

For the special case that \( t \) is diagonal: \( t_{ij} = \varepsilon_i \delta_{ij} \)
\[ \sim H_0 = \sum_i \varepsilon_i \hat{a}_i^\dagger \hat{a}_i \]

Analogously, one shows for the two-particle operators

\[ F = \frac{1}{2} \sum_{\alpha \neq \beta} f^{(2)}(r_\alpha, r_\beta) \]

that they can be written as

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

with

\[ f_{ijkm} = \langle i, j \mid f^{(2)} \mid k, m \rangle = \int dr \int dr' \phi_i^*(r) \phi_j^*(r) f^{(2)}(r, r') \phi_k(r') \phi_m(r') \]

Proof:
\[ (+) \text{ means in the } N\text{-particle space} \]
\[ F = \frac{1}{2} \sum_{\alpha \neq \beta} \sum_{i,j,k,m} \langle i, j \mid f^{(2)} \mid k, m \rangle \langle i \mid \alpha \rangle \langle j \mid \beta \rangle \langle k \mid \alpha \rangle \langle m \mid \beta \rangle \]

Now it is

\[ \sum_{\alpha \neq \beta} \langle i \mid \alpha \rangle \langle j \mid \beta \rangle \langle k \mid \alpha \rangle \langle m \mid \beta \rangle = \sum_{\alpha \neq \beta} \langle i \mid \alpha \rangle \langle k \mid \alpha \rangle \langle j \mid \beta \rangle \langle m \mid \beta \rangle - \langle k \mid j \rangle \delta_{kj} \sum_{\alpha} \langle i \mid \alpha \rangle \langle m \mid \alpha \rangle \]
\[ = \hat{a}_i^\dagger \hat{a}_k \hat{a}_j^\dagger \hat{a}_m - \hat{a}_i^\dagger \left[ \hat{a}_k, \hat{a}_j^\dagger \right] \hat{a}_m \]
\[ = \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k \]

\[ \blacksquare \]
1.4 Fermions

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

$$S_- |i_1 i_2 \cdots i_N\rangle = \frac{1}{\sqrt{N!}} \left| \begin{array}{cccc} |i_1\rangle & |i_1\rangle & \cdots & |i_1\rangle \\ \vdots & \vdots & \ddots & \vdots \\ |i_N\rangle & |i_N\rangle & \cdots & |i_N\rangle \end{array} \right| \quad \text{(Slater determinant)}$$

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

Here, too, we shall characterize the states by specifying their occupation numbers, which now can take the values 0 and 1. The state with $n_1$ particles in state 1, $n_2$ particles in state 2, etc is $\{|n_1 n_2 \cdots \rangle\}$, which forms the basis of the Fock space. $\mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_N \oplus \cdots$. Scalar product and completeness relation as for Bosons.

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

**Definition:**

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

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

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

and therefore also

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

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

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

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

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

The adjoined relation is

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

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

With this we compute

$$\hat{a}_i |\cdots, n_i', \cdots\rangle = \sum_{n_i} |n_i\rangle \langle n_i | \hat{a}_i |n_i'\rangle$$

$$= \begin{cases} 0 & \text{for } n_i' = 0 \\ (-1)^{\sum_{j<i} n_j} \delta_{n_i, 0} & \text{for } n_i' = 1 \end{cases}$$

$$= \begin{cases} 0 & \text{for } n_i' = 0 \\ (-1)^{\sum_{j<i} n_j} |\cdots, n_i' - 1, \cdots\rangle & \text{for } n_i' = 1 \end{cases}$$
Therefore
\[ \hat{a}_i | \cdots, n_i, \cdots \rangle = n_i (-1)^{\sum_{j<i} n_j} | \cdots, n_i - 1, \cdots \rangle \]

It follows
\[ \hat{a}_i \hat{a}_i^\dagger \cdots, n_i, \cdots \rangle = (1 - n_i) (-1)^{\sum_{j<i} n_j} (n_i + 1) | \cdots, n_i, \cdots \rangle = (1 - n_i) | \cdots, n_i, \cdots \rangle \]
\[ \hat{a}_i^\dagger \hat{a}_i \cdots, n_i, \cdots \rangle = n_i (-1)^{\sum_{j<i} n_j} (1 - n_i + 1) | \cdots, n_i, \cdots \rangle = n_i | \cdots, n_i, \cdots \rangle \]

\[ \hat{a}_i^\dagger \hat{a}_i \]

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

One shows the relation \( \sum_{\alpha} | i \rangle_{\alpha} \langle j |_{\alpha} = \hat{a}_i^\dagger \hat{a}_j \) as follows: (wlog \( i_1 < i_2 < \cdots < i_N \))
\[ \sum_{\alpha} | i \rangle_{\alpha} \langle j |_{\alpha} S_- | i_1, i_2, \cdots, i_N \rangle = S_- \left( \sum_{\alpha} | i \rangle_{\alpha} \langle j |_{\alpha} \right) | i_1, i_2, \cdots, i_N \rangle = n_j (1 - n_i) S_- | i_1, i_2, \cdots, i_N \rangle | j \rightarrow i \rangle \]

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

Thus one has for one-particle and two-particle operators – for fermions and for bosons
\[ T = \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j \]
\[ F = \frac{1}{2} \sum_{ijkm} \langle i, j | f^{(2)} | k, m \rangle \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k \]
e.g.
\[ \hat{H} = \sum_{ij} \left( \frac{h_{ij}}{E_{\text{kin}}} + \frac{U_{ij}}{E_{\text{pot}}} \right) \hat{a}_i^\dagger \hat{a}_j + \frac{1}{2} \sum_{ijkm} f_{ijkm} \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k \]
1.5 Field operators

Let \{\ket{i}\} and \{\ket{\xi}\} be two complete orthogonal bases of one-particle states. Then one has \(\ket{\xi} = \sum_i \ket{i} \bra{i} \ket{\xi}\).

\[
\Leftrightarrow \quad \hat{a}_\xi^\dagger = \sum_i \hat{a}_i^\dagger \bra{i} \hat{a}_\xi \kappa \quad \text{b.c.} \quad \hat{a}_\xi \left( \hat{a}_\xi^\dagger \right) \quad \text{creates a particle in} \quad \ket{i} \left( \ket{\xi} \right)
\]

\[
\hat{a}_\xi = \sum_i \hat{a}_i \bra{\xi} \hat{\kappa} \quad \text{follows from the adjugated relation}
\]

Important special case: Eigenstates of the position operator \(\ket{r}\):

\[
\bra{r} \hat{a}_i \ket{r} = \phi_i(r) \quad \text{one-particle wave function in position representation}
\]

Definition: Field operators

\[
\hat{\psi}(r) = \sum_i \phi_i(r) \hat{a}_i \quad \hat{\psi}^\dagger(r) = \sum_i \phi_i^*(r) \hat{a}_i^\dagger
\]

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

\[
\left[ \hat{\psi}(r), \hat{\psi}(r') \right]_\pm = 0
\]

\[
\left[ \hat{\psi}^\dagger(r), \hat{\psi}^\dagger(r') \right]_\pm = 0
\]

\[
\left[ \hat{\psi}(r), \hat{\psi}^\dagger(r') \right]_\pm = \sum_{i,j} \phi_i(r) \phi_j^*(r') \left[ \hat{a}_i^\dagger, \hat{a}_j^\dagger \right]_\pm = \delta(r - r')
\]

where

\[
\left[ \bullet, \bullet \right]_+ = \left[ \bullet, \bullet \right] \quad \text{commutator}
\]

\[
\left[ \bullet, \bullet \right]_- = \{ \bullet, \bullet \} \quad \text{anti-commutator}
\]

Operator can be expressed via field operators:

Kinetic energy:

\[
\sum_{i,j} \hat{a}_i^\dagger T_{ij} \hat{a}_j = \sum_{i,j} \int dr \ \hat{a}_i^\dagger \phi_i^*(r) \left( -\frac{\hbar^2}{2m} \Delta \right) \phi_j(r) \hat{a}_j \quad \psi_{(r \to \infty)} \rightarrow 0 \int dr \ \nabla \hat{\psi}^\dagger(r) \cdot \nabla \hat{\psi}(r)
\]

One-particle potential:

\[
\sum_{i,j} \hat{a}_i^\dagger U_{ij} \hat{a}_j = \sum_{i,j} \int dr \ \hat{a}_i^\dagger \phi_i^*(r) U(r) \phi_j(r) \hat{a}_j \quad = \int dr \ U(r) \hat{\psi}^\dagger(r) \hat{\psi}(r)
\]
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Two-particle interaction:

\[
\frac{1}{2} \sum_{i,j,k,m} \int \! \! \! dr \, dr' \, \phi_i(r) \phi_j(r') \, V(r, r') \, \phi_k(r) \phi_m(r') \, \hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_m \hat{a}_k \\
= \frac{1}{2} \int \! \! \! dr \, dr' \, V(r, r') \, \hat{\psi}^\dagger(r) \, \hat{\psi}^\dagger(r') \, \hat{\psi}(r') \, \hat{\psi}(r)
\]

Hamiltonian:

\[
\hat{H} = \int \! \! \! dr \, \left( \frac{\hbar^2}{2m} \nabla \hat{\psi}^\dagger \nabla \hat{\psi} + U \hat{\psi}^\dagger \hat{\psi} \right) \\
+ \frac{1}{2} \int \! \! \! dr \, dr' \, \hat{\psi}^\dagger(r) \, \hat{\psi}^\dagger(r') \, V(r, r') \, \hat{\psi}(r') \, \hat{\psi}(r)
\]

Particle density:

\[
n(r) = \sum_{\alpha} \delta(r - r_\alpha) \\
= \sum_{\alpha} \sum_{i,j} |i\rangle_\alpha \langle j| \langle \delta(r - r_\alpha) \rangle \langle j|_\alpha \langle j|_\alpha \\
= \int \! \! \! dr' \, \phi_i^\dagger(r') \delta(r - r') \phi_j(r) \\
= \sum_{i,j} \sum_{\alpha} |i\rangle_\alpha \langle j|_\alpha \phi_i^\dagger(r) \phi_j(r) \\
\Rightarrow n(r) = \hat{\psi}^\dagger(r) \hat{\psi}(r)
\]

Particle number operator:

\[
\hat{N} = \int \! \! \! dr \, \hat{n}(r) = \int \! \! \! dr \, \hat{\psi}^\dagger(r) \hat{\psi}(r)
\]

\[\sim \text{ e.g. current density operator } \hat{j}(r) = \frac{\hbar}{2m} \left\{ \hat{\psi}^\dagger(r) \left( \nabla \hat{\psi}(r) \right) - \left( \nabla \hat{\psi}^\dagger(r) \right) \hat{\psi}(r) \right\} \]

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

\[
\hbar \frac{\partial}{\partial t} \hat{\psi}(r, t) = \left( -\frac{\hbar^2}{2m} \Delta + U(r) \right) \hat{\psi}(r, t) + \int \! \! \! dr' \, \hat{\psi}^\dagger(r', t) \, V(r, r') \, \hat{\psi}(r', t) \, \hat{\psi}(r, t)
\]

Proof (see exercise): using Heisenberg equation of motion \( \hbar \frac{\partial}{\partial t} \hat{\psi}(r, t) = -\left[ \hat{H}, \hat{\psi}(r, t) \right] \)

analogous for \( \hat{\psi}^\dagger(r, t) \) (yields a minus sign on the right hand side)

From this follows the equation of motion of the density operator:

\[
\frac{\partial}{\partial t} \hat{n}(r, t) = \hat{\psi}^\dagger \hat{\psi} + \hat{\psi} \hat{\psi}^\dagger = \frac{\hbar}{i} \left( -\frac{\hbar^2}{2m} \Delta \hat{\psi} \right) - \left( \Delta \hat{\psi} \right) \hat{\psi}
\]

\[\text{i.e.} \quad \frac{\partial}{\partial t} \hat{n}(r, t) = -\nabla \hat{j}(r, t)\]
1.6 Momentum representation

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

\[
\sim \int dr \, \phi_k^*(r) \phi_{k'}(r) = \delta_{kk'} \quad \text{(orthogonality)}
\]

Representation of the Hamiltonian in second quantization:

The matrix elements read

\[
E_{\text{kin}}: \int dr \, \phi_{k'}^*(r) (-\Delta) \phi_k(r) = k^2 \delta_{kk'}
\]

\[
E_{\text{pot}}: \int dr \, \phi_{k'}^*(r) U(r) \phi_k(r) = \frac{1}{V} \sum \phi_{k'}^*(r) U_{k',-k}(r)
\]

\( E_{\text{int}}: \) Consider two-particle potentials \( V(r, r') \) which only depend on the distance \( r - r' \)

Define: \( V_q := \int dr \, e^{-i q \cdot r} V(r) \quad (~V(r) = \frac{1}{V} \sum_q V_q e^{i q \cdot r}) \)

The two-particle matrix element then reads

\[
\langle p', k' | V(r - r') | p, k \rangle = \frac{1}{V^2} \int dr \, dr' \, e^{-i p' \cdot r} e^{-i k' \cdot r'} V(r - r') e^{i k \cdot r'} e^{i p \cdot r}
\]

\[
= \frac{1}{V^3} \sum_q V_q \int dr \, dr' \, e^{-i p' \cdot r} e^{-i k' \cdot r'} + i q \cdot (r - r') + i k \cdot r' + i p \cdot r
\]

\[
= \frac{1}{V^3} \sum_q V_q \delta_{q = p' - k'} \delta_{q = p} \delta_{q = 0} \delta_{k' = k}
\]

Combining the above results leads to:

\[
\hat{H} = \sum_k \frac{(\hbar k)^2}{2m} \hat{a}_k^\dagger \hat{a}_k + \frac{1}{V} \sum_{k,k'} U_{k'-k} \hat{a}_{k'}^\dagger \hat{a}_k + \frac{1}{2V} \sum_{q,p,k} V_q \hat{a}_{p+q}^\dagger \hat{a}_{k-q}^\dagger \hat{a}_k \hat{a}_p
\]

\( \hat{a}_k^\dagger (\hat{a}_k) \) creates (annihilates) a particle with wave number \( k \), where the following commutation relations apply:

\[
[\hat{a}_k, \hat{a}_{k'}] = 0, \quad [\hat{a}_k^\dagger, \hat{a}_{k'}^\dagger] = 0, \quad [\hat{a}_k, \hat{a}_{k'}^\dagger] = \delta_{kk'}
\]

Visualization of the interaction term:

\[\text{2nd order perturbation theory: (double dispersion of two particles)}\]
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Fourier transformation of the density:

\[ \hat{n}_q = \int dr \hat{n}(r)e^{-iq\cdot r} = \int dr \hat{\psi}^\dagger(r)\hat{\psi}(r)e^{-iq\cdot r} \]

Using the expressions \( \hat{\psi}(r) = \frac{1}{\sqrt{V}} \sum_p e^{ip\cdot r}\hat{a}_p \) and \( \hat{\psi}^\dagger(r) = \frac{1}{\sqrt{V}} \sum_p e^{-ip\cdot r}\hat{a}_p^\dagger \) gives

\[ \hat{n}_q = \sum_p \hat{a}_p^\dagger\hat{a}_{p+q} \]

Consideration of spin:

\[ \hat{\psi}(r) \rightarrow \hat{\psi}_\sigma(r) \]
\[ \hat{a}_p \rightarrow \hat{a}_{p,\sigma} \]

\[ \rightarrow \quad n(r) = \sum_\sigma \hat{\psi}_\sigma^\dagger(r)\hat{\psi}_\sigma(r) \]
\[ n_q = \sum_{p,\sigma} \hat{a}_{p,\sigma}^\dagger\hat{a}_{p+q,\sigma} \]

In the case of spin-\( \frac{1}{2} \) fermions \( \sigma = \pm \frac{1}{2} \).

Spin density operator:

\[ \hat{S}(r) = \sum_i \delta(r - r')\hat{S}_i = \frac{\hbar}{2} \sum_{\sigma,\sigma'} \hat{\psi}_\sigma^\dagger(r)\sigma_{\sigma\sigma'}\hat{\psi}_{\sigma'}(r), \]

where \( \sigma_{\sigma\sigma'} \) are the matrix elements of the Pauli matrices. Otherwise everything remains the same with spin index \( \sigma \).

1.7 Summary of second quantization

The most important facts about second quantization are summarized in the Table 1.1. Some of the relations are identical for bosons and fermions: in those cases we use the generic notation \( \hat{a} \) for the annihilation operator. Otherwise we denote it \( \hat{b} \) for bosons and \( \hat{c} \) for fermions.

Let us end this chapter with a few practical tips concerning the creation-annihilation permutations (CAPs). In all applications of the second quantization, you run into expressions consisting of a long product of CAPs, stacked between two basis vectors of the Fock-space. In order to derive any useful result, you must be able to manipulate those products of CAPs, i.e. you must master the definition and commutation relations of the CAPs at an operational level. You can handle the following simple rules:

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

b) Try to reduce the number of operators by converting them to occupation number operators

\[ \hat{a}_i^\dagger\hat{a}_i \{n_k\} = n_i \{n_k\}. \]

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

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

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

\[ \langle \{n_k\} | \hat{c}_{i_1}^\dagger \hat{c}_{i_2}^\dagger \hat{c}_{i_3} \hat{c}_{i_4} | \{n_k\} \rangle \]

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

\[
i_1 = i_3, \quad i_2 = i_4, \quad i_1 \neq i_2,
\]

or

\[
i_1 = i_4, \quad i_2 = i_3, \quad i_1 \neq i_2.
\]

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

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

\[
\langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_2}^{\dagger} \hat{c}_{i_1} \hat{c}_{i_2} | \{n\} \rangle = -\langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_1} ^{\dagger} \hat{c}_{i_2} \hat{c}_{i_2} | \{n\} \rangle
\]

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

\[
\langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_2}^{\dagger} \hat{c}_{i_1} \hat{c}_{i_2} | \{n\} \rangle = -n_{i_2} \langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_1} | \{n\} \rangle = -n_{i_2} n_{i_1}.
\]

Treating the second possibility in the same way, we find

\[
\langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_2}^{\dagger} \hat{c}_{i_3} \hat{c}_{i_4} | \{n\} \rangle = -\langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_2}^{\dagger} \hat{c}_{i_1} \hat{c}_{i_2} | \{n\} \rangle = \langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_1} \hat{c}_{i_2}^{\dagger} \hat{c}_{i_2} | \{n\} \rangle
\]

where we permute (i) the third and the fourth terms, and (ii) the second and the third terms.

We now use the reduction rule twice:

\[
\langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_2}^{\dagger} \hat{c}_{i_3} \hat{c}_{i_4} | \{n\} \rangle = n_{i_2} \langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_1} | \{n\} \rangle = n_{i_1} n_{i_2}
\]

We finally obtain:

\[
\langle \{n\} | \hat{c}_{i_1}^{\dagger} \hat{c}_{i_2}^{\dagger} \hat{c}_{i_3} \hat{c}_{i_4} | \{n\} \rangle = -n_{i_1} n_{i_2} \delta_{i_1,i_3} \delta_{i_2,i_4} + n_{i_1} n_{i_2} \delta_{i_1,i_4} \delta_{i_2,i_3}.
\]
### CHAPTER 1. SECOND QUANTIZATION

#### Bosons

| Many-particle wave function | \( \Psi(|r_i\rangle, t) \) | fully symmetric | Fermions |
|-----------------------------|-----------------------------|-----------------|----------|
| Fock-space, where the basis states are labeled by the sets \( \{n_k\} \) of occupations numbers | non-negative integers | fully antisymmetric |
| Creation and annihilation operators | commute \( [\hat{b}_k, \hat{b}_k'] = 0 \) \( \{\hat{c}_k, \hat{c}_k'\} = 0 \) | anticommutate: \( [\hat{c}_k, \hat{c}_k'] = 0 \) \( \{\hat{c}_k, \hat{c}_k'\} = 0 \) |
| Occupation number operator | \( \hat{n}_k = \hat{a}_k^\dagger \hat{a}_k \) | \( \hat{N} = \sum_k \hat{n}_k = \sum_k \hat{a}_k^\dagger \hat{a}_k \) |
| total number of particles: | | |
| Hamiltonian with particle-particle interactions | \( \hat{H} = \sum_k \epsilon_k \hat{b}_k^\dagger \hat{b}_k + \frac{1}{2V} \sum_{k,k',q} V_{k,k'+q} \hat{b}_{k+q}^\dagger \hat{b}_{k'}^\dagger \hat{b}_{k'} \hat{b}_k \) | the same, with spins |
| Field operators: dynamics (without interactions): | \( \Psi(r) = \sum_k \hat{a}_k \phi_k(r) \) | Schrödinger equation for the wave function: \( i\hbar \partial_t \hat{\Psi}(r, t) = \left[-\frac{\hbar^2}{2m} \nabla^2 + V(r)\right] \hat{\Psi}(r, t) \) |
| Heisenberg equation: | | |

| Table 1.1: Summary of second quantization |
Chapter 2

Application of second quantization

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

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

$$|\phi_0\rangle = \prod_p \prod_\sigma \hat{c}_{p,\sigma}^\dagger \hat{c}_{p,\sigma} |0\rangle_{\sigma = \pm \frac{\hbar}{2}}$$

Expectation value of particle number operator in momentum space:

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

For $|q| > p_F$ one has

$$\hat{c}_{q,\sigma} |\phi_0\rangle = \prod_p \prod_\sigma \hat{c}_{p,\sigma}^\dagger \hat{c}_{q,\sigma} |0\rangle = 0$$

The total particle number is connected to the Fermi momentum by

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

$$(*)$: $\sum_k f(k) = \sum_k \frac{\Delta k}{(2\pi)^3} f(k) = \frac{V}{2\pi} \int \Delta k f(k)$$

With this it follows

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

$h p_F$: the Fermi momentum, and $\varepsilon_F = (h p_F)^2/2m$: the Fermi energy.
The total energy is

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

The relation with the Fermi energy is then:

\[
\frac{E}{V} = \frac{\varepsilon_F}{p_F} \frac{p_F^3}{5\pi^2} = \frac{3}{5} n \varepsilon_F \quad \text{and} \quad \frac{E}{N} = \frac{3}{5} \varepsilon_F,
\]

and the relation with the density \( n \) is:

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

**Expectation value of particle density:**

\[
\langle \hat{n} \rangle = \sum_{\sigma} \langle \phi_0 | \hat{\psi}_\sigma^\dagger (\mathbf{r}) \hat{\psi}_\sigma (\mathbf{r}) | \phi_0 \rangle = \sum_{\mathbf{p}, \mathbf{p}'} \sum_{\sigma} \frac{e^{-ip\cdot r + ip'\cdot r}}{V} \langle \phi_0 | \hat{\psi}_{\mathbf{p}, \sigma}^\dagger \hat{\psi}_{\mathbf{p}', \sigma} | \phi_0 \rangle = \frac{1}{V} \sum_{\mathbf{p}, \sigma} n_{\mathbf{p}, \sigma} = \frac{N}{V} = n.
\]

**Excitation of a Fermi gas:**

\[
|\phi \rangle = \hat{c}_{k_2, \sigma_2}^\dagger \hat{c}_{k_1, \sigma_1} |\phi_0 \rangle \equiv \text{particle hole pair}
\]

\[
\hat{b}_{k, \sigma} = \hat{c}_{-k, -\sigma}^\dagger \quad \text{hole annihilator}
\]

\[
\hat{b}_{k, \sigma}^\dagger = \hat{c}_{-k, -\sigma} \quad \text{hole creator}
\]

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

\[
G_{\sigma} (\mathbf{r} - \mathbf{r}') = \langle \phi_0 | \hat{\psi}_\sigma^\dagger (\mathbf{r}) \hat{\psi}_\sigma (\mathbf{r}') | \phi_0 \rangle = \frac{n}{2} \times \text{prob. amp. for} \quad \hat{\psi}_\sigma (\mathbf{r}') | \phi_0 \rangle \rightarrow \hat{\psi}_\sigma (\mathbf{r}) | \phi_0 \rangle \quad \text{particle missing at pos.} \ \mathbf{r}' \quad \text{particle missing at pos.} \ \mathbf{r}
\]

b.c. \quad \left( \langle \phi_0 | \hat{\psi}_\sigma^\dagger (\mathbf{r}') \hat{\psi}_\sigma (\mathbf{r}') | \phi_0 \rangle = \frac{n}{2} \right)
CHAPTER 2. APPLICATION OF SECOND QUANTIZATION

\[ G_\sigma (\mathbf{r} - \mathbf{r}') = \sum_{\mathbf{p}, \mathbf{p}'} \frac{1}{V} e^{-i\mathbf{p} \cdot \mathbf{r} + i\mathbf{p}' \cdot \mathbf{r}'} \langle \phi_0 | \hat{c}_{\mathbf{p}', \sigma} \hat{c}_{\mathbf{p}, \sigma} | \phi_0 \rangle \]

\[ = \frac{1}{V} \sum_{|\mathbf{p}| < p_F} e^{-i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} = \int_{|\mathbf{p}| < p_F} \frac{d\mathbf{p}}{(2\pi)^3} e^{-i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}')} \]

\[ = \frac{1}{(2\pi)^2} \int_0^{p_F} dp \int_0^1 d\eta e^{i\eta|\mathbf{r}' - \mathbf{r}|} \theta(|\mathbf{r} - \mathbf{r}'|) \]

\[ = \frac{1}{2\pi^2r} \int_0^{p_F} dp \sin(pr) \]

\[ = -\frac{\partial}{\partial r} \int_0^{p_F} dp \cos(pr) \]

\[ = -\frac{p_F}{r^2} \sin(p_Fr) - p_F \cos(p_Fr) \]

\[ = \frac{\sin(p_Fr) - p_Fr \cos(p_Fr)}{2\pi^2r^3} \]

i.e. \[ G_\sigma (\mathbf{r}) = \frac{3n \sin(p_Fr) - p_Fr \cos(p_Fr)}{(p_Fr)^3} \]

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

\[ \langle \phi'(\mathbf{r}, \sigma)|\hat{\psi}_\sigma^\dagger(\mathbf{r}') \hat{\psi}_{\sigma'}(\mathbf{r}')|\phi'(\mathbf{r}, \sigma)\rangle = \langle \phi_0 | \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_\sigma(\mathbf{r}) | \phi_0 \rangle \]

\[ = \left( \frac{n}{2} \right)^2 \frac{g_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}')}{\text{pair distribution function}} \]

It is

\[ \left( \frac{n}{2} \right)^2 g_{\sigma\sigma'}(\mathbf{r} - \mathbf{r}') = \langle \phi_0 | \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_{\sigma'}(\mathbf{r}') \hat{\psi}_\sigma(\mathbf{r}') | \phi_0 \rangle - \delta_{\sigma\sigma'} \delta(\mathbf{r} - \mathbf{r}') \langle \phi_0 | \hat{\psi}_\sigma^\dagger(\mathbf{r}) \hat{\psi}_{\sigma'}(\mathbf{r}') | \phi_0 \rangle \]

\[ = \langle \phi_0 | \hat{n}_\sigma(\mathbf{r}) \hat{n}_{\sigma'}(\mathbf{r}') | \phi_0 \rangle - \delta_{\sigma\sigma'} \delta(\mathbf{r} - \mathbf{r}') \langle \phi_0 | \hat{n}_\sigma(\mathbf{r}) | \phi_0 \rangle \]
In the Fourier-space we have

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

It is non zero only if \( p = p' \), \( k = k' \) or \( p = k' \), \( k = p' \). These conditions give

\[
\left( \frac{n}{2} \right)^2 g_{\sigma\sigma'}(r - r') = \frac{1}{V^2} \sum_{k p} \langle \phi_0 | \hat{c}_{k,\sigma}^\dagger \hat{c}_{p,\sigma'}^\dagger \hat{c}_{p,\sigma} \hat{c}_{k,\sigma} | \phi_0 \rangle 
\]

\[
= \langle \phi_0 | \hat{c}_{k,\sigma}^\dagger \hat{c}_{k,\sigma} \hat{c}_{p,\sigma}^\dagger \hat{c}_{p,\sigma} - \delta_{\sigma\sigma'} \delta_{p k} \delta_{p', k} \rangle + \frac{1}{V^2} \sum_{k p} e^{-i k \cdot (r - r')} e^{-i p \cdot (r' - r)} \langle \phi_0 | \hat{c}_{k,\sigma} \hat{c}_{p,\sigma'} \hat{c}_{p', \sigma'} \hat{c}_{k', \sigma} | \phi_0 \rangle
\]

\[
= \frac{1}{V^2} \langle \phi_0 | \hat{n}_{k,\sigma} \hat{n}_{p,\sigma'} | \phi_0 \rangle - \delta_{\sigma\sigma'} \frac{1}{V^2} \sum_{k p} e^{-i k \cdot (r - r')} e^{-i p \cdot (r' - r)} \langle \phi_0 | \hat{n}_{k,\sigma} \hat{n}_{p,\sigma} | \phi_0 \rangle.
\]

For \( \sigma \neq \sigma' \), we find

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

which gives \( g_{\sigma\sigma'}(r - r') = 1 \).

For \( \sigma = \sigma' \), we find

\[
\left( \frac{n}{2} \right)^2 g_{\sigma\sigma}(r - r') = \left( \frac{n}{2} \right)^2 - \frac{1}{V} \sum_{k} e^{-i k \cdot (r - r')} \hat{n}_{k,\sigma} \frac{1}{V} \sum_{p} e^{-i p \cdot (r - r')} \hat{n}_{p,\sigma} \langle \phi_0 | \phi_0 \rangle 
\]

\[
= \left( \frac{n}{2} \right)^2 - [G_{\sigma}(r - r')]^2.
\]

Combining these results leads to

\[
\Rightarrow g_{\sigma\sigma'}(r - r') = 1 - \frac{9}{(p_F r)^6} \left( \sin(p_F r) - p_F r \cos(p_F r) \right)^2 \delta_{\sigma\sigma'}, \quad r = |r - r'|.
\]
Because of the above relation, the pair distribution function represents the probability density for pair of particles to be at a distance $r$. The reduction of $g(r)$ for distances $\lesssim p_F^{-1}$ is called the correlation or exchange hole. It is an effect of the antisymmetry of the $N$-particle state.

Density correlation function:

$$\tilde{G}(r) = \langle \hat{n}(r)\hat{n}(0) \rangle = \frac{1}{V} \int dr' \langle \hat{n}(r + r')\hat{n}(r') \rangle$$

$$= \frac{1}{V} \sum_{\alpha,\beta} \int dr' \langle \delta(r + r' - r_\alpha)\delta(r' - r_\beta) \rangle = \frac{1}{V} \sum_{\alpha,\beta} \langle \delta(r - r_\alpha + r_\beta) \rangle$$

$$\sum_{\alpha \neq \beta} \delta(r - r_\alpha + r_\beta) \rightarrow \int dr' dr'' \hat{\psi}^\dagger(r')\hat{\psi}^\dagger(r'')\delta(r - r' + r'')\hat{\psi}(r'')\hat{\psi}(r')$$

$$= \int dr' \hat{\psi}^\dagger(r'')\hat{\psi}^\dagger(r' - r)\hat{\psi}(r'')\hat{\psi}(r' - r)$$

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

Static structure factor:

$$S(q) := \frac{1}{N} \left\langle \sum_{\alpha,\beta} e^{-i\mathbf{q} \cdot (r_\alpha - r_\beta)} \right\rangle - N\delta_{q,0} = \frac{1}{N} \langle \hat{n}_q \hat{n}_{-q} \rangle - N\delta_{q,0}$$

$$= \frac{N}{V} \int dr e^{-iq\cdot r} g(r) + 1 - N\delta_{q,0},$$

i.e.

$$S(q) - 1 = n \int dr e^{-iq\cdot r} (g(r) - 1),$$

and

$$g(r) - 1 = \frac{1}{n} \int \frac{dq}{(2\pi)^3} e^{iq\cdot r} (S(q) - 1).$$
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2.2 Magnetic (polarized) ground state of interacting Fermi gas

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

\[
\hat{H}_{\text{kin}} = \sum_{k,\sigma} \frac{\hbar^2 k^2}{2m} c_{k,\sigma}^\dagger c_{k,\sigma} \quad \text{and} \quad \hat{H}_{\text{int}} = \frac{1}{2V} \sum_{k,k',q,\sigma,\sigma'} U_q c_{k+q,\sigma}^\dagger c_{k',-q,\sigma'}^\dagger c_{k',\sigma'} c_{k,\sigma}.
\]

The polarization is defined by

\[
P = \frac{N_\uparrow + N_\downarrow}{N}
\]

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

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

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

\[
|g_P\rangle = \left( \prod_{|k|<k_{F,\uparrow}} c_{k,\uparrow}^\dagger \right) \left( \prod_{|k|<k_{F,\downarrow}} c_{k,\downarrow}^\dagger \right) |0\rangle,
\]

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

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

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

**Kinetic energy:**

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

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

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

and we have

\[
n_{\uparrow} = \frac{N_\uparrow}{V} = 1 \cdot \int_{|k|<k_{F,\uparrow}} \frac{d^3k}{(2\pi)^3} = \frac{k_{F,\uparrow}^3}{2 \cdot 3\pi^2}, \quad n_{\downarrow} = 1 \cdot \frac{k_{F,\downarrow}^3}{2 \cdot 3\pi^2},
\]

which give the Fermi momenta:

\[
k_{F,\uparrow\downarrow} = (2 \cdot 3\pi^2 n_{\uparrow\downarrow})^{1/3}.
\]
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Remember we have
\[
\frac{E_K}{V} = \frac{E(P = 0)}{V} = (3\pi^{2/3} \frac{3h^2}{10m}) \left( \frac{N}{V} \right)^{5/3} \equiv C \quad \Rightarrow \quad C = \frac{E_K}{V} \left( \frac{V}{N} \right)^{5/3}.
\]

\[
\frac{E_{\text{kin}}(P)}{V} = \frac{C}{2} \left[ (2n_\uparrow)^{5/3} + (2n_\downarrow)^{5/3} \right]
\]

\[
= \frac{E_K}{2V} \left( \frac{V}{N} \right)^{5/3} \left[ \left( \frac{2N_\uparrow}{V} \right)^{5/3} + \left( \frac{2N_\downarrow}{V} \right)^{5/3} \right]
\]

\[
= \frac{E_K}{2V} \left[ \left( \frac{2N_\uparrow}{N} \right)^{5/3} + \left( \frac{2N_\downarrow}{N} \right)^{5/3} \right]
\]

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

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

**Potential energy:**

The Coulomb potential is
\[
U(r) = \frac{e^2}{4\pi r} \Rightarrow U(q) = \frac{e^2}{q^2}.
\]

Since electron-electron interaction is screened (Yukawa potential):
\[
U(r) = \frac{e^2}{4\pi r} \exp(-r/r_c) \Rightarrow U(q) = \frac{e^2}{q^2 + r_c^2}.
\]

We use here a simpler model (very strongly screened \( |q| r_c \ll 1 \):
\[
U(r) = U\delta(r) \Rightarrow U(q) = U.
\]

The potential energy is then
\[
\langle g_P | \hat{H}_{\text{int}} | g_P \rangle = \frac{U}{2V} \sum_{k,k',q} \sum_{\sigma,\sigma'} \langle g_P | c_{k+q,\sigma} c_{k',-q,\sigma'}^\dagger c_{k',\sigma'}^\dagger c_k a | g_P \rangle
\]

\[
\neq 0 \text{ only for } \begin{cases} (A) k' - q = k', \quad k + q = k \Rightarrow q = 0 \\ (B) k' - q = k, \quad k + q = k', \quad \sigma = \sigma' \end{cases}
\]

Diagrams of corresponding interactions:
(A) Hartree term:

\[ E_H = \frac{U}{2V} \sum_{k,k'} \sum_{\sigma} \langle g_P | c_{k',\sigma} c_{k,\sigma} | g_P \rangle \]

\[ = \langle g_P | c_{k,\sigma} c_{k,\sigma} c_{k',\sigma} c_{k,\sigma} | g_P \rangle - \delta_{k,k'} \delta_{\sigma,\sigma'} \langle g_P | c_{k',\sigma} c_{k,\sigma} | g_P \rangle \]

\[ = n_{k',\sigma} n_{k,\sigma} - \delta_{k,k'} \delta_{\sigma,\sigma'} n_{k,\sigma} \]

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

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

(B) Fock term:

\[ E_{\text{Fock}} = \frac{U}{2V} \sum_{k,k'} \sum_{\sigma} \langle g_P | c_{k',\sigma} c_{k,\sigma} c_{k',\sigma} c_{k,\sigma} | g_P \rangle \]

\[ = - \langle g_P | c_{k,\sigma} c_{k,\sigma} c_{k',\sigma} c_{k,\sigma} | g_P \rangle + \delta_{k,k'} \langle g_P | c_{k',\sigma} c_{k,\sigma} | g_P \rangle \]

\[ = -n_{k',\sigma} n_{k,\sigma} + \delta_{k,k'} n_{k,\sigma} \]

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

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

\( E_{\text{Fock}} \) is minimal for \( |P| = 1 \). It comes from the Pauli principle.

Total energy:

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

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

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

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

Although it is impossible to solve this equation analytically with respect to \( P \), it suffices to plot the optimal polarization versus \( E_H/E_K \), as in the figure below.
From the plot we understand the following:

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

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

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

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

Pair distribution function for free bosons. We assume non-interacting bosons with spin zero. 

Only quantum number is the momentum. Consider the $N$-particle state

$$|\phi\rangle = |n_{p_0}, n_{p_1}, \ldots\rangle \quad n_{p_i} \in \{0, 1, 2, \ldots\}$$

Particle density:

$$\langle \phi | \hat{\psi}^\dagger (r) \hat{\psi} (r') | \phi \rangle = \frac{1}{V} \sum_{k, k'} e^{-i k r + i k' r'} \langle \phi | \hat{b}^\dagger_k \hat{b}_{k'} | \phi \rangle = \frac{1}{V} \sum_k n_k = \frac{N}{V} = n.$$ 

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

Pair distribution function:

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

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

$$\langle \phi | \hat{b}^\dagger_k \hat{b}^\dagger q \hat{b}_q \hat{b}_{k'} | \phi \rangle = (1 - \delta_{kk'}) (\delta_{kk'} \delta_{qq'} \langle \phi | \hat{b}^\dagger_k \hat{b}^\dagger q \hat{b}_q \hat{b}_{k'} | \phi \rangle + \delta_{kq} \delta_{k'q'} \langle \phi | \hat{b}^\dagger_k \hat{b}^\dagger q \hat{b}_q \hat{b}_{k'} | \phi \rangle)$$

$$+ \delta_{kq} \delta_{kk'} \delta_{qq'} \langle \phi | \hat{b}^\dagger_k \hat{b}^\dagger q \hat{b}_q \hat{b}_{k'} | \phi \rangle = (1 - \delta_{kk'}) (\delta_{kk'} \delta_{qq'} + \delta_{kq} \delta_{k'q'}) n_k n_q + \delta_{kq} \delta_{kk'} \delta_{qq'} n_k (n_k - 1)$$

With this it follows

$$\langle \phi | \hat{\psi}^\dagger (r) \hat{\psi}^\dagger (r') \hat{\psi} (r') \hat{\psi} (r) | \phi \rangle = \frac{1}{V^2} \left[ \sum_{k, q} \left( 1 - \delta_{k, q} \right) \left( 1 + e^{-i(k - q)(r - r')} \right) n_k n_q + \sum_k n_k (n_k - 1) \right]$$

$$= \frac{1}{V^2} \left[ \sum_{k, q} n_k n_q - \sum_k n_k^2 + \left| \sum_k e^{-i k(r - r')} n_k \right|^2 - \sum_k n_k^2 + \sum_k n_k^2 - \sum_k n_k \right]$$

$$= n^2 + \left| \frac{1}{V} \sum_k e^{-i k(r - r')} n_k \right|^2 - \frac{1}{V^2} \sum_k n_k (n_k + 1) \quad (*)$$

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

Looking at two examples:

1) All bosons occupying the same state $p_0$. Then

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

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

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

\[ n_k = \frac{(2\pi)^3 n}{(\sqrt{\pi} \Delta)^3} e^{-(k-k_0)^2/\Delta^2} \quad \text{with} \quad \int \frac{dp}{(2\pi)^3} n_p = n \quad \text{(normalization)} \]

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

\[ \int \frac{dk}{(2\pi)^3} e^{-ik(r-r')} n_k = n e^{-\frac{\Delta^2}{4} (r-r')^2} e^{-ik_0(r-r')} \]

and

\[ \frac{1}{V} \int \frac{dk}{(2\pi)^3} n_k^2 = \frac{1}{V} \left[ \frac{(2\pi)^3 n}{(\sqrt{\pi} \Delta)^3} \right]^2 \int \frac{dk}{(2\pi)^3} e^{-2(k-k_0)^2/\Delta^2} \sim \frac{n^2 \Delta^3}{V \Delta^6} \sim \frac{n^2}{V \Delta^3} \]

For \( n = \text{const.} \) and \( \Delta = \text{const.} \) disappears the third term in \((*)\) when \( V \to \infty \).

\[ n^2 g(r - r') = n^2 \left( 1 + e^{-\frac{\Delta^2}{4} (r-r')^2} \right) \]

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


2.4 Weakly interacting Bosons

Non-interacting Bose gas

The Hamiltonian for non-interacting bosons (NIB) is

\[ \hat{H}^{(1)} = \sum_k E(k) \hat{b}_k^\dagger \hat{b}_k; \quad E(k) = \frac{\hbar^2 k^2}{2m}. \]

Ground state: all particles are in \( k = 0 \)-level:

\[ |N\rangle = \frac{(b_0)^N}{\sqrt{N!}} |0\rangle = |N, 0, 0, 0, \ldots \rangle. \]

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

\[ |\phi\rangle = \sum_N |N\rangle. \]

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

Weakly interacting Bosons

Hamiltonian:

\[ \hat{H} = \sum_k \frac{\hbar^2 k^2}{2m} \hat{b}_k^\dagger \hat{b}_k + \frac{1}{2V} \sum_{k,p,q} U_{q} \hat{b}_{k+q}^\dagger \hat{b}_{p-q}^\dagger \hat{b}_p \hat{b}_k, \quad (2.1) \]

where \( \hat{b}_k \) and \( \hat{b}_k^\dagger \) are bosonic annihilator/creator.

Low temperatures: Bose-Einstein-condensation in the \( (k = 0)\)-mode, i.e. even with a weak interaction \( U(r) \) is present, we assume that in the ground state \( |N\rangle \) the single-particle state with \( k = 0 \) is macroscopically occupied.

\[ N_0 = \langle N|\hat{b}_0^\dagger \hat{b}_0|N\rangle \ll N, \]

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

\[ N - N_0 \ll N_0 \ll N. \]

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

\[ \hat{H} = \sum_k \frac{\hbar^2 k^2}{2m} \hat{b}_k^\dagger \hat{b}_k + \frac{1}{2V} U_0 \hat{b}_0^\dagger \hat{b}_0 \hat{b}_0 \hat{b}_0 + \frac{1}{V} \sum_{k \neq 0} (U_0 + U_k) \hat{b}_0^\dagger \hat{b}_0 \hat{b}_k^\dagger \hat{b}_k + \frac{1}{2V} \sum_{k \neq 0} U_k \left( \hat{b}_k^\dagger \hat{b}_{-k}^\dagger \hat{b}_0 \hat{b}_0 + \hat{b}_0^\dagger \hat{b}_0 \hat{b}_k \hat{b}_{-k} \right) + O(\hat{b}_k^3) \]

\( (k = p = q = 0 \text{ in } (2.1)) \)

\( (\text{resp. } p = q = 0, \quad p = q, k = 0 \text{ in } (2.1)) \)

\( (\text{resp. } k = 0, \quad p = 0) \)

\( (\text{resp. } k = -q, \quad p = q \text{ in } (2.1)) \)
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Because

\[ \hat{b}_0 | \ldots , N_0 , \ldots \rangle = \sqrt{N_0} | \ldots , N_0 - 1 , \ldots \rangle \]
\[ \hat{b}_0^\dagger | \ldots , N_0 , \ldots \rangle = \sqrt{N_0 + 1} | \ldots , N_0 + 1 , \ldots \rangle \]
\[ \hat{b}_0 \hat{b}_0^\dagger - \hat{b}_0^\dagger \hat{b}_0 = 1 \]

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

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

\[ \Rightarrow \hat{H} = \sum_{k \neq 0} \frac{\hbar^2 k^2}{2m} \hat{b}_k^\dagger \hat{b}_k + \frac{U_0}{2V} N_0^2 U_0 + \frac{N_0}{V} \sum_{k \neq 0} \left( (U_0 + U_k) \hat{b}_k^\dagger \hat{b}_k + \frac{1}{2} U_k \left( \hat{b}_k^\dagger \hat{b}_{-k} + \hat{b}_k \hat{b}_{-k} \right) \right) + \ldots \]

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

\[ \hat{N} = N_0 + \sum_{k \neq 0} \hat{b}_k^\dagger \hat{b}_k \]

\[ \left( \text{total particle number} = \text{#(condensated bosons)} + \text{#(excited particles)} \right) \]

It is for example

\[ \frac{U_0}{2V} N_0^2 = \frac{U_0}{2V} N_0^2 - \frac{N U_0}{V} \sum_{k \neq 0} \hat{b}_k^\dagger \hat{b}_k + \frac{U_0}{2V} \sum_{k,k' \neq 0} \hat{b}_k^\dagger \hat{b}_k \hat{b}_k^\dagger \hat{b}_k' \]

and

\[ \hat{H} = \sum_{k \neq 0} \frac{\hbar^2 k^2}{2m} \hat{b}_k^\dagger \hat{b}_k + \frac{U_0}{2V} N_0^2 U_0 + \frac{N_0}{V} \sum_{k \neq 0} U_0 \hat{b}_k^\dagger \hat{b}_k + \frac{N_0}{V} \sum_{k \neq 0} U_0 \left( \hat{b}_k^\dagger \hat{b}_{-k} + \hat{b}_k \hat{b}_{-k} \right) \]

\[ \approx \sum_{k \neq 0} \frac{\hbar^2 k^2}{2m} \hat{b}_k^\dagger \hat{b}_k + \frac{N^2}{2V} U_0 + \frac{N}{V} \sum_{k \neq 0} U_k \hat{b}_k^\dagger \hat{b}_k + \frac{N}{2V} \sum_{k \neq 0} U_k \left( \hat{b}_k^\dagger \hat{b}_{-k} + \hat{b}_k \hat{b}_{-k} \right) + \hat{H}' \]

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

\[ \frac{N}{V} = n. \]

\( \hat{H} \) is a quadric form (in \( \hat{b}_k^\dagger \hat{b}_k \)), which still has to be diagonalized (\( \sim \) Bogolivbov transformation).

**Ansatz:**

\[ \hat{b}_k = U_k \hat{\alpha}_k + v_k \hat{\alpha}_{-k}^\dagger \]
\[ \hat{b}_k^\dagger = U_k \hat{\alpha}_k^\dagger + v_k \hat{\alpha}_{-k} \]
CHAPTER 2. APPLICATION OF SECOND QUANTIZATION

If \( u_k^2 - v_k^2 = 1 \) fulfilled, then \( \hat{\alpha}_k \) and \( \hat{\alpha}_k^\dagger \) are again bosonic operators:

\[
[\hat{\alpha}_k, \hat{\alpha}_{k'}] = [\hat{\alpha}_k^\dagger, \hat{\alpha}_{k'}^\dagger] = 0 \\
[\hat{\alpha}_k, \hat{\alpha}_{k'}^\dagger] = \delta_{k,k'}
\]

(Proof: see exercise)

The inverse transformation reads

\[
\hat{\alpha}_k = U_k \hat{b}_k - v_k \hat{b}_k^\dagger \\
\hat{\alpha}_k^\dagger = U_k \hat{b}_k^\dagger - v_k \hat{b}_k
\]

A longer calculation (see exercise) leads to

\[
\hat{H} = \frac{1}{2V} N^2 U_0 + \sum_{k \neq 0} \left( \frac{\hbar^2 k^2}{2m} + nU_k \right) \left[ u_k^2 \hat{\alpha}_k \hat{\alpha}_k^\dagger + v_k^2 \hat{\alpha}_k^\dagger \hat{\alpha}_k + u_k v_k \left( \hat{\alpha}_k^\dagger \hat{\alpha}_{-k}^\dagger + \hat{\alpha}_k \hat{\alpha}_{-k} \right) \right] \\
+ \frac{N}{2V} \sum_{k \neq 0} U_k \left[ u_k^2 + v_k^2 \right] \left( \hat{\alpha}_k^\dagger \hat{\alpha}_{-k}^\dagger + \hat{\alpha}_k \hat{\alpha}_{-k} \right) + 2 u_k v_k \left( \hat{\alpha}_k^\dagger \hat{\alpha}_k + \hat{\alpha}_k \hat{\alpha}_k^\dagger \right)
\]

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

\[
\left( \frac{\hbar^2 k^2}{2m} + nU_k \right) u_k v_k + \frac{n}{2} U_k \left( u_k^2 + v_k^2 \right) = 0
\]

With the condition \( u_k^2 - v_k^2 = 1 \) one calculates

\[
u_k^2 = \frac{\omega_k + \left( \frac{\hbar^2 k^2}{2m} + nU_k \right)}{2\omega_k} \\
\]

\[
v_k^2 = \frac{-\omega_k + \left( \frac{\hbar^2 k^2}{2m} + nU_k \right)}{2\omega_k},
\]

where

\[
\omega_k = \left[ \left( \frac{\hbar^2 k^2}{2m} + nU_k \right)^2 - (nU_k)^2 \right]^{1/2} = \left[ \left( \frac{\hbar^2 k^2}{2m} \right)^2 + \frac{n\hbar^2 k^2 U_k}{m} \right]^{1/2}
\]

It follows

\[
\frac{u_k U_k}{\hbar} = \frac{\left( \frac{\hbar^2 k^2}{2m} + nU_k \right)^2 - \omega_k^2}{\frac{2\omega_k}{\omega_k}} = -\frac{nU_k}{2\omega_k}
\]
We can now further calculate $\hat{H}$

$$\hat{H} = \frac{N^2 U_0}{2V} + \sum_{k \neq 0} \left( \frac{\hbar^2 k^2}{2m} + nU_k \right) \left( u_k^2 \hat{\alpha}_k \hat{\alpha}_k + v_k^2 \left( 1 + \hat{\alpha}_k \hat{\alpha}_k \right) \right)$$

$$+ \frac{n}{2} U_k^2 \left( - \frac{nU_k}{2\omega_k} \left( \hat{\alpha}_k \hat{\alpha}_k + 1 + \hat{\alpha}_k \hat{\alpha}_k \right) \right)$$

$$= \frac{N^2 U_0}{2V} + \sum_{k \neq 0} \left( u_k^2 + v_k^2 \right) \hat{\alpha}_k \hat{\alpha}_k + \left( \frac{h^2 k^2}{2m} + nU_k \right) v_k^2 - \frac{n^2 V^2_k}{\omega_k} \hat{\alpha}_k \hat{\alpha}_k - \frac{n^2 V^2_k}{2\omega_k}$$

$$= \frac{N^2 U_0}{2V} + \sum_{k \neq 0} \frac{1}{\omega_k} \left[ \left( \frac{h^2 k^2}{2m} + nU_k \right)^2 - (nU_k)^2 \right] \hat{\alpha}_k \hat{\alpha}_k - \frac{1}{2} \left( \frac{h^2 k^2}{2m} + nU_k \right)$$

$$+ \frac{1}{2\omega_k} \left( \frac{h^2 k^2}{2m} + nU_k \right)^2 - \frac{n^2 V^2_k}{\omega_k}$$

$$\implies \hat{H} = \frac{N^2 U_0}{2V} - \frac{1}{2} \sum_{k \neq 0} \left( \frac{h^2 k^2}{2m} + nU_k - \omega_k \right) + \sum_{k \neq 0} \left( \omega_k \hat{\alpha}_k \hat{\alpha}_k \right)$$

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

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

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

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

Exited states are generated by $\hat{\alpha}_k^\dagger |N\rangle$. Their energy is $\hbar \omega_k$. One finds the dispersion relation
\[ \omega_k = \left[ \left( \frac{\hbar^2 k^2}{2m} \right)^2 + \frac{n\hbar^2 k^2 U_k}{m} \right]^{1/2} \]

\[ = \begin{cases} 
  ck & \text{for } k \to 0 \text{ where } c = \sqrt{\frac{nU_0}{m}} \\
  \frac{\hbar^2 k^2}{2m} + nU_k & \text{for } k \to \infty 
\end{cases} \]

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

Distinctive feature: \( \min \left\{ \frac{\omega_k}{k} \right\} =: v_{\text{crit}} \neq 0 \) leads to superfluidity.
Chapter 3

Superfluidity

3.1 Landau’s model Helium 4 superfluid

Quasiparticle excitation in superfluid He

Area I:
Excitations: phonons
\[ \varepsilon_p = cp, \quad c = 238 \text{ m/s} \]

Area II:
Minimum at \( p_0 = 1.91 \, \text{Å}^{-1} \hbar \)
Excitations: rotons
\[ \varepsilon_p = \Delta + \left( \frac{|p| - p_0}{2\mu} \right)^2, \quad \mu = 0.16 \, \text{m}_{\text{He}}, \quad \Delta/k = 8.6 \text{ K} \]

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

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

If there is no excitation present, then:
Rest frame (of fluid):

\[ P_0 = 0, \quad E = E_{gs} \]

Lab frame (fluid moving, vel. \( v \)):

\[ P = Mv, \quad E = E_{gs} + \frac{Mv^2}{2} \]

Assuming now there exist excitations with (total) momentum \( p \) and energy \( \varepsilon(p) \).

Rest frame:

\[ P_0 = p, \quad E = E_{gs} + \varepsilon(p) \]

Lab frame:

\[ P = Mv + p, \quad E = \frac{Mv^2}{2} + v \cdot p + E_{gs} + \varepsilon(p) \]

\[ \Rightarrow \Delta E = \varepsilon(p) + v \cdot p \]

Is it energetically beneficial to excite quasiparticles, i.e. \( \Delta E < 0 \)?

Because \( \varepsilon(p) > 0 \), the energy difference assumes it smallest value when \( p \) and \( v \) are antiparallel.

For an excitation to have an energetic benefit the following inequality must be satisfied:

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

The critical velocity is therefore given by

\[ v_{crit} = \min_p \left\{ \frac{\varepsilon(p)}{|p|} \right\} \]

**Implication:** For \( |v| < v_{crit} \) there is no excitation possible and the fluid flows frictionless \( \Leftrightarrow \) superfluidity.

\( T > 0 \): There already exist some excitations which can collide with the wall and can interchange energy and momentum \( \Leftrightarrow \) friction caused by the noncondensated particles. But up to \( T_U \) there is a macroscopic condensate present.
3.2 Field theory for interacting Bose gas

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

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

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

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

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

The commutators give:

$$\left[ \hat{\Psi}(r), \hat{H}^{(1)} \right] = -\frac{\hbar^2}{2m} \int d^3r' \hat{\Psi}^\dagger(r') \left\{ \hat{\Psi}(r), \hat{\Psi}^\dagger(r') \right\} \Delta \hat{\Psi}(r') = 0$$

and

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

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

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

and the evolution equation (or Heisenberg Equation) becomes

$$i\hbar \frac{\partial}{\partial t} \hat{\Psi} = -\frac{\hbar^2}{2m} \Delta \hat{\Psi} + U \hat{\Psi}^\dagger \hat{\Psi} \hat{\Psi}. \quad (3.1)$$

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

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

Since $N \gg 1$ we have:

$$\langle \hat{b}_0^\dagger \hat{b}_0 \rangle \simeq \langle \hat{b}_0 \hat{b}_0^\dagger \rangle \gg (|\hat{b}_0^\dagger \hat{b}_0^\dagger|).$$

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

$$\hat{\Psi}(r,t) = \sum_{\text{number}} \hat{b}_0 \psi_r(t) + \sum_{k \neq 0_{\text{operator!}}} \hat{b}_k \psi_k(r,t). \quad (3.2)$$
CHAPTER 3. SUPERFLUIDITY

**Simplest solution** of Eq. (3.1):
The condensate (ground state) is
\[
\hat{\Psi}(\mathbf{r}, t) = b_0 \psi(\mathbf{r}, t) = \psi(t) \quad \text{(classical field)}
\]
This corresponds to the state \( \psi(\mathbf{r}, t) \) with momentum \( \mathbf{k} = 0 \), and it does not depend on \( \mathbf{r} \).
Eq. (3.1) then becomes:
\[
\hbar \frac{\partial \psi}{\partial t}(t) = U |\psi(t)|^2 \psi(t). \tag{3.3}
\]
The solution of Eq. (3.3) with time-independent modulus is:
\[
\psi(t) = \psi_0 e^{-\frac{i}{\hbar} \mu t}, \quad |\psi(t)|^2 = |\psi_0|^2
\]
Remember that \( \hat{\Psi} \hat{\Psi}^\dagger \) is the density operator hence the solution describes the Bose condensate with density \( \rho(\mathbf{r}) = |\psi_0|^2 \). The parameter \( \mu \) is related to the density via Eq. (3.3):
\[
\mu = U \rho.
\]
It is the chemical potential of the condensate: adding one more particle to the condensate absorbs the interaction energy \( U \) multiplied by the local density of bosons \( \rho \).

### 3.3 Oscillatory excitations

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

**Ansatz**:
\[
\hat{\Psi}(\mathbf{r}, t) = \psi(\mathbf{r}, t) + \delta \hat{\Psi}(\mathbf{r}, t) e^{-\frac{i}{\hbar} \mu t}.
\]
Inserting this expression of \( \hat{\Psi} \) in Eq. (3.1) (Heisenberg equation) and keeping only the terms to first order in \( \delta \hat{\Psi} \), we obtain:
\[
\hbar \frac{\partial}{\partial t} \delta \hat{\Psi} + \mu \delta \hat{\Psi} = -\frac{\hbar^2}{2m} \Delta \delta \hat{\Psi} + U \psi_0^2 \delta \hat{\Psi}^\dagger + 2U |\psi_0|^2 \delta \hat{\Psi}.
\]
To simplify, we assume that \( \psi_0 \) is real:
\[
U \psi_0^2 = U |\psi_0|^2 = U \rho = \mu.
\]
Therefore,
\[
\hbar \frac{\partial}{\partial t} \delta \hat{\Psi} = -\frac{\hbar^2}{2m} \Delta \delta \hat{\Psi} + \mu \left( \delta \hat{\Psi}^\dagger + \delta \hat{\Psi} \right). \tag{3.4}
\]
Obviously plane waves satisfy this equation. Expressing the corrections to the condensate operators as in Eq. (3.2), we can search for a solution of the form
\[
\delta \hat{\Psi}(\mathbf{r}, t) = \frac{1}{\sqrt{V}} \sum_k \hat{b}_k(t) e^{i \mathbf{k} \cdot \mathbf{r}}.
\]
Inserting in Eq. (3.4) we obtain:
\[
\frac{1}{\sqrt{V}} \sum_k e^{i \mathbf{k} \cdot \mathbf{r}} \left( \hbar \frac{\partial}{\partial t} \hat{b}_k \right) = \frac{1}{\sqrt{V}} \sum_k e^{i \mathbf{k} \cdot \mathbf{r}} \left[ E(\mathbf{k}) + \mu \right] \hat{b}_k + \frac{1}{\sqrt{V}} \sum_k e^{-i \mathbf{k} \cdot \mathbf{r}} \mu \hat{b}_k^\dagger
\]
Multiply both sides with $\frac{1}{\sqrt{V}} e^{-i q \cdot r}$ and then sum over $r$:

$$
\frac{1}{V} \sum_k \sum_r e^{i (k - q) \cdot r} \left( i \hbar \frac{\partial}{\partial t} \hat{b}_k \right) = \frac{1}{V} \sum_k \sum_r e^{i (k - q) \cdot r} \left[ E(k) + \mu \right] \hat{b}_k + \frac{1}{V} \sum_k \sum_r e^{-i (k + q) \cdot r} \mu \hat{b}_k^\dagger
$$

which gives:

$$
\hbar \frac{\partial}{\partial t} \hat{b}_q = [E(q) + \mu] \hat{b}_q + \mu \hat{b}_q^\dagger.
$$  (3.5)

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

Bogoliubov introduced the following new Bose-operators:

$$
\hat{b}_k = u_k \hat{\alpha}_k + v_k \hat{\alpha}_k^\dagger
$$

$$
\hat{b}_k^\dagger = u_k \hat{\alpha}_k^\dagger + v_k \hat{\alpha}_k
$$  (3.6)

such that Eq. (3.5) transforms into:

$$
\hbar \frac{\partial}{\partial t} \hat{\alpha}_k = \varepsilon_k \hat{\alpha}_k.
$$  (3.7)

where $u_k$ and $v_k$ are real coefficients and $u_k^2 - v_k^2 = 1$ due to Bose operator $\hat{\alpha}_k$.

The “wrong” creation/annihilation-operators $\hat{b}_k$, $\hat{b}_k^\dagger$ describe particles and the “right” c/a operators $\hat{\alpha}_k$, $\hat{\alpha}_k^\dagger$ describe quasi-particles.

To find the quasiparticle energies $\varepsilon_k$ along with the coefficients $u_k$ and $v_k$, one substitutes Eq. (3.6) into Eq. (3.5) and requires that it can be written as Eq. (3.7) (see exercise). One then obtains a linear algebra problem for an unknown vector with eigenvalues $\varepsilon_k$.

The quasi particles energies, the energies of the elementary excitations of the interacting Bose condensate, are given by:

$$
\varepsilon_k = \sqrt{E(k)[E(k) + 2\mu]} = \sqrt{\frac{\hbar^2 k^2}{2m} \left( \frac{\hbar^2 k^2}{2m} + 2\mu \right)}
$$

$$
= \hbar k \sqrt{\frac{\mu}{m} \left( 1 + \frac{\hbar^2 k^2}{4\mu m} \right)} = \hbar k \sqrt{\frac{\mu}{m} + O(k^2)}.
$$

Hence

$$
\frac{\varepsilon_k}{\mu} = \frac{k}{k_B} \sqrt{1 + \frac{k^2}{2k_B^2}}, \quad k_B = \frac{\sqrt{2\mu m}}{\hbar}
$$

Small-$k$ behavior:

$$
\varepsilon_k = \hbar v_p k + O(k^2),
$$

$$
\omega_k = v_p k + O(k^2),
$$

$$
v_p = \frac{\mu}{m} = \lim_{k \to 0} \frac{\partial \varepsilon_k}{\partial k}.
$$

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

It turns out that many field theories possess excitations not captured by a Taylor expansion: topological excitations. Configurations of quantum fields in such theories can be separated into classes such that no infinitesimally small change of the field configuration would cause a change from one class to the other.

In superfluidity the relevant configurations of the complex field $\langle \hat{\Psi}(r,t) \rangle$ have constant modulus (related to the particle density) while the phase can change rather freely. There exist topologically non-trivial configurations of the phase which are called vortices: emergent excitations.

Simplification: Resort to a closed equation for $\langle \hat{\Psi}(r,t) \rangle = \psi(r,t)$: “quasiclassical approximations”.

From Heisenberg equation (3.1), with mean field approximation:

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

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

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

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

$$\xi \equiv \sqrt[3]{\frac{\hbar^2}{2mU\rho}} = \frac{\hbar}{\sqrt{2mU\rho}}.$$

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

GP is a classical Hamiltonian equation, can be obtained from Hamiltonian:

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

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

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

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

**How to relate $\psi(r,t)$ to more classical quantities characterizing a liquid?**

It is clear that density $\rho(r,t) = \langle \hat{\Psi}^\dagger(r,t) \hat{\Psi}(r,t) \rangle \simeq |\psi(r,t)|^2 \Rightarrow$ modulus of $\psi$!

What about the phase? With Eq. (3.8) one finds:

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

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

$$\mathbf{j}(r,t) = -\frac{i\hbar}{2m} [\psi^*(r,t) \nabla \psi(r,t) - \psi(r,t) \nabla \psi^*(r,t)].$$
then the particle density satisfy the continuity equation

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

Since \( \mathbf{j} \) is on one hand a particle current density, \( \mathbf{j} = \rho \mathbf{v}_s \), with \( \mathbf{v}_s \) the local velocity field and on the other hand with \( \psi = \sqrt{\rho} e^{i\phi} \):

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

Hence the velocity is

\[
\mathbf{v}_s(\mathbf{r}, t) = \frac{\hbar}{m} \nabla \phi(\mathbf{r}, t),
\]

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

\[
\mathbf{v}_s = \frac{\hbar}{m} \mathbf{k} = \frac{\mathbf{p}}{m}.
\]

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

\[
\int dx \frac{\partial \phi}{\partial x} = 2\pi n, \quad n \in \mathbb{Z}.
\]

The integer \( n \) is a topological number, it cannot be changed by a small variation of \( \psi \).

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

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

\[\Rightarrow \phi'' = \frac{m}{\hbar} v_s' = 0 \quad \Rightarrow v_s = \text{const}.
\]

The condensate moves with a constant velocity \( v_s \) along the ring.
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Each field configuration with a non-zero constant density in all points of the ring is characterized by a certain $n$, and those that differ in $n$ belong to different sectors. For $\psi = \sqrt{\rho} e^{in\theta}$,

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

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

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

To understand this: compute total angular momentum $L_n$ of the superfluid with respect to the symmetry axis of the ring: 

Momentum of an infinitesimal element of the fluid: $dl = v_n m \rho s dx$

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

with $N_p = 2\pi R s \rho$, the number of particles in the condensate.  

In a topological sector $n$, each particle of the superfluid acquires a quantized value of the angular momentum $\hbar n$. It is different from the angular momentum quantization of non-interacting bosons: clear manifestation of the collective nature of topological excitations.

3.4.1 Vortices

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

$$\phi(r, \theta) = n \theta \quad \Rightarrow \quad \mathbf{v}_s(r, \theta) = \frac{n \hbar}{mr} \mathbf{e}_\theta.$$  

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

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

$n$ is also called the winding number of the vortex. Note that $\mathbf{v}_s$ diverges for $r \rightarrow 0$ and the phase becomes undefined at $r = 0$: something special goes on close to the center of the vortex (i.e. tornado, whirlpool sink, ...).

Go back to GP and seek for cylindrically symmetric solutions of the form

$$\psi(r) = \sqrt{\rho_0} f(r) e^{in\theta}$$

when $\rho_0$ is the equilibrium density of the superfluid that is reached far away from the vortex center, and $f(r)$ is a dimensionless function. The continuity of $\psi$ gives $f(r) \simeq r^n$ for $r \rightarrow 0$, i.e. the density of the condensate must reach zero precisely in the vortex center!

From the stationary form of the Eq. (3.8):

$$0 = \left[ \frac{\hbar^2}{2m} \Delta - \mu + U |\psi|^2 \right] \psi$$
with the Laplace operator in polar coordinates
\[ \Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2}. \]

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

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

\[ 0 = -\frac{\hbar^2}{2m\xi^2} \left( f''(u) + \frac{1}{u} f'(u) - \frac{n^2}{u^2} f(u) \right) - \mu f(u) + U \rho_0 f(u) \]
\[ \Rightarrow \frac{1}{u} \frac{df}{du} \left( u \frac{df}{du} \right) + \left( 1 - \frac{n^2}{u^2} \right) f - f^3 = 0. \]

This equation indeed has a solution satisfying \( f \simeq u^n \) for \( u \to 0 \):
\[ \frac{1}{u} \frac{df}{du} \left( u \frac{df}{du} \right) = n^2 u^{n-2}, \quad \left( 1 - \frac{n^2}{u^2} \right) f = -n^2 u^{n-2} + O(u^n) \]

and \( f \simeq 1 \) for \( u \to \infty \):
\[ \frac{df}{du} = 0, \quad \frac{n^2}{u^2} f \to 0, \quad \text{and} \quad f - f^3 \to 0. \]

Estimate the (kinetic) energy stored in a single vortex in a 3d slab of height \( b \):
\[ E_n = \int d^3r \frac{mv(r)^2}{2} \rho(r) = \int_0^b dz \int dr \int_0^{2\pi} d\theta \frac{m}{2} \frac{\hbar^2 n^2}{m^2 r^2} \rho_0 = n^2 b \pi \frac{\hbar^2 \rho_0}{m} \int \frac{dr}{r}. \]

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

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

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

Total velocity:
\[ v_{\text{tot}}(r) = v_1(r) + v_2(r) + \cdots. \]

Total kinetic energy of the fluid is prop. to \( v_{\text{tot}}^2 \): pairwise vortex-vortex interactions.

(a) Assume we have \( N_v \) vortices of winding number \( n = +1 \) (or \( n = -1 \)). They all carry separately the same energy \( E_1 \), since all circulate in the same way. Full energy including interactions:
\[ E = b \frac{dE}{dl} \left[ N_v \ln \frac{L}{\xi} + \frac{1}{2} \sum_{i \neq j} \ln \frac{L}{|r_i - r_j|} \right], \]
with \( r_i \) are the vortex coordinates. Interaction energy is lowest when the vortices are far apart. Hence for fixed concentration of vortices, they form a regular lattice.

(b) Pair of vortices with opposite winding number. Energy:
\[ E \propto b \frac{dE}{dl} \ln \frac{d}{\xi}, \]
with \( d \) the distance between the two vortex centers. attraction, independent of the system size \( L \): zero topological charge. Then topologically connected to the ground state. Hence it can be seen as a superposition of elementary excitations (sound quanta) of the ground state.

(c) Several vortex arrangement.

3.4.2 Vortex lines (in 3d)

In a realistic 3d liquid, the vortex cores are long lines that must start and end at the boundaries of the superfluid and penetrate the whole volume of the fluid:
\[ E_1 = L \frac{dE}{dl} \ln \frac{L}{\xi}. \]
These vortex lines can be simply produced by setting the superfluid into rotation.
Rotating a normal rigid body: \( \mathbf{v} = \omega_0 \times \mathbf{r} \).
Given \( \mathbf{v}(x, y, z) \), consider surface \( \Omega \):
\[
\int_{\Omega} (\nabla \times \mathbf{v}) \cdot d\mathbf{S} = \int_{\partial \Omega} \mathbf{v} \cdot d\mathbf{r} = \Gamma.
\]
Clearly this contour integral is a measure of the circulation \( \Gamma \) of the field \( \mathbf{v} \) along the contour \( \partial \Omega \). For a normal rotating rigid body, the vorticity is:
\[
\omega \equiv \nabla \times \mathbf{v} = \nabla \times (\omega_0 \times \mathbf{r}) = (\nabla \cdot \mathbf{r})\omega_0 - (\omega_0 \cdot \nabla)\mathbf{r} \\
= 3\omega_0 - \omega_0 = 2\omega_0.
\]
The vorticity is thus simply twice the angular frequency of the rotation.

**Superflow:**
The vorticity is
\[
\omega = 2\pi N_v \frac{\hbar}{m},
\]
with \( N_v \) is the number of vortices penetrating the surface.
Remember: for one vortex:
\[
\mathbf{v} = \frac{\hbar}{m} \nabla \phi, \quad \oint \mathbf{v} \cdot d\mathbf{r} = 2\pi \frac{\hbar}{m}.
\]
\[\Rightarrow\] Superflow without vortices: zero vorticity, zero angular momentum, non-rotating.  
\[\Rightarrow\] Superfluid in a rotating vessel just slips along the vessel walls.

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

Note: The picture is the same for \(^4\)He and \(^3\)He.

O. V. Lounasmaa and E. Thuneberg,  
*Vortices in rotating superfluid \(^3\)He*,  
Chapter 4

Quantization of the classical radiation field

4.1 Classical Fields

Chain of coupled oscillators

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

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

where the Hamilton's equations of motion read:

\[
\dot{x}_n = \frac{\partial H}{\partial p_n}, \quad \dot{p}_n = -\frac{\partial H}{\partial x_n}.
\]

which further implies:

\[
\frac{d^2 x_n}{dt^2} = \frac{K}{m} (x_{n+1} - 2x_n + x_{n-1}).
\] (4.1)

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

\[
x_n(t) = u_n \exp\{i(\omega_k t - k_n)\} + u_n^* \exp\{-i(\omega_k t - k_n)\}
\] (4.2)

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

\[-\omega_k^2 = 2\frac{K}{m} (\cos k - 1),
\]

\[
\Rightarrow \omega_k = 2\sqrt{\frac{K}{m} \sin \frac{k}{2}} \approx |k| \sqrt{\frac{K}{m}}.
\] (4.3)

It is the dispersion relation.

Note: Eq. (4.2) and Eq. (4.3) are periodic in \(k\) with period \(2\pi \Rightarrow k \in [-\pi, \pi]\).

Boundary condition: allowed \(k\)-values are discrete.
Periodic boundary condition (for $N$ oscillators):

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

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

$$x_n(t) = \sum_k \left[ u_k e^{i(kn - \omega t)} + u_k^* e^{-i(kn - \omega t)} \right].$$  \hspace{1cm} (4.4)

## Continuous elastic string

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

### Hamiltonian:

Let us first discretize:

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

$$\Delta u = u_{n+1} - u_n,$$

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

Momentum:

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

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

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

Potential energy:

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

The Hamiltonian then takes the form:

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

It gives the equation of motion:

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

### Continuum limit: $d \to 0$

$\kappa d = K = \text{const.}$ is the string tension.

Definition of momentum density:

$$p(x) = \frac{p_n}{d} \quad \text{for} \quad d \to 0.$$
CHAPTER 4. QUANTIZATION OF THE CLASSICAL RADIATION FIELD

Hamiltonian for the continuous elastic string:

\[
H = \int dx \left[ \frac{p^2(x)}{2\rho} + \frac{K}{2} \left( \frac{\partial u}{\partial x} \right)^2 \right].
\] (4.5)

Equation of motion:

\[
\begin{align*}
\frac{\partial u}{\partial t} &= \frac{\delta H}{\delta p(x)} = \frac{p(x)}{\rho}, \\
\frac{\partial p}{\partial t} &= -\frac{\delta H}{\delta u(x)} = K \frac{d^2 u(x, t)}{dx^2}.
\end{align*}
\]

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

\[
\frac{d^2 u(x, t)}{dt^2} = K \frac{d^2 u(x, t)}{dx^2}.
\] (4.6)

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

Solution:

Consider

\[
u_k(x, t) = u_k e^{i(kx - \omega_k t)} + u_k^* e^{-i(kx - \omega_k t)}.
\] (4.7)

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

\[
\omega_k = |k| \sqrt{\frac{K}{\rho}}.
\]

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

\[k = \frac{2\pi l}{L}, \quad l = 0, \pm 1, \pm 2, \ldots\.
\]

General solution:

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

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

Definition:

\[
u_k(t) = u_k e^{-i\omega_k t}, \quad u_k^*(t) = u_k^* e^{i\omega_k t}.
\]

Then,

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

\[
\Rightarrow \frac{\partial u}{\partial x} = \sum_k ik \left[ u_k(t) e^{ikx} - u_k^*(t) e^{-ikx} \right],
\]

\[
\Rightarrow \frac{\partial u}{\partial t} = \sum_k i\omega_k \left[ u_k(t) e^{ikx} - u_k^*(t) e^{-ikx} \right].
\]
And,
\[
\left( \frac{\partial u}{\partial x} \right)^2 = \sum_{k, k'} (-k k') \left[ u_k(t) e^{ikx} - u_k^*(t) e^{-ikx} \right] \left[ u_{k'}(t) e^{ik'x} - u_{k'}^*(t) e^{-ik'x} \right],
\]
\[
\left( \frac{\partial u}{\partial t} \right)^2 = \sum_{k, k'} (-\omega_k \omega_{k'}) \left[ u_k(t) e^{ikx} - u_k^*(t) e^{-ikx} \right] \left[ u_{k'}(t) e^{ik'x} - u_{k'}^*(t) e^{-ik'x} \right].
\]

Now use:
\[
\frac{1}{L} \int_0^L dx e^{i(k-k')} = \delta_{k,k'}, \quad \frac{1}{L} \int_0^L dx e^{i(k+k')} = \delta_{-k,k'},
\]
and from Eq. (4.5), we obtain
\[
H = \int_0^L dx \left[ \frac{\rho^2}{2\rho} \left( \frac{\partial u}{\partial t} \right)^2 + \frac{K}{2} \left( \frac{\partial u}{\partial x} \right)^2 \right] = \frac{\rho}{2} L \sum_k \omega_k^2 \left[ -u_k(t) u_{-k}(t) + u_k(t) u_k^*(t) + u_k^*(t) u_k(t) - u_k^*(t) u_{-k}(t) \right] + \frac{K}{2} L \sum_k k^2 \left[ -u_k(t) u_{-k}(t) + u_k(t) u_k^*(t) + u_k^*(t) u_k(t) + u_k^*(t) u_{-k}(t) \right] = \sum_k 2\rho \omega_k^2 (u_k u_k^* + u_k^* u_k),
\]
where we use the dispersion relation \( Kk^2 = \rho \omega_k^2 \).

Definition:
\[
d_k = u_k \sqrt{4L\rho \omega_k} \quad \Rightarrow \quad u_k = \frac{d_k}{\sqrt{4L\rho \omega_k}}.
\]

Then, \( H \) could be written as:
\[
H = \frac{1}{2} \sum_k \omega_k (d_k^* d_k + d_k d_k^*).
\]
As long as \( d_k \) and \( d_k^* \) are complex numbers:
\[
H = \sum_k \omega_k d_k^* d_k.
\]

\( d_k \) = normal coordinates of the field \( u(x, t) \).

Time dependence of the field can be assigned to the \( d_k \)
\[
d_k(t) = d_k e^{-i\omega_k t}, \quad \dot{d}_k(t) = -i\omega_k^2 d_k(t)
\]

One can introduce real variables:
\[
Q_k = \frac{1}{\sqrt{2\omega_k}} (d_k + d_k^*), \quad \text{and} \quad P_k = -i \sqrt{\frac{\omega_k}{2}} (d_k - d_k^*).
\]

Then, for a set of oscillators
\[
H = \sum_k \frac{1}{2} \left( P_k^2 + \omega_k^2 Q_k^2 \right) \quad (4.8)
\]
\[ P_k, Q_k = \text{generalized coordinates/momenta of the displacement field } u(x, t). \]

Note: All oscillators in nature (electromagnetic wave, sound, pendula, skee ball hanging on a spring) are very similar and can be regarded in a unified way.

Eq. (4.8) is a classical Hamiltonian function, so the equation of motions are:

\[
\dot{Q}_k = \frac{\partial H}{\partial P_k}, \quad \dot{P}_k = -\frac{\partial H}{\partial Q_k},
\]

fully equivalent to Eq. (4.6).

**Quantization rules:**

\[ Q_k, P_k \rightarrow \hat{Q}_k, \hat{P}_k \]

with the commutation rules:

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

Equivalent to:

\[ d_k, d_k^* \rightarrow \hat{d}_k, \hat{d}_k^\dagger \]

with bosonic commutation rules:

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

### 4.2 Quantization of the free electromagnetic field

**Free electromagnetic fields:**

Expressed in the Coulomb gauge (\( \nabla \cdot A = 0 \)), Maxwell’s equations for the vector potential \( A(x, t) \) and the scalar potential \( \phi(x, t) \) in vacuum (without sources) are reduced to

\[
\nabla^2 \phi = 0, \quad \Box A = 0,
\]

\[
\Box \equiv \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2.
\]

The corresponding fields are obtained through

\[
\mathbf{B} = \nabla \times \mathbf{A} \quad \text{and} \quad \mathbf{E} = -\frac{1}{c} \frac{\partial \mathbf{A}}{\partial t} - \nabla \phi.
\]

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

**Transversal electromagnetic fields:**

The fields \( \mathbf{E} \) and \( \mathbf{B} \) are *transversal* fields like \( \mathbf{A} \), because for a plane wave

\[
\mathbf{A} = A_0 e^{i(k \cdot x - \omega t)}
\]

results \( \nabla \cdot \mathbf{A} = 0 \) in \( k \cdot \mathbf{A} = 0 \). Hence the Coulomb gauge is also called *transversal gauge*. It proved favorable to use the Coulomb gauge in the quantization process.
Field energy:
No quantization without Hamilton operator, and for this we need the expression for the total energy
\[ E_{\text{cl}} = \frac{1}{8\pi} \int (E^2 + B^2) d^3 r \]
of the radiation field. We are now looking for an operator \( \hat{A}_{\text{op}} \) for the vector potential so that
\[ i\hbar \frac{d}{dt} \hat{A}_{\text{op}} = [\hat{A}_{\text{op}}, \hat{H}] \quad \iff \quad \Box \hat{A}_{\text{op}} = 0 \quad (4.11) \]
where \( \hat{H} = E_{\text{cl}} \) applies.

Periodic boundary conditions:
The quantization is easier to do if there are only countable many degrees of freedom. But the vector field is continuous and have uncountable many degrees of freedom. Therefore we use periodic boundary conditions
\[ A(x + L, y, z, t) = A(x, y, z, t) \]
for a finite volume \( V = L^3 \). At the end of the calculations, we will expand it to infinity.

Fourier Series:
Fields which exist on a finite hypercube can be expanded in a Fourier series. The general solution of (4.9) then reads
\[ A(r, t) = \sum_k \sum_\lambda \sqrt{\frac{2\pi \hbar c}{k}} \frac{1}{\sqrt{V}} \left( A_\lambda(k, t)e^{ik \cdot r} + A^*_\lambda(k, t)e^{-ik \cdot r} \right) u_\lambda(k) \]
The \( k \) sum runs over all valid \( k \) vectors. In the case of periodic boundary conditions they are given by
\[ k = \frac{2\pi}{L} (n_1, n_2, n_3), \quad \text{with} \quad n_i \in \mathbb{Z}. \]
The index \( \lambda \) runs over 1 and 2 and accounts for the polarization. The prefactor under the root will be usefull later but has no further physical meaning. The unit vectors \( u_1 \) and \( u_2 \) are orthogonal to each other and together with the wave vector \( k \) they form an orthogonal trihedron (transversal gauge):
\[ k \cdot u_\lambda(k) = 0, \quad \text{and} \quad u_\lambda(k) \cdot u_\mu(k) = \delta_{\mu\lambda}. \]
Additionally we chose without loss of generality \( u_\lambda(k) = u_\lambda(-k) \).

Harmonic Oscillator:
It is important to note that due to (4.9) every Fourier coefficient \( A_\lambda(k, t) \) satisfies the equation
\[ \Box A = 0 \quad \Rightarrow \quad \frac{\partial^2 A_\lambda}{\partial t^2}(k, t) = -c^2 k^2 A_\lambda(k, t) \quad (4.12) \]
which corresponds to the differential equation of a harmonic oscillator. This fact will later on provide the basis for the quantization of the light field.
General solution of the Wave Equation:
To satisfy (4.12), we set
\[ A_\lambda(k, t) = A_\lambda(k)e^{-i\omega_k t}, \quad \omega_k = c|k| \]
The general solution of the wave equation (4.9) is then given by
\[
A(r, t) = \sum_k \sum_{\lambda} \sqrt{\frac{2\pi\hbar c}{k}} \frac{1}{\sqrt{\pi}} \left( A_\lambda(k)e^{i(k\cdot r -\omega_k t)} + A^*_\lambda(k)e^{-i(k\cdot r -\omega_k t)} \right) u_\lambda(k)
\] (4.13)
The time-independent field amplitudes \( A_\lambda(k) \) will become operators in the Schrödinger picture when the quantization is carried out.

Energy of the light field:
With the help of (4.13) we want to express the total energy of the radiation field through the \( A_\lambda(k) \) only. With (4.10) and \( \phi = 0 \) follows
\[
E_{\text{cl}} = \frac{1}{8\pi} \int (E^2 + B^2) \, d\mathbf{r} = \frac{1}{8\pi} \int \left[ \frac{1}{c^2} \left( \frac{\partial A}{\partial t} \right)^2 + (\nabla \times A)^2 \right] \, d^3\mathbf{r} \quad (4.14)
\]
We will calculate both parts of the integrals in separate steps.

The \( \partial_t A \)-term of the field energy:
It is
\[
\frac{1}{8\pi c^2} \int \left( \frac{\partial A}{\partial t} \right)^2 \, d^3\mathbf{r} = \frac{1}{8\pi c^2} \int \frac{2\pi\hbar c^2}{V} \sum_{k, k'} \sum_{\lambda, \lambda'} \left[ -\frac{\omega_k \omega_{k'}}{\sqrt{\omega_k \omega_{k'}}} u_\lambda(k) \cdot u_{\lambda'}(k') \right]
\times (A_\lambda(k, t)e^{ik\cdot r} - A^*_\lambda(k, t)e^{-i\kappa_{k'} r})(A_{\lambda'}(k', t)e^{i\kappa_{k'} r} - A^*_{\lambda'}(k', t)e^{-i\kappa_{k'} r}) \, d^3\mathbf{r}
\] (4.15)
One can make use of the relation
\[
\frac{1}{V} \int e^{i(k-k')\cdot r} \, d^3\mathbf{r} = \delta_{k,k'} \quad \text{and} \quad \frac{1}{V} \int e^{-i(k+k')\cdot r} \, d^3\mathbf{r} = \delta_{k,-k'}.
\] (4.16)
Furthermore
\[
\sum_{\lambda, \lambda'} u_\lambda(k) \cdot u_{\lambda'}(k) = \sum_{\lambda}
\]
because \( u_\lambda(k) \cdot u_{\lambda'}(k) = \delta_{\lambda, \lambda'} \). After this (4.15) transforms to
\[
\frac{1}{8\pi c^2} \int (\partial_t A)^2 \, d^3\mathbf{r} = \frac{1}{4} \sum_{k, \lambda} h\omega_k [A_\lambda(k, t)A^*_\lambda(k, t) + A^*_\lambda(k, t)A_\lambda(k, t)]
- A_\lambda(k, t)A_\lambda(-k, t) - A^*_\lambda(-k, t)A^*_{\lambda}(k, t).
\]
The \( \nabla \times A \)-term of the field energy:
The second integral provides the same result (except for the sign) as the first
\[
\frac{1}{8\pi} \int (\nabla \times A)^2 \, d^3\mathbf{r} = \frac{1}{4} \sum_{k, \lambda} h\omega_k [A_\lambda(k, t)A^*_\lambda(k, t) + A^*_\lambda(k, t)A_\lambda(k, t)]
+ A_\lambda(k, t)A_\lambda(-k, t) + A^*_\lambda(-k, t)A^*_{\lambda}(k, t).
\]
The last two terms will therefore cancel out and we find

\[
E_{cl} = \frac{1}{2} \sum_k \sum_\lambda \hbar \omega_k \left[ A_\lambda(k)A_\lambda^*(k) + A_\lambda^*(k)A_\lambda(k) \right]
\]

\[
\omega_k = c|k|
\]

(4.17)

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

### 4.3 Quantization of the light field

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

**Photons are Bosons:**

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

\[
A_\lambda(k) \rightarrow \hat{a}_\lambda(k),
\]

\[
A_\lambda^*(k) \rightarrow \hat{a}_\lambda^*(k)
\]

(4.18)

where the ladder operators satisfy the bosonic commutation relation

\[
[\hat{a}_\lambda(k), \hat{a}_\lambda^*(k')] = \delta_{k,k'}\delta_{\lambda,\lambda'}.
\]

(4.19)

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

\[
[\hat{a}_k, \hat{a}_k^*] = \delta_{k,k'}.
\]

**Hamiltonian:**

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

\[
\hat{H}_{em} = \sum_k \hbar \omega_k \left( \hat{a}_k^\dagger \hat{a}_k + \frac{1}{2} \right) = \sum_k \hbar \omega_k \left( \hat{N}_k + \frac{1}{2} \right).
\]

(4.20)

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

**Operator of the vector potential:**

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

\[
\hat{A}_{\text{op}}(\mathbf{r}, t) = \sum_k \sqrt{\frac{2\pi \hbar c^2}{V \omega_k}} \left( \hat{a}_k e^{i(k \cdot \mathbf{r} - \omega_k t)} + \hat{a}_k^\dagger e^{-i(k \cdot \mathbf{r} - \omega_k t)} \right) \mathbf{u}_k,
\]

\[
\omega_k = c|k|
\]

(4.21)
all properties of the quantized light field can be derived directly from this representation.

**Equation of motion in the Heisenberg picture:**

The Heisenberg equation

\[
\frac{i\hbar}{\hbar} \frac{\partial \hat{A}_{\text{op}}}{\partial t} = [\hat{A}_{\text{op}}, \hat{H}],
\]

(4.22)

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

\[
\Box \hat{A}_{\text{op}}(\mathbf{r},t) = 0, \quad \Box e^{\pm i(k \cdot r - \omega_k t)} = 0
\]

which is already satisfied for every single wave.

Considering every separate term and using \([\hat{a}^\dagger \hat{a}, \hat{a} \hat{a}^\dagger] = -\hat{a}^\dagger \hat{a}\):

\[
i\hbar(\pm \omega_k)\hat{a}_k + \hbar \omega_k [\hat{a}_k, \hat{N}_k] = \hbar \omega_k \hat{a}_k - \hbar \omega_k \hat{a}_k = 0.
\]

Therefore the equation of motion is satisfied too.

**Time dependence:**

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

\[
\hat{a}_k(t) = e^{i\hat{H}t/\hbar} \hat{a}_k e^{-i\hat{H}t/\hbar}.
\]

Then is

\[
\frac{d}{dt} \hat{a}_k(t) = \frac{1}{i\hbar} e^{i\hat{H}t/\hbar} [\hat{a}_k, \hat{H}] e^{-i\hat{H}t/\hbar} = \frac{1}{i\hbar} e^{i\hat{H}t/\hbar} (\hbar \omega_k \hat{a}_k) e^{-i\hat{H}t/\hbar} = -i\omega_k \hat{a}_k,
\]

which leads to

\[
\hat{a}_k(t) = e^{-i\omega_k t} \hat{a}_k
\]

and

\[
\hat{a}^\dagger_k(t) = e^{i\omega_k t} \hat{a}^\dagger_k.
\]

This is obviously consistent with (4.21).

**Field operators:**

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

\[
\hat{\mathbf{E}}_{\text{op}}(\mathbf{r},t) = i \sum_k \sqrt{\frac{2\pi \hbar \omega_k}{V}} \left( \hat{a}_k e^{i(k \cdot r - \omega_k t)} - \text{h.c.} \right) \mathbf{u}_k,
\]

(4.23)

\[
\hat{\mathbf{B}}_{\text{op}}(\mathbf{r},t) = i \sum_k \mathbf{k} \times \sqrt{\frac{2\pi \hbar c^2}{V \omega_k}} \left( \hat{a}_k e^{i(k \cdot r - \omega_k t)} - \text{h.c.} \right) \mathbf{u}_k.
\]

(4.24)

The abbreviation “h.c.” describes the Hermitic conjugate of the first expression in brackets, in this case \( \hat{a}^\dagger_k e^{-i(k \cdot r - \omega_k t)} \).

**Momentum:**

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

\[
\mathbf{P} = \frac{1}{4\pi c} \int \mathbf{E} \times \mathbf{B} \, d^3 \mathbf{r}.
\]
From (4.23) and (4.24)

\[
\hat{P}_{op} = \sum_{k} \hbar k \hat{a}^\dagger_k \hat{a}_k = \sum_{k} \hbar k \hat{N}_k.
\]

The momentum of a single photon is given by \(\hbar k\).

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

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

\[
\hat{a}_k |0\rangle = 0 \quad \forall k \quad \text{and} \quad \langle 0|0 \rangle = 1.
\]

(4.25)

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

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

\[
\left(\hat{a}^\dagger_{k_1}\right)^{n_{k_1}} \left(\hat{a}^\dagger_{k_2}\right)^{n_{k_2}} \cdots |0\rangle = \prod_{i=0}^{\infty} \left(\frac{\hat{a}^\dagger_{k_i}}{\sqrt{n_{k_i}}}\right)^{n_{k_i}} |0\rangle.
\]

Or in short \(|n_{k_1}, n_{k_2}, \cdots\rangle\) or \(|\{n_{k_i}\}\rangle\).

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

\[
\hat{N}_{k_i} |\cdots, n_{k_i}, \cdots\rangle = n_{k_i} |\cdots, n_{k_i}, \cdots\rangle.
\]

(4.27)

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

\[
|n_{k_1}\rangle \otimes |n_{k_2}\rangle \otimes \cdots = |n_{k_1}\rangle |n_{k_2}\rangle \cdots
\]

(4.28)

For every mode \(k\) the \(|n_k\rangle\) \(\forall n_k\) form a complete set of orthonormal states. If one is interested in a single mode, one writes for the considered state only \(|n_k\rangle\).

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

**Zero Point Energy**:

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

\[
\langle 0|\hat{H}_{em}|0\rangle = \frac{1}{2} \sum_{k} \hbar \omega_k \rightarrow \infty.
\]

(4.29)

The energy of the vacuum seems to be divergent!

- In general we only consider energy differences where an infinite vacuum energy is of no concern.

- The vacuum energy is dependent of the boundary conditions and changes within restricted geometries, e.g. the intermediate space between two conducting plates, which can be experimentally seen in the *Casimir effect*. 
4.4 Properties of the radiation field: Coherent states

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

\[ \hat{E}_{\text{op}}(r, t) = -\frac{1}{c} \frac{\partial \hat{A}_{\text{op}}}{\partial t} = i \sum_k \sqrt{\frac{2\pi \hbar \omega_k}{V}} \left( \hat{a}_k e^{i(k \cdot r - \omega_k t)} - \text{h.c.} \right) u_k. \]

We are now only interested in a single mode \( k \). For this mode the above equation simply reads

\[ \hat{E}_{\text{op}}(k, t) = i \sqrt{\frac{2\pi \hbar \omega_k}{V}} \left( \hat{a}_k e^{i(k \cdot r - \omega_k t)} - \text{h.c.} \right) u_k. \]

The expectation value of this operator in a state \( |n_k\rangle \) with fixed population \( n_k \) of photons is

\[ \langle n_k | \hat{E}_{\text{op}}(k, t) | n_k \rangle = 0 \]

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

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

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

\[ \langle n_k | \frac{1}{8\pi} (\hat{E}_{\text{op}}^2 + \hat{B}_{\text{op}}^2) | n_k \rangle = \langle n_k | \frac{1}{4\pi} \hat{E}_{\text{op}}^2 | n_k \rangle = \frac{1}{V} \hbar \omega_k \left( n_k + \frac{1}{2} \right), \]

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

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

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

\[ \hat{a} = \sqrt{\hat{N}} + 1 e^{i\hat{\phi}}, \quad \hat{a}^\dagger = e^{-i\hat{\phi}^\dagger} \sqrt{\hat{N}} + 1, \quad \hat{N} = \hat{a}^\dagger \hat{a} \]

which corresponds to a separation of the creation and annihilation operators in amplitude and phase. \( \hat{N} = \hat{a}^\dagger \hat{a} \) is verified even if not obvious. This procedure can be in general performed in a bosonic system. We will further see, that the phase operator is almost self-adjoint, \( \hat{\phi} \simeq \hat{\phi}^\dagger \), special care has only to be taken when looking at the vacuum state \( |0\rangle \).
First we have to show that the representation (4.30) is unitary. We face the task to find such commutation relations, so that

\[ [\hat{N}, \hat{\phi}] =? \iff [\hat{a}, \hat{a}^\dagger] = 1. \] (4.31)

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

\[ \left( \sqrt{\hat{N} + 1} \right)^{-1} \hat{a} = e^{i\hat{\phi}} \quad \hat{a}^\dagger \left( \sqrt{\hat{N} + 1} \right)^{-1} = e^{-i\hat{\phi}^\dagger}. \] (4.32)

Reminder:
\[ \hat{a} |n\rangle = \sqrt{n} |n - 1\rangle \quad \hat{a}^\dagger |n\rangle = \sqrt{n + 1} |n + 1\rangle \]

This gives:
\[ e^{i\hat{\phi}} |n\rangle = \left( \sqrt{\hat{N} + 1} \right)^{-1} \hat{a} |n\rangle = (1 - \delta_{n,0}) \left( \sqrt{(n - 1) + 1} \right)^{-1} \sqrt{n} |n - 1\rangle = \begin{cases} |n - 1\rangle & : n > 0 \\ 0 & : n = 0 \end{cases}, \]

and
\[ e^{-i\hat{\phi}^\dagger} |n\rangle = \hat{a}^\dagger \left( \sqrt{\hat{N} + 1} \right)^{-1} |n\rangle = (n + 1)^{-1/2} \hat{a}^\dagger |n\rangle = |n + 1\rangle. \]

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

\[ \langle n|e^{i\hat{\phi}}|m\rangle = \delta_{n,m-1}, \]
\[ \langle n|e^{-i\hat{\phi}^\dagger}|m\rangle = \delta_{n-1,m}, \]

and therefore

\[ \langle m|e^{i\hat{\phi}}e^{-i\hat{\phi}^\dagger}|n\rangle = \delta_{m,n} \quad \langle m|e^{-i\hat{\phi}^\dagger}e^{i\hat{\phi}}|n\rangle = (1 - \delta_{n,0})\delta_{m,n}. \] (4.33)

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

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

\[ \sin \hat{\phi} \equiv \frac{e^{i\hat{\phi}} - e^{-i\hat{\phi}^\dagger}}{2i}, \quad \cos \hat{\phi} \equiv \frac{e^{i\hat{\phi}} + e^{-i\hat{\phi}^\dagger}}{2}. \] (4.34)

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

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

\[ 1 = \hat{a}\hat{a}^\dagger - \hat{a}^\dagger\hat{a} = \sqrt{\hat{N} + 1}e^{i\hat{\phi}}e^{-i\hat{\phi}^\dagger}\sqrt{\hat{N} + 1} - e^{-i\hat{\phi}^\dagger}(\hat{N} + 1)e^{i\hat{\phi}} = \hat{N} - e^{-i\hat{\phi}^\dagger}\hat{N}e^{i\hat{\phi}} \]
Multiplying both sides with $e^{i\phi}$ yields:

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

Therefore:

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

With this we obtain

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

and

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

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

$$[\hat{N}, \hat{\phi}] = i$$  

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

**Uncertainty Relation:**

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

One brings to mind the Heisenberg uncertainty principle

$$(\Delta \hat{A})(\Delta \hat{B}) \geq \frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle| = \frac{1}{2}, \quad [\hat{A}, \hat{B}] = i,$$

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

**Digression: Superconductivity:**

This result is essential for superfluidity (see chapter 3, where we discussed the meaning of the phase of the condensate wave function) and for superconductivity. Superconductivity comes into being through singlet pairing of electrons and one can – in a very crude approximation – view this pairs as bosons, because following the spin statistics theorem, this particles possess integer spin – like bosons.

The superconductive condensate is characterized by a fixed phase, one also speaks of a spontaneous breaking of the global gauge invariance.

But when the phase is fixed, then the particle number cannot be according to (4.35). Therefore the BCS wave function is

$$|\psi_{BCS}\rangle = \prod_k (u_k + v_k \tikz[baseline=-1pt]{
ode (e) {$\tikz{\draw[thick] (-0.25mm,-0.25mm) -- (0.25mm,0mm) -- (0mm,0.25mm);}$};}) \langle 0 |$$

given by a coherent superposition of states with a different number of singlet pairs.
CHAPTER 4. QUANTIZATION OF THE CLASSICAL RADIATION FIELD

Variance:
In a pure state \( |n\rangle \) with fixed photon number, the natural fluctuation of the occupation number operator vanishes:
\[
\Delta N = \sqrt{\langle n|\hat{N}^2|n\rangle - \langle n|\hat{N}|n\rangle^2} = 0
\]
In contrast, \( \cos \phi \) has a finite fluctuation. It is \( \langle \cos \phi \rangle = 0 \) and
\[
\langle \cos^2 \phi \rangle = \frac{1}{4} (e^{i\phi}e^{-i\phi} + e^{-i\phi}e^{i\phi}) = 2 - \frac{\delta_{n,0}}{4}
\]
in a pure state \( |n\rangle \), and therefore \( \Delta \cos \phi = \Delta \sin \phi \):
\[
\Delta \cos \phi = \sqrt{\langle \cos^2 \phi \rangle - \langle \cos \phi \rangle^2} = \begin{cases} 1/\sqrt{2} & ; n > 0, \\ 1/2 & ; n = 0. \end{cases}
\]

Coherent States:
One can do a linear combination of states with different particle numbers to achieve a transition to macroscopic electrodynamics. One defines a coherent state \( |c\rangle \) (also called a Glauber state, Nobel price 2005) through
\[
|c\rangle \equiv e^{-|c|^2/2} \sum_{n=0}^{\infty} \frac{c^n}{\sqrt{n!}} |n\rangle \quad \text{with} \quad c \in \mathbb{C}, \quad c = |c|e^{i\theta}
\]
By using the representation (4.26) for the state \( |n\rangle \), one can write in a more compact fashion:
\[
|c\rangle = e^{-|c|^2/2} \sum_{n=0}^{\infty} \frac{c^n}{\sqrt{n!}} (\hat{a}^\dagger)^n |0\rangle = \exp \left( -\frac{|c|^2}{2} + c\hat{a}^\dagger \right) |0\rangle
\]
A Glauber state \( |c\rangle \) only contains the \( \{|n\rangle\} \) of a single mode, so \( \mathbf{k} \) is still sharply defined.

Properties of a Glauber state:
The coherent states are eigenstates of \( \hat{a} \). Proof:
\[
\hat{a} |c\rangle = e^{-|c|^2/2} \sum_{n=0}^{\infty} \frac{c^n}{\sqrt{n!}} \hat{a} |n\rangle = e^{-|c|^2/2} \sum_{n=1}^{\infty} \frac{c^n}{\sqrt{(n-1)!}} |n-1\rangle = e^{-|c|^2/2} \sum_{n=0}^{\infty} \frac{c^{n+1}}{\sqrt{n!}} |n\rangle = c|c\rangle.
\]
The Glauber state is thus an eigenstate of the annihilation operator. We summarize the relations:
\[
\hat{a} |c\rangle = c|c\rangle, \quad \langle c|\hat{a}|c\rangle = c, \quad \langle c|\hat{a}^\dagger|c\rangle = c^*, \quad \langle c|c\rangle = 1 \quad (4.36)
\]
We notice that the coherent states do not build an orthogonal basis, because in general \( \langle c|c'\rangle \neq 0 \).

Electric field of a coherent state:
The expectation value
\[
\langle c|\hat{E}_{\text{op}}|c\rangle = i \sqrt{\frac{2\pi\hbar\omega_k}{V}} \left( e^{i(k \cdot r - \omega_k t)} - \text{c.c.} \right) \mathbf{u}_k = i \sqrt{\frac{2\pi\hbar\omega_k}{V}} |c| \left( e^{i(k \cdot r - \omega_k t + \theta)} - \text{c.c.} \right) \mathbf{u}_k
\]
\[
= -2 \sqrt{\frac{2\pi\hbar\omega_k}{V}} |c| \sin(k \cdot r - \omega_k t + \theta) \mathbf{u}_k. \quad (4.37)
\]
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of the electrical field in a coherent state is equivalent to the classical value. Hence there exists a one-to-one relation between the plane waves of classical electrodynamics and the coherent states |c⟩, because through c = |c|e^{iθ} the amplitude as well as the phase of the plane wave can be determined by use of Eq. (4.37).

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

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

and

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

so that

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

The relative fluctuation of the photon number is therefore

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

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

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

which matches a Poisson distribution.

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

Proof:

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

hence

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

Since

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

one has

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

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

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

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

**Fluctuations of the phase:**

We assume the uncertainty relation of to general Hermitian operators \( A \) and \( B \):

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

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

\[ \Delta \hat{N} \Delta \sin \hat{\phi} \geq \frac{1}{2} \left| \langle \cos \hat{\phi} \rangle \right| \]

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

\[ \frac{\Delta \cos \hat{\phi}}{|\langle \cos \hat{\phi} \rangle|} \geq \frac{1}{2|c|}. \quad (4.40) \]

This estimate provides strictly speaking only a lower bound of the relative fluctuations of the phase, but saves the need of costly calculations. In general, the actual fluctuations are determined by two operators of the same magnitude as the corresponding uncertainty relation.

The relative fluctuations of the phase thus vanish in the limit of large photon numbers \(\langle \hat{N} \rangle = |c|^2\), just as the relative fluctuations of the photon numbers itself, see Eq. (4.39).

**Classical Limit:**

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

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

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

**Minimal coupling:**

The total Hamiltonian of matter and radiation reads

\[ \hat{H} = \hat{H}_{\text{em}} + \hat{H}_{\text{mat}} + \hat{H}_I, \]

(4.41)

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

\[ \hat{H}_{\text{em}} = \sum_k \hbar \omega_k \left( \hat{N}_k + \frac{1}{2} \right), \quad \hat{H}_{\text{mat}} = \sum_i \frac{\hat{p}_i^2}{2m_i} + \hat{V}(r_1, r_2, \ldots). \]

We will neglect spin effects. The index \( i \) runs over all particles. After the introduction of electromagnetic field, the interaction \( H_I \) results from minimal coupling in Coulomb gauge via:

\[ \hat{p}_i \rightarrow \hat{p}_i - \frac{e}{c} \hat{A}_{\text{op}}(r_i, t), \]

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

**Light-Matter Interaction:**

By using \( \hat{A}_{\text{op}}^i \equiv \hat{A}_{\text{op}}(r_i, t) \), one arrives at

\[ \hat{H}_I = \sum_i \left[ -\frac{e}{2m_i c} \left( \hat{p}_i \cdot \hat{A}_{\text{op}}^i + \hat{A}_{\text{op}}^i \cdot \hat{p}_i \right) + \frac{e^2}{2m_i c^2} \left( \hat{A}_{\text{op}}^i \right)^2 \right] \]

\[ = -\sum_i \frac{e}{m_i c} \hat{A}_{\text{op}}^i \cdot \hat{p}_i + \sum_i \frac{e^2}{2m_i c^2} \left( \hat{A}_{\text{op}}^i \right)^2 \equiv \hat{H}_I' + \hat{H}_I''. \]

(4.42)

for the interaction between light and matter. Due to \( \nabla \cdot A = 0 \), it is possible to set

\[ \hat{p} \cdot \hat{A} = \frac{\hbar}{i} \nabla \cdot \hat{A} + \hat{A} \cdot \hat{p} = \hat{A} \cdot \hat{p}. \]

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

**State Space:**

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

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

**Perturbation operator for a single electron:**

In the following we will consider a special case: we ask for the transition rates of a single bound
electron in an atom (e.g. the hydrogen atom) which are introduced through the presence of a radiation field. The Hamiltonian of the interaction reads now:

$$\hat{H}'_I = -\frac{e}{mc} \sum_k \sqrt{\frac{2\pi \hbar c^2}{V \omega_k}} \left( \hat{a}_k e^{i \hat{k} \cdot \hat{r}} + \text{h.c.} \right) \mathbf{u}_k \cdot \hat{p}. $$

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

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

$$\Gamma_{i\rightarrow f} = \frac{2\pi}{\hbar} \delta(E_i - E_f) |\langle f | \hat{H}_I' |i\rangle|^2.$$

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

$$\hat{H}_{mat} |\varepsilon_i\rangle = \varepsilon_i |\varepsilon_i\rangle, \quad \hat{H}_{mat} |\varepsilon_f\rangle = \varepsilon_f |\varepsilon_f\rangle,$$

$$\hat{H}_{em} |\{n^i_k\}\rangle = \sum_k \hbar \omega_k \left( n^i_k + \frac{1}{2} \right) |\{n^i_k\}\rangle, \quad \hat{H}_{em} |\{n^f_k\}\rangle = \sum_k \hbar \omega_k \left( n^f_k + \frac{1}{2} \right) |\{n^f_k\}\rangle.$$

The states then read

$$|i\rangle = |\varepsilon_i\rangle \otimes |\{n^i_k\}\rangle, \quad |f\rangle = |\varepsilon_f\rangle \otimes |\{n^f_k\}\rangle.$$

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

**Emission of a photon $\hbar \omega$:**
The energies of initial and final state are given by

$$E_i = \varepsilon_i + \sum_{k'} \hbar \omega_{k'} \left( n^i_{k'} + \frac{1}{2} \right),$$

$$E_f = \varepsilon_f + \sum_{k'} \hbar \omega_{k'} \left( n^f_{k'} + \frac{1}{2} \right) + \hbar \omega_k,$$

because exactly one photon of energy $\hbar \omega_k$ should be emitted. The state vectors read:

$$|i\rangle = |\varepsilon_i\rangle \otimes |\cdots, n_k, \cdots\rangle,$$

$$|f\rangle = |\varepsilon_f\rangle \otimes |\cdots, n_k + 1, \cdots\rangle.$$

The Golden Rule states, that a corresponding transition must satisfy

$$E_i - E_f = \varepsilon_i - (\varepsilon_f + \hbar \omega_k) = 0.$$
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This is exactly the conservation of energy. Further applies
\[
\langle f | \hat{H}'_I | i \rangle = -\frac{e}{mc} \sum_{k'} \sqrt{\frac{2\pi \hbar c^2}{V \omega_{k'}}} \langle \varepsilon_f | e^{-i\mathbf{k}' \cdot \hat{\mathbf{r}}} \mathbf{u}_{k'} \cdot \hat{\mathbf{p}} | \varepsilon_i \rangle \langle \cdot, \cdot, n_k + 1, \cdot, \cdot | \hat{a}_{k'}^\dagger | \cdot, \cdot, n_k, \cdot \rangle.
\]

The annihilators do not appear anymore, because the corresponding matrix elements will disappear (more photons appear on the left hand side than on the right hand side). Only the summand with \( k = k' \) survives. Only then is a photon in the right state created and the inner product will not vanish. The second term in the brackets reads therefore
\[
\langle \cdot, \cdot, n_k + 1, \cdot, \cdot | \hat{a}_{k'}^\dagger | \cdot, \cdot, n_k, \cdot \rangle = \sqrt{n_k + 1} \delta_{k,k'}
\]
and the transition rate of the emission is given by:
\[
\Gamma_{e,i \rightarrow f} = \frac{4\pi^2 e^2}{m^2 V \omega_k} \delta(\varepsilon_i - \varepsilon_f - \hbar \omega_k)(n_k + 1) | \langle \varepsilon_f | e^{-i\mathbf{k} \cdot \hat{\mathbf{r}}} \mathbf{u}_{k} \cdot \hat{\mathbf{p}} | \varepsilon_i \rangle |^2.
\]

**Absorption of a photon \( \hbar k \):**
The energies of initial and final states are
\[
E_i = \varepsilon_i + \sum_{k'} \hbar \omega_{k'} \left( n_{k'} + \frac{1}{2} \right),
\]
\[
E_f = \varepsilon_f + \sum_{k'} \hbar \omega_{k'} \left( n_{k'} + \frac{1}{2} \right) - \hbar \omega_k,
\]
because now a photon will be "extracted" from the light field. The state vectors are given by
\[
|i\rangle = |\varepsilon_i \rangle \otimes |\cdot, \cdot, n_k, \cdot \rangle,
\]
\[
|f\rangle = |\varepsilon_f \rangle \otimes |\cdot, \cdot, n_k - 1, \cdot \rangle.
\]
In this case, the creation operators do not contribute to the calculation of the matrix elements \( \langle f | \hat{H}'_I | i \rangle \). Furthermore, only the annihilation operator with \( k = k' \) remains. Analogous to the emission one finds:
\[
\Gamma_{a,i \rightarrow f} = \frac{4\pi^2 e^2}{m^2 V \omega_k} \delta(\varepsilon_i - \varepsilon_f + \hbar \omega_k)n_k | \langle \varepsilon_f | e^{i\mathbf{k} \cdot \hat{\mathbf{r}}} \mathbf{u}_{k} \cdot \hat{\mathbf{p}} | \varepsilon_i \rangle |^2.
\]

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

- **Spontaneous emission:** One speaks of a spontaneous emission if a photon is emitted in absence of other photons. Spontaneous emission is possible, because the factor \( n_k + 1 \) in Eq. (4.43) will not disappear if a external photon field is missing (\( n_k = 0 \)).

- **Stimulated emission:** The factor \( n_k + 1 \) in Eq. (4.43) implies, that in presence of a external field with the same quantum numbers, the emission probability is increased, proportional to the intensity of the external light field. One speaks of stimulated emission – which is essential for the laser – because a mode \( \hbar k \) can only stimulate an emission of a photon of the same wave length \( \lambda = 2\pi/|k| \). One obtains coherent radiation.
Absorption: The interpretation of the occupation factor $n_k$ in Eq. (4.44) of the absorption process is relatively trivial. Photons can only be absorbed, if any are present.

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

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

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

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

and find

$$\langle \varepsilon_f | \hat{p} | \varepsilon_i \rangle = \langle \varepsilon_f | \frac{im}{\hbar} [\hat{H}_{\text{mat}}, \hat{r}] | \varepsilon_i \rangle = \frac{im}{\hbar} \langle \varepsilon_f | \hat{H}_{\text{mat}} \hat{r} - \hat{r} \hat{H}_{\text{mat}} | \varepsilon_i \rangle = \frac{im}{\hbar} \langle \varepsilon_f | \hat{r} | \varepsilon_i \rangle (\varepsilon_f - \varepsilon_i).$$

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

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

as interaction term.

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

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

$$e^{\pm ik\cdot\hat{r}} \simeq 1 \pm ik \cdot \hat{r} + \ldots.$$ 

The next order (linear in $k \cdot \hat{r}$) describes magnetic dipole and electric quadrupole transitions.
4.6 Lifetime of an excited state

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

**Lifetime of an excited state:**

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

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

(4.46)

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

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

**Thermodynamic limit:**

$V$ will now approach infinity. This is done by the substitution

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

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

**Summation over different polarizations:**

First we will perform the $\lambda$-summation. We have to calculate:

$$
\sum_{\lambda=1}^{2} \left| u_{\lambda}(k) \cdot \langle \varepsilon_f | \hat{r} | \varepsilon_i \rangle \right|^2
$$

Other than building an orthogonal trihedron with $k$, $u_{\lambda}$ can be chosen freely. E.g. one can choose $u_2$ to be perpendicular to the dipole matrix element $d$, which will result in a dependence of the sum on $u_1$ alone. Let the angle between $d$ and $u_1$ be $\xi$, the angle between $d$ and $k$ reads $\theta = \pi/2 - \xi$. The above sum then yields

$$
| \langle \varepsilon_f | \hat{r} | \varepsilon_i \rangle |^2 \sin^2 \theta.
$$
The orthogonal trihedron consisting of the two polarization vectors $\mathbf{u}_1$, $\mathbf{u}_2$ and the wave vector of the photon $\mathbf{k}$ can be arranged in such a way, so that the dipole matrix element $\mathbf{d}$ lies within the plane spanned by $\mathbf{u}_1$ and $\mathbf{k}$.

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

$$
\frac{1}{\tau} = \sum_f \frac{4\pi^2 e^2}{\hbar^2} (\varepsilon_f - \varepsilon_i)^2 |\langle \varepsilon_f | \hat{r} | \varepsilon_i \rangle|^2 \frac{1}{(2\pi)^3} \int k^2 \sin \theta \sin^2 \theta \frac{\delta(\varepsilon_f - \varepsilon_i + \hbar \omega_k)}{\omega_k} dk d\theta d\varphi
$$

$$
= \sum_f \frac{e^2}{2\pi \hbar^4 c^3} (\varepsilon_f - \varepsilon_i)^2 |\langle \varepsilon_f | \hat{r} | \varepsilon_i \rangle|^2 \int_{8\pi/3} \sin^3 \theta d\theta d\varphi \int_{\varepsilon_f - \varepsilon_i}^{\varepsilon_f + \varepsilon_i} \varepsilon \delta(\varepsilon - \varepsilon_i) d\varepsilon
$$

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

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

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

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

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

This principle is applied in every laser. The matrix element $r_{if} = |\langle \varepsilon_f | \hat{r} | \varepsilon_i \rangle|^2$ contains selection rules for electric dipole transitions → cf. Stark effect.

Hydrogen atom: $\tau(2p \to 1s) = 1.6 \cdot 10^{-9}$ s, lifetime of magnetic dipole or electric quadrupole transitions is four times longer. Interestingly $2s \to 1s$: forbidden in every multipole expansion ⇒ long lifetime of $1/7$ s, multi-photon process.
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Light scattering on atoms:
In such a process the photon number is conserved

$$|i⟩ = \langle(\mathbf{k}, \varepsilon, \omega), \frac{A}{1 \text{ photon atomic state}} \rangle,$$

$$|f⟩ = \langle(\mathbf{k'}, \varepsilon', \omega'), B⟩.$$

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

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

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

Elastic scattering: $\omega' = \omega$, $B = A$.
Limiting case $\omega \ll \omega_{1A} \equiv (E_I - E_A)/\hbar$: Rayleigh scattering. Expansion in powers of $\omega/\omega_{1A}$:

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

Limiting case $\omega \gg \omega_{1A}$: Thomson scattering

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

also applies when $\omega_{1A} = 0$, i.e. for free electrons, the Compton scattering.

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

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

Special situation: $E_I = E_A + \hbar \omega \rightarrow$ resonant Raman scattering, KH-formula fails. Energy uncertainty has to be considered.
4.7 Interaction between light and matter in Second Quantization

Our goal is now, in association with the first part of the lesson, to examine the interaction of light and matter. The representation of matter states in the second quantization formalism will allow us to introduce the concept of Feynman diagrams, which play an important role in the theory of many particles as well as the theory of fundamental particles.

Because everything will be expressed as an operator now, we will neglect emphasis of operators via bold letters.

Light-matter Hamiltonian in second quantization:

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

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

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

$$\hat{H}_{\text{mat}} = \int \text{d} r \hat{\psi}^\dagger(r) \left( -\frac{\hbar^2}{2m} \Delta + V(r) \right) \hat{\psi}(r)$$

$$\hat{H}_I = \int \text{d} r \hat{\psi}^\dagger(r) \left[ \frac{e}{mc} \hat{A}_{\text{op}} \cdot \mathbf{p} + \frac{e^2}{2mc^2} \left( \hat{A}_{\text{op}} \right)^2 \right] \hat{\psi}(r)$$

$$\hat{H}_\text{em} = \sum_q \hbar \omega_q \left( \hat{a}_q^\dagger \hat{a}_q + \frac{1}{2} \right),$$

where

$$\hat{A}_{\text{op}} = \sum_q \sqrt{\frac{2\pi \hbar c^2}{V \omega_q}} \left( \hat{a}_q e^{i\mathbf{q} \cdot \mathbf{r}} + \hat{a}_q^\dagger e^{-i\mathbf{q} \cdot \mathbf{r}} \right) \mathbf{u}_q.$$ 

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

Field operators:

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

$$\hat{\psi}_k(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k e^{i\mathbf{k} \cdot \mathbf{r}} \hat{c}_k$$

$$\hat{\psi}^\dagger_k(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_k e^{-i\mathbf{k} \cdot \mathbf{r}} \hat{c}^\dagger_k$$
where the following (anti-)commutation rules apply:
\[
\{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r'})\} = 0, \quad \{\hat{\psi}(\mathbf{r}), \hat{\psi}(\mathbf{r'})\} = 0, \quad \{\hat{\psi}(\mathbf{r}), \hat{\psi}^\dagger(\mathbf{r'})\} = \delta(\mathbf{r} - \mathbf{r'})
\]
\[
\{\hat{c}_k, \hat{c}_k'\} = 0, \quad \{\hat{c}_k, \hat{c}_k^\dagger\} = 0, \quad \{\hat{c}_k, \hat{c}_k'^\dagger\} = \delta_{k,k'}.
\]

Dispersion relation:
Thus we are able to express \(\hat{H}_{\text{mat}}\) completely in terms of ladder operators:
\[
\hat{H}_{\text{mat}} = \sum_{k,k'} \frac{1}{V} \int d\mathbf{r} e^{-i k \cdot \mathbf{r}} \left( -\frac{\hbar^2}{2m} \right) e^{i k' \cdot \mathbf{r}} \hat{c}_k^\dagger \hat{c}_{k'}
\]
\[
\quad \quad \quad = \frac{\hbar^2 k^2}{2m} \epsilon_k \hat{n}_k
\]

where \(\epsilon_k = \hbar^2 k^2 / 2m\) is called dispersion relation.

\[
\hat{H}_{\text{mat}} = \sum_{k} \frac{\hbar^2 k^2}{2m} \hat{c}_k^\dagger \hat{c}_k = \sum_{k} \epsilon_k \hat{n}_k \tag{4.47}
\]

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

\[
H_1' = \frac{1}{V} \int d\mathbf{r} \sum_{k_1} e^{-i k_1 \cdot r} \hat{c}_k^\dagger \left( -\frac{e \hbar c}{m c} \sum_{\mathbf{q}} \sqrt{\frac{2 \pi \hbar c^2}{V \omega}} a_\mathbf{q} e^{i \mathbf{q} \cdot \mathbf{r}} + a_\mathbf{q}^\dagger e^{-i \mathbf{q} \cdot \mathbf{r}} \right) \mathbf{u}_\mathbf{q} \cdot \nabla \right) \sum_{k_2} e^{i k_2 \cdot r} \hat{c}_k^\dagger
\]
\[
= \sum_{k_1,k_2,\mathbf{q}} \left( M_1(k_1,k_2,\mathbf{q}) \hat{c}_k^\dagger \hat{c}_k^\dagger \hat{c}_k^\dagger + M_1(k_1,k_2,-\mathbf{q}) \hat{c}_k^\dagger \hat{c}_k^\dagger \hat{c}_k^\dagger \right) \tag{4.48}
\]

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

\[
M_1(k_1,k_2,\mathbf{q}) = \frac{1}{V} \int d\mathbf{r} e^{-i k_1 \cdot r} \left( -\frac{e \hbar c}{m c} \sqrt{\frac{2 \pi \hbar c^2}{V \omega}} \mathbf{u}_\mathbf{q} \cdot (\mathbf{i} k_2) e^{i k_2 \cdot r} \right)
\]
\[
= -\frac{e \hbar}{V mc} \sqrt{\frac{2 \pi \hbar c^2}{V \omega}} \mathbf{u}_\mathbf{q} \cdot \mathbf{k}_2 \int d\mathbf{r} e^{i \mathbf{q} + \mathbf{k}_2 - \mathbf{k}_1 \cdot \mathbf{r}}
\]
\[
= -\frac{e \hbar}{mc} \sqrt{\frac{2 \pi \hbar c^2}{V \omega}} \mathbf{u}_\mathbf{q} \cdot \mathbf{k}_2 \delta_{k_1,\mathbf{q} + \mathbf{k}_2}. \tag{4.49}
\]

The last expression in (4.49) represents the conservation of momentum. The partial Hamiltonian \(H_1'\) describes two kinds of processes via its two terms in (4.48):

- The first term destroys a photon \(\mathbf{q}\) and an electron \(k_2\) and creates on the other hand an electron \(k_1\). The total momentum is thereby conserved: \(k_1 = \mathbf{q} + k_2\).
- The second term creates a photon \(\mathbf{q}\) and an electron \(k_1\) but destroys on the other hand an electron \(k_2\). Again the total momentum is conserved via \(k_2 = \mathbf{q} + k_1\).
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Simplification:
It is easy to show that the second term in (4.48) is the Hermitian conjugate of the first term. This is because the first term reads

\[ u_q \cdot k_2 = u_q \cdot (k_1 - q) = u_q \cdot k_1 , \]

so one can instead of \( q \rightarrow -q \) do the substitution \( k_1 \leftrightarrow k_2 \) when doing the transition to the second term. The Hermitian conjugate of the second term satisfies then

\[
\left( \sum_{k_1, k_2, q} M_1(k_2, k_1, q) c_{k_1}^\dagger c_{k_2} a_q^\dagger \right) = \sum_{k_1, k_2, q} M_1(k_2, k_1, q) c_{k_2}^\dagger c_{k_1} a_q \\
= \sum_{k_1, k_2, q} M_1(k_1, k_2, q) c_{k_1}^\dagger c_{k_2} a_q
\]

and this corresponds to the first term. The paramagnetic part of \( \hat{H}'_I \) of the light-matter interaction can therefore be written as

\[
\hat{H}'_I = \sum_{k_1, k_2, q} \left( M_1(k_1, k_2, q) c_{k_1}^\dagger c_{k_2} a_q + \text{h.c.} \right). \tag{4.50}
\]

Feynman diagrams:
Both processes described by \( \hat{H}'_I \) can be visualized by simple diagrams. Fig. 4.1 shows on the left the first process: the annihilation of a photon \( q \) while scattering an electron from the state \( k_2 \) to \( k_1 \). The diagram on the right hand side represents the hermetic conjugated process, namely the creation of a photon under scattering of an electron.

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

**Feynman diagrams:**
Feynman diagrams are a graphical representation of perturbation theoretical processes. Lines represent participating incoming or outgoing particles and the vertices correspond to the matrix elements of the interaction.
Feynman diagrams do not only serve the purpose of visualisation. In many body theory and the theory of fundamental particles every Feynman diagram represents a precise mathematical expression of perturbation theory.

**Conservation of momentum at the vertices:**
A point were different particle lines meet is called a vertex. The Kronecker delta in \( M_1 \) demands at a vertex that the total momentum of annihilated particles is equal to the total momentum of created particles.

**Diamagnetic perturbation term:**
\( \tilde{H}_I'' \) as part of the whole Hamiltonian contains four terms which arise from the product \( \hat{A}^2 \):

\[
\tilde{H}_I'' = \sum_{k_1,k_2} \sum_{q_1,q_2} \left( M_2(k_1,k_2,q_1,q_2) \hat{c}_{k_1} \hat{c}_{k_2} \hat{a}_{q_1} \hat{\alpha}_{q_2} + M_2(k_1,k_2,-q_1,q_2) \hat{c}_{k_1} \hat{c}_{k_2} \hat{a}_{q_1} \hat{\alpha}_{q_2} \\
+ M_2(k_1,k_2,-q_2) \hat{c}_{k_1} \hat{c}_{k_2} \hat{a}_{q_1} \hat{\alpha}_{q_2} + M_2(k_1,k_2,-q_1,-q_2) \hat{c}_{k_1} \hat{c}_{k_2} \hat{a}_{q_1} \hat{\alpha}_{q_2} \right)
\]

\[
= \sum_{k_1,k_2} \sum_{q_1,q_2} \left( M_2(k_1,k_2,q_1,q_2) \hat{c}_{k_1} \hat{c}_{k_2} \hat{a}_{q_1} \hat{\alpha}_{q_2} + M_2(k_1,k_2,-q_1,q_2) \hat{c}_{k_1} \hat{c}_{k_2} \hat{a}_{q_1} \hat{\alpha}_{q_2} + \text{h.c.} \right)
\]

(4.51)

Where

\[
M_2(k_1,k_2,q_1,q_2) = \frac{2\pi \hbar c^2}{V} \frac{1}{\sqrt{\omega_{q_1} \omega_{q_2}}} \frac{1}{2mc^2} \int dr \, e^{i\mathbf{k}_1 \cdot \mathbf{r} - i\mathbf{q}_1 \cdot \mathbf{r}} e^{i\mathbf{k}_2 \cdot \mathbf{r}} (\mathbf{u}_{q_1} \cdot \mathbf{u}_{q_2})
\]

\[
= \frac{2\pi \hbar c^2}{V} \frac{1}{\sqrt{\omega_{q_1} \omega_{q_2}}} \frac{e^2}{2mc^2} (\mathbf{u}_{q_1} \cdot \mathbf{u}_{q_2}) \, \delta_{k_1,k_2,q_1+q_2+2}
\]

(4.52)

The four terms in (4.51) describe vertices, at which two electrons and two photons are involved each. Fig. 4.2 shows the corresponding Feynman graphs. The quantities \( M_1 \) and \( M_2 \) determine the probability of the occurrence of these processes.

![Figure 4.2: Processes associated with first order perturbation theory in \( \tilde{H}_I'' \). Both graphs in the middle describe contributions to Compton scattering. The two diagrams to the right are the Hermitian conjugate of the left ones.](image)

**Compton Scattering:**
Both graphs in the middle of the Fig. 4.2 show the scattering of a photon on a (free) electron,
what is called *Compton scattering* (note that basically we are not looking at one “single photon”, a photon gets annihilated while another is created - at least this is a good visualisation). The other diagrams describe emission and absorption processes involving two photons: Always two photon lines are involved at a vertex created via $H_{1}''$.

### 4.8 Non-relativistic Bremsstrahlung

In the following we will examine the scattering of an electron at a potential, e.g. at a static (because much heavier compared to the electron) nucleus. The charged particle will be hereby accelerated and will radiate energy in the form of photons. This effect is known as *Bremsstrahlung* and is for example used in a dentist’s office to produce the appropriate radiation for a X-ray scan. We will assume that $v/c \ll 1$, namely we are looking at the non-relativistic limiting case.

**Perturbation terms:**

We are interested in the emission of a single photon, therefore the interaction term is given by $H_{I}'$. Furthermore we will consider the potential $V_{\text{Nuc}}(r)$ of a nucleus from the target as a perturbation. The complete operator of the perturbation then reads

$$\hat{V}_{0} = \hat{H}_{I}' + V_{\text{Nuc}}(r).$$

We note that $\hat{H}_{I}''$ is not appearing, because the diamagnetic term of lowest order describes the Rutherford scattering process. We find in second quantization:

$$H_{I}' = \sum_{k_1, k_2, q} \left( M_{I}(k_1, k_2, q) \hat{c}_{k_1}^{\dagger} \hat{c}_{k_2} \hat{a}_{q} + \text{h.c.} \right)$$

and

$$V_{\text{Nuc}} = \int dr \hat{\psi}^{\dagger}(r)V_{\text{Nuc}}(r)\hat{\psi}(r), \quad \text{with} \quad \hat{\psi}(r) = \frac{1}{\sqrt{V}} \sum_{k} e^{i k \cdot r} \hat{c}_{k}.$$

**No conservation of momentum:**

The explicit for of the perturbation potential reads

$$V_{\text{Nuc}} = \frac{1}{V} \sum_{k_1, k_2} \int dr e^{i(k_1 - k_2) \cdot r} V_{\text{Nuc}}(r) \hat{c}_{k_1}^{\dagger} \hat{c}_{k_2} = \frac{1}{V} \sum_{k_1, k_2} \tilde{V}_{\text{Nuc}}(k_1 - k_2) \hat{c}_{k_1}^{\dagger} \hat{c}_{k_2}$$

with $\tilde{V}_{\text{Nuc}}(k) = \int dr V_{\text{Nuc}}(r) e^{-i k \cdot r}$.

The potential $V_{\text{Nuc}}$ is real, therefore the Fourier transform $\tilde{V}_{\text{Nuc}}$ is Hermitian symmetric, i.e. $\tilde{V}_{\text{Nuc}}(-k) = \tilde{V}_{\text{Nuc}}(k)$. We notice, that the total momentum is not conserved, because the Hamiltonian has no translation invariance. Momentum can be transferred to the lattice when scattering at $V_{\text{Nuc}}$.

**Golden rule:**

Using the perturbation operator $V_{0}$, we want to induce transitions. Fermi’s golden rule for transitions reads:

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} \delta(E_{i} - E_{f})|M_{i f}|$$

(4.54)
with

\[ M_{if} = M_{if}^{(1)} + M_{if}^{(2)}. \]

The energies \( E_i \) and \( E_f \) stand for the total energies of electrons and radiation field before and after the transition. Initial and final states are:

\[
\begin{align*}
|i\rangle &= \hat{c}_k^\dagger |0\rangle: \text{no photon, one electron } \hbar k, \quad E_i = \frac{\hbar^2 k^2}{2m} \\
|f\rangle &= \hat{c}_k'\hat{a}_q^\dagger |0\rangle: \text{one photon } \hbar q, \text{ one electron } \hbar k', \quad E_F = \frac{\hbar^2 k'^2}{2m} + \hbar c|q|
\end{align*}
\]

(4.55) \hspace{5cm} (4.56)

Differential cross-section

\[ \Delta N(p, \theta) \]

\[ \Delta \Omega \]

\[ \Delta \theta \]

Current \( j \)

Figure 4.3: Geometry of the elastic scattering. The area \( \Delta \sigma \) of the incoming ray reads \( \Delta \sigma = 2\pi \Delta b \). Also shown the solid angle \( \Delta \Omega \).

Suppose a particle stream of density \( j_i \) (describes particle number per area and time, “initial”) is hitting a scattering potential. In this event, a detector counting the scattered particles at the solid angle \( d\Omega \) and in the momentum range between \( k' \) and \( k' + dk' \) will measure a certain counting rate (events per second). This rate is given by

\[
\frac{V}{(2\pi)^3} \frac{\hbar^2}{dk'} dk' d\Omega \Gamma_{i\rightarrow f} = j_i d\sigma ,
\]

where \( d\sigma \) is a differential area element perpendicular to the incoming particle stream \( j_i \). \( \Gamma_{i\rightarrow f} \) describes the transition rate to the final state \( k' \), see Fig. 4.3.

**General scattering cross-section:**

In the following we have to specify more precisely what a detector will be measuring. In the case of a wavelength-dispersive detector, the interesting quantity is

\[
\frac{d^2 \sigma}{dk'^2 d\Omega} (k', \Omega) = \frac{1}{j_i (2\pi)^3} \frac{V}{\hbar^2} \Gamma_{i\rightarrow f}.
\]
The scattering cross-section is a measure for the magnitude of scattering coming from a centre of diffraction inside a solid angle \( d\Omega \) and into the momentum range between \( k' \) and \( k' + dk' \).

**Differential cross-section:**
Assuming the detector is not sensitive in a certain momentum range \( dk' \) around \( k' \) alone but is just counting all scattered particles in \( d\Omega \), without regard for their energy. Then we have to integrate over the left hand side of (4.57) with respect to \( dk' \) and we are calling

\[
\frac{d\sigma}{d\Omega}(\Omega) := \frac{1}{j_i (2\pi)^3} \int dk' k'^2 \Gamma_{i\rightarrow f}
\]

differential cross-section with regard to a scattering into the solid angle \( \Omega \).

**Final states regarding Bremsstrahlung:**
In the case of Bremsstrahlung one is confronted with one obstacle: After the scattering one has to deal with two particles, the electron \( \hbar k' \) and the photon \( \hbar q \). The energy of the photon is not fixed but follows a certain distribution. A detector for photons should work wavelength-dispersive, a detector for the scattered electrons however should not. In the case of Bremsstrahlung we are mainly concerned with the wavelength of the generated photons (important for application like X-ray scans), but we are not interested in the energy of the scattered electrons.

Therefore we are asking for the differential cross-section of the scattering of an electron into the solid angle \( d\Omega_k' \) under emission of a photon carrying a momentum between \( \hbar q \) and \( \hbar(q + \Delta q) \) into the solid angle \( d\Omega_q \). This quantity is written as

\[
\frac{d^3\sigma}{d\Omega_k'd\Omega_qdq} (\Omega_{k'}, q, \Omega_q).
\]

**Velocities:** \( \nu := \frac{\hbar k}{m} \) and \( \nu' = \frac{\hbar k'}{m} \) \( \Rightarrow \) particle stream: \( j_i = \frac{\nu}{V} \)

\[
\Rightarrow \text{cross-section: } \frac{d^3\sigma}{d\Omega_k'd\Omega_qdq} (\Omega_{k'}, q, \Omega_q) = \frac{V}{\nu} \left( \frac{V}{(2\pi)^3} \right)^2 q^2 \int dk' k'^2 \Gamma_{i\rightarrow f}.
\]

(4.58)

**Perturbation theory of first order:**
The part \( V_{Nuc} \) is not containing any creators of photons which is why it cannot cause transitions between (4.55) and (4.56) in first order. The only contribution will come from the Hermitian conjugate inside of \( H'_I \). The terms concerned are proportional to \( \hat{c}_{ki}, \hat{c}_k \hat{a}_q^\dagger \) and the corresponding Feynman diagram is shown on the right of Fig 4.1. However conservation of momentum and energy apply and both requirements can’t be satisfied simultaneously. This can be seen via the following:

Let be \( p'^\mu \) and \( (p')^\mu \) the four-momentum of the arriving respectively emitting electron. Furthermore let \( q^\mu \) be the four-momentum of the photon (we will set \( \hbar = 1 \)). Then we find

\[
m^2 c^2 = p'^\mu p_\mu = ((p')^\mu + q^\mu)((p')_\mu + q_\mu).
\]

The right hand side gives, considering \( q^\mu q_\mu = 0 \) (photons own no mass):

\[
m^2 c^2 + 0 + (p')^\mu q_\mu + q^\mu (p')_\mu = m^2 c^2 + 2(p')^\mu q_\mu.
\]
This leads to \((p')^\mu q_\mu = 0\). In the resting frame of the escaping electron is
\[
(p')^\mu = (mc, 0) \quad \text{and} \quad q^\mu = (\hbar \omega_q/c, q),
\]
which gives
\[
(p')^\mu q_\mu = mc\hbar \omega_q = 0.
\]
The energy of the photon vanishes, the considered process does not exist. Bremsstrahlung is an effect of second order perturbation theory in \(V_0\).

**Second order perturbation theory:**

The matrix element \(M_i^{(2)}\) reads
\[
M_i^{(2)} = \sum_m \frac{\langle f | V_0 | m \rangle \langle m | V_0 | i \rangle}{E_i - E_m + \eta \hbar}, \quad \text{where} \quad V_0 = H'_I + V_{\text{Nuc}},
\]
which we already know from Quantum Mechanics I (with \(\eta \ll 1\)). It needs a little bit of bookkeeping to not lose track of the calculations. For an intermediate state \(|m\rangle\) exist two possibilities, so that the numerator of the sum is not vanishing.

**a) Intermediate state without photon:**

The intermediate state has no photon in it, but only an “intermediate” electron carrying momentum \(\hbar k_z\),
\[
|m_a\rangle = c_{k_z}^\dagger 0\rangle, \quad E_m = \frac{\hbar^2 k_z^2}{2m}.
\]
The numerator of (4.59) then reads
\[
\langle f | H'_I + V_{\text{Nuc}} | m_a \rangle \langle m_a | H'_I + V_{\text{Nuc}} | i \rangle = \langle f | H'_I | m_a \rangle \langle m_a | V_{\text{Nuc}} | i \rangle
\]
because \(H'_I\) generates exactly the required photon of the final state (via its h.c. part), \(V_{\text{Nuc}}\) on the other hand generates none. The corresponding Feynman graph is shown on the right.

**b) Intermediate state with photon:**

The intermediate state contains a photon carrying momentum \(\hbar q\) and an electron carrying momentum \(\hbar k_z\):
\[
|m_b\rangle = c_{k_z}^\dagger \hat{a}^\dagger_{q} 0\rangle, \quad E_m = \frac{\hbar^2 k_z^2}{2m} + \hbar c q.
\]
The numerator of (4.59) reads
\[
\langle f | V_{\text{Nuc}} | m_b \rangle \langle m_b | H'_I | i \rangle
\]
and the Feynman graph is shown in fig. 4.8 on the right hand side. Only the Hermitian conjugate part of \( H'_I \) plays a role again in the calculations of the matrix elements, the other part is not contributing. The sum appearing in \( M_{if}^{(2)} \) is running over all \( k_z \) of intermediate electrons and over the cases \( a) \) and \( b) \).

\[
\begin{align*}
\text{a) } & k_z = k' + q \\
\text{b) } & k_z = k - q
\end{align*}
\]

The emission of Bremsstrahlung is carried out in two phases: the scattering at a nucleus and the emission of a photon (or vice versa). The calculation of the matrix elements is following:

\textbf{a) Matrix elements - Intermediate state without photon:}

One has to calculate (4.60). It is

\[
\langle m_a | V_{\text{Nuc}} | i \rangle = \langle 0 | \hat{c}_{k_1}^\dagger \hat{V}_{\text{Nuc}}(k_1 - k_2) \hat{c}_{k_2} \hat{c}_k^\dagger | 0 \rangle
\]

\[
= \sum_{k_1, k_2} \langle 0 | \left( \hat{c}_{k_2} \hat{c}_k^\dagger \right) \hat{V}_{\text{Nuc}}(k_1 - k_2) \left( \hat{c}_{k_2} \hat{c}_k^\dagger \right) | 0 \rangle
\]

\[
= \sum_{k_1, k_2} \delta_{k_2, k_1} \hat{V}_{\text{Nuc}}(k_1 - k_2) \delta_{k_2, k}
\]

\[
= \hat{V}_{\text{Nuc}}(k_z - k)
\]

and

\[
\langle f | H_I' | m_a \rangle = \langle 0 | \hat{c}_{k'} \hat{a}_q \sum_{k_1, k_2, q_1} M_1(k_1, k_2, -q_1) \hat{c}_{k_1}^\dagger \hat{c}_{k_2} \hat{a}_q^\dagger \hat{c}_{q_1}^\dagger \hat{c}_{k_2}^\dagger | 0 \rangle
\]

\[
= \sum_{k_1, k_2, q_1} \langle 0 | \left( \hat{c}_{k'} \hat{a}_q^\dagger \right) \left( \hat{a}_q\hat{c}_{q_1}^\dagger \right) \left( \hat{c}_{k_2} \hat{c}_k^\dagger \right) | 0 \rangle M_1(k_1, k_2, -q_1)
\]

\[
= \sum_{k_1, k_2, q_1} \delta_{k', k_1} \delta_{q, q_1} \delta_{k_2, k_z} M_1(k_1, k_2, -q_1)
\]

\[
= -\frac{eh}{mc} \sqrt{\frac{2\pi h c^2}{V \omega_q}} \delta_{k_z, q + k'} (u_q \cdot k_z).
\]

The first contribution to \( M_{if}^{(2)} \) is therefore, taking into account that \( u_q \cdot q = 0 \), given by:

\[
M_{if}^{(2,a)} = \sum_{k_z} \frac{\langle f | H_I' | m_a \rangle \langle m_a | V_{\text{Nuc}} | i \rangle}{E_i - E_m^a + mh} \eta \to 0
\]

\[
= -\frac{eh}{mc} \sqrt{\frac{2\pi h c^2}{V \omega_q}} \frac{\hat{V}_{\text{Nuc}}(q + k' - k)(u_q \cdot k')}{\frac{\hbar^2}{2m}(k_z^2 - (q + k')^2)}.
\]
Because of energy conservation,

\[ E_f = \frac{\hbar^2 k'^2}{2m} + \hbar c |q| = E_i = \frac{\hbar k^2}{2m}, \]

the denominator also writes

\[ N_a = \hbar c |q| - \frac{\hbar q^2}{2m} - \frac{\hbar^2 q \cdot k'}{m} = \hbar c |q| \left( 1 - \frac{\hbar q \cdot k'}{mc|q|} - \frac{\hbar q^2}{2mc|q|} \right). \quad (4.62) \]

But the second term in brackets gives

\[ \frac{\hbar k'}{m} \cdot \frac{q}{c|q|} \leq \frac{\nu'}{mc|q|} \approx \frac{\nu'}{c}, \]

where \( \nu' \) is the velocity of the electron after the collision. The third term of (4.62) is again one magnitude smaller in \( \frac{\nu}{c} \), because \( |q| \) is assumed far smaller than the electron momentum. Therefore the non-relativistic case is approximated by \( N_a \approx \hbar c |q| = \hbar \omega_q \). Hence

\[ M_{i_f}^{(2,a)} = - \frac{e}{mc} \sqrt{\frac{2\pi \hbar c^2}{V_{\omega_q}}} \frac{\tilde{V}_{\text{Nuc}}(q + k' - k)(u_q \cdot k')}{\hbar \omega_q}. \]

**b) Matrix elements - Intermediate state containing a photon:**

The calculation is carried out analogous to case \( a \) and the result for the second contribution of \( M_{i_f}^{(2)} \) reads

\[ M_{i_f}^{(2,b)} = \sum_{k_z} \frac{\langle f | V_{\text{Nuc}} | m_a \rangle \langle m_a | H_{i_f}^0 | i \rangle}{E_i - E_m^0 + \eta \hbar} = - \frac{e}{mc} \sqrt{\frac{2\pi \hbar c^2}{V_{\omega_q}}} \frac{\tilde{V}_{\text{Nuc}}(q + k' - k)(u_q \cdot k)}{\hbar \omega_q}. \]

The denominator one finds then:

\[ N_b = \frac{\hbar k^2}{2m} - \left( \frac{\hbar q^2}{2m} + \frac{\hbar k^2}{2m} - \frac{\hbar q \cdot k}{m} \right) - \hbar c |q| = -\hbar c |q| \left( 1 + \frac{\hbar q^2}{2mc|q|} - \frac{\hbar q \cdot k}{mc|q|} \right) \approx -\hbar \omega_q. \]

Hence

\[ M_{i_f}^{(2,b)} = - \frac{e}{mc} \sqrt{\frac{2\pi \hbar c^2}{V_{\omega_q}}} \frac{\tilde{V}_{\text{Nuc}}(q + k' - k)(u_q \cdot k)}{-\hbar \omega_q}. \]

**Sum of the matrix elements - Nucleus potential:**

Both intermediate states (with and without photon) together result in:

\[ M_{i_f}^{(2)} = M_{i_f}^{(2,a)} + M_{i_f}^{(2,b)} = - \frac{e}{mc} \sqrt{\frac{2\pi \hbar c^2}{V_{\omega_q}}} \frac{(k' - k) \cdot u_q}{\hbar \omega_q} \tilde{V}_{\text{Nuc}}(q + k' - k). \quad (4.63) \]

Until now we didn’t specify the nucleus potential. From now on we choose

\[ V_{\text{Nuc}}(r) = -\frac{Ze^2}{r}. \]
The Fourier transform $\tilde{V}_{\text{Nuc}}(k)$ gives

$$\tilde{V}_{\text{Nuc}}(k) = -\frac{Ze^2}{V} \int_V \frac{e^{ik \cdot r}}{r} dV = -\frac{Ze^2}{V} \int_V \frac{\Delta e^{ik \cdot r}}{r}. \tag{4.64}$$

Two times partial integration and the substitution

$$\Delta \frac{1}{r} = -4\pi \delta(r)$$

results in

$$\tilde{V}_{\text{Nuc}}(k) = -\frac{Ze^2}{Vk^2} \int_V \frac{\Delta \left(\frac{1}{r}\right) e^{ik \cdot r}}{r} = -\frac{4\pi Ze^2}{Vk^2}.\tag{4.64}$$

Finally we arrive at

$$M_{if}^{(2)} = \frac{4\pi Z e^2 h}{mc} \sqrt{\frac{2\pi \hbar c^2}{V \omega_q}} \frac{(k' - k) \cdot u_q}{V \hbar \omega_q (q + k' - k)^2 \Delta \nu}. \tag{4.64}$$

**Low energy scattering:**

We will now assume that the energy of the photon $\omega := \omega_q$ is much smaller compared to the electron’s and we set

$$(q + k' - k)^2 \approx (k' - k)^2 := (\Delta k)^2 = \frac{m^2}{\hbar^2} (\Delta \nu)^2.\tag{4.64}$$

Simultaneously we find that $|\nu| = |\nu'|$ because when the photon is neglected we are confronted with elastic scattering of the electrons. For the transition rate we find

$$\Gamma_{i \rightarrow f} = \frac{2\pi}{\hbar} \delta(E_f - E_i) \left| M_{if}^{(2)} \right|^2 = \frac{64\pi^2 Z^2 \delta(\nu \cdot \Delta \nu)^2}{V^3 \omega^4 \hbar^6 \sin^4(\theta/2)} \delta(E_i - E_f).\tag{4.64}$$

If $\theta$ is the angle between the velocities $\nu$ and $\nu'$ before respectively after the collision, we also find

$$|\Delta \nu| = 2|\nu| \sin \frac{\theta}{2}.\tag{4.64}$$

**Differential cross-section of Bremsstrahlung:**

The differential cross-section (4.58) can now be calculated:

$$\frac{d^3 \sigma}{d\Omega_{k'} d\Omega_q dq} = \frac{V}{\nu} \left( \frac{V}{(2\pi)^3} \right)^2 q^2 \int dk' k'^2 \Gamma_{i \rightarrow f}$$

$$= \frac{64\pi^4 Z^2 \hbar^2 \delta(\nu \cdot \Delta \nu)^2}{(2\pi)^6 \omega^4 \hbar^6} \int dk' \frac{(k' - k) \cdot u_q}{16 \nu^4 \sin^4(\theta/2)} \delta(E_i - E_f).$$

We see a Rutherford cross-section is already looming in this result. The integrand is only dependent on $k'^2$, and the $\delta$-distribution only of $k'$. Further it is

$$\delta(E_i - E_f) = \delta \left( \frac{\hbar^2 k'^2}{2m} - \frac{\hbar^2 k^2}{2m} \right) = \frac{2m}{\hbar^2} \delta(k'^2 - k^2).\tag{4.64}$$
Now it is easy to calculate the integral:

\[
\int dk' k'^2 \delta(k'^2 - k^2) = \int d\xi \frac{\xi}{2\sqrt{\xi}} \delta(\xi - k^2) = \frac{k}{2} = \frac{m\nu}{2\hbar}.
\]

Along with \( q = \omega/c \) we arrive at

\[
\frac{d^3\sigma}{d\Omega_k d\Omega_q d\omega} = \frac{Z^2 e^4}{m^2 \nu^4 \sin^4(\theta/2)} \frac{(\mathbf{u} \cdot \Delta \nu)^2 e^2}{16\pi^2 c^2 \hbar \omega}.
\] (4.65)

In the first factor, one recognizes the Rutherford cross-section. The second factor represents the probability density of observing an additional photon carrying energy \( \hbar \omega_q \) at the solid angle \( d\Omega_q \).
Chapter 5

Relativistic quantum mechanics

5.1 Invariances of the Schrödinger equation

Consider a free particle:

\[ \hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} = -\frac{\hbar^2}{2m} \nabla^2 = -\frac{\hbar^2}{2m} \Delta \]

Coordinate transformations:

a) Translation: \( x' = x - a, \ y' = y, \ z' = z, \ t' = t \).

b) Rotation: \( x'_j = \sum_l a_{jl} x_l \).

Rotations do not change the length:

\[ \sum_j x_j'^2 = \sum_j \sum_{k,l} a_{jk} a_{jl} x_k x_l = \sum_j x_j^2. \]

Thus

\[ \sum_j a_{jk} a_{jl} = \delta_{kl} \quad \text{and} \quad \sum_k a_{ik} a_{jk} = \delta_{ij} \]

or more compact

\[ \mathbf{A} \cdot \mathbf{A}^T = \mathbf{A}^T \cdot \mathbf{A} = \mathbf{1} \quad \text{with} \quad \mathbf{A} = (a_{jl}). \]

c) Galilean transformation: The primed coordinate system moves with a constant speed \( v \) relative to the unprimed system: \( x' = x - vt, \ y' = y, \ z' = z, \ t' = t \).

Schrödinger equation

\[ i\hbar \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = -\frac{\hbar^2}{2m} \Delta \psi(\mathbf{r}, t) \]

is covariant under the transformations mentioned above, i.e. it is form-invariant during a change of coordinates:

\[ i\hbar \frac{\partial}{\partial t'} \psi'(\mathbf{r}', t') = -\frac{\hbar^2}{2m} \Delta' \psi'(\mathbf{r}', t'). \]

Proof:

a) Translation: Use the chain rule:

\[ \frac{\partial}{\partial x'} = \frac{\partial x}{\partial x'} \frac{\partial}{\partial x} = \frac{\partial}{\partial x}. \]

and analogous for \( y, z \) and \( t \). With \( \psi'(x') = \psi'(x - a) = \psi(x) \) the covariance under translation becomes obvious.
b) **Rotation:** Use the chain rule:

\[
\frac{\partial}{\partial x_k} = \sum_j \frac{\partial x'_j}{\partial x_k} \frac{\partial}{\partial x'_j} = \sum_j a_{jk} \frac{\partial}{\partial x'_j}.
\]

Thus the Laplacian transforms as

\[
\Delta = \sum_k \frac{\partial^2}{\partial x'_k} = \sum_{k,j,l} a_{jk} a_{lk} \frac{\partial}{\partial x'_j} \frac{\partial}{\partial x'_l} = \sum_j \frac{\partial^2}{\partial x'_j} = \Delta'.
\]

With \( \psi'(\mathbf{r}',t') = \psi(\mathbf{r},t) \) the covariance under rotation is clear.

c) **Galilean transformation:** The momenta in both systems satisfy

\[
p'_x = p_x - mv, \quad p'_y = p_y, \quad p'_z = p_z.
\]

The momentum operators in both systems reads as

\[
\hat{p}_x = \frac{\hbar}{i} \frac{\partial}{\partial x}, \quad \hat{p}'_x = \frac{\hbar}{i} \frac{\partial}{\partial x'}.
\]

Below, we will show that the Schrödinger equation is covariant under Galilean transformation if the following transformation of the wave function is used

\[
\psi(\mathbf{r},t) = e^{-\frac{i}{\hbar}mvx'} \psi'(\mathbf{r}',t'). \tag{5.1}
\]

It is

\[
\hat{p}_x \psi(\mathbf{r},t) = (p'_x + mv) \psi(\mathbf{r},t) = \left[ \frac{\hbar}{i} \frac{\partial}{\partial x} + m \right] e^{-\frac{i}{\hbar}mvx'} \psi'(\mathbf{r}',t')
\]

and thus

\[
\hat{p}'_x \psi'(\mathbf{r}',t') = e^{-\frac{i}{\hbar}mvx'} \hat{p}'_x \psi'(\mathbf{r}',t').
\]

Inserting this into the the Schrödinger equation leads to

\[
0 = \left[ \frac{i\hbar}{\partial t} - \frac{1}{2m} \left( \hat{p}'_x^2 + \hat{p}'_y^2 + \hat{p}'_z^2 \right) \right] \psi'(\mathbf{r}',t')
\]

This equation is fulfilled if

\[
\frac{i\hbar}{\partial t'} \psi'(\mathbf{r}',t') = \frac{1}{2m} \left[ \hat{p}'_x^2 + \hat{p}'_y^2 + \hat{p}'_z^2 \right] \psi'(\mathbf{r}',t').
\]

Importantly, it follows from Eq. \( 5.1 \) that

\[
|\psi(\mathbf{r},t)|^2 = |\psi'(\mathbf{r}',t')|^2,
\]

i.e. the probability densities of the original and transformed wave functions are the same and thus also the physics they describe.

We have shown that the Schrödinger equation is form-invariant under the transformations mentioned above. In particular, it fulfills the **classical principle of relativity:** two persons, that move with a speed \( v \) relative to each other, observe physical processes in the same way.

However, we know from classical mechanics that Galilean transformations are only valid for \( v \ll c \). A correct formulation of the principle of relativity must account for the equality of the speed of light \( c \) in all reference frames.
5.2 Recap of special relativity

Before combining special relativity and quantum mechanics we recap the required formalism of relativity. This enables us to generalize Galilean invariance to Lorentz invariance.

Please note, that we have to use Lorentz transformations

\[ x' = \frac{x - vt}{\sqrt{1 - \frac{v^2}{c^2}}} = \gamma(x - \beta ct), \quad y' = y, \quad z' = z, \quad ct' = \frac{ct - \frac{v}{c}x}{\sqrt{1 - \frac{v^2}{c^2}}} = \gamma(ct - \beta x) \tag{5.2} \]

instead of Galilean transformations.

\[ \gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{1}{\sqrt{1 - \beta^2}} \]

is the so-called Lorentz factor.

It turns out that the Schrödinger equation is not invariant under Lorentz transformations and thus a relativistic generalization of this equation is needed.

Let's repeat the formalism of relativity. We define a (contravariant) four-vector as

\[ x^\mu = (x^0, x^1, x^2, x^3) = (t, x, y, z) \]

where

\[ x^0 = ct, \quad x^1 = x, \quad x^2 = y, \quad x^3 = z. \]

Later we will introduce a (covariant) four-vector \( x_\mu \) which is distinct from \( x^\mu \).

We define a metric in this four-dimensional Minkowski space via a squared distance

\[ s^2 = c^2t^2 - x^2 - y^2 - z^2 = c^2t^2 - r = g_{\mu\nu}x^\mu x^\nu \tag{5.3} \]

with the Minkowski metric tensor

\[ g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \]

More precisely, it is a pseudo-Euclidean metric, because it is not positive-definite. Distances with \( s^2 < 0 \) are called spacelike. Events with a spacelike distance are causally independent. On the other hand, events with a timelike distance, \( s^2 > 0 \), can influence each other. For events with a lightlike distance, \( s^2 = 0 \), a communication is only possible via signals that propagate at the speed of light.

Note that, in Eq. (5.3) we have used the so-called Einstein summation convention: we sum (from 0 to 3) over indices occurring twice, one of which is a upper and the other a lower index.

In analogy to rotations, we want to describe Lorentz transformations via a real matrix \( \Lambda^\mu_\nu \) as

\[ x'^\mu = \Lambda^\mu_\nu x^\nu \tag{5.4} \]
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The Lorentz transformation should leave the distance \( s^2 \) unchanged. Just like for rotations, the condition for the matrix \( \Lambda^{\mu}_{\nu} \) reads as

\[
s^{\prime 2} = g_{\mu \nu} x^{\prime \mu} x^{\prime \nu} = g_{\mu \nu} \Lambda^{\mu}_{\rho} x^{\rho} \Lambda^{\nu}_{\lambda} x^{\lambda} = \frac{1}{g_{\rho \lambda} x^{\rho} x^{\lambda}} = s^{2}.
\]

Thus

\[
g_{\mu \nu} \Lambda^{\mu}_{\rho} \Lambda^{\nu}_{\lambda} = g_{\rho \lambda}
\]  

or in matrix representation

\[
\Lambda^{T} g \Lambda = g.
\]

All Lorentz transformations form a group, the so-called Lorentz group.

In particular, the matrix representation of the basic Lorentz transformation (5.2) reads as

\[
\Lambda^{\mu}_{\nu} = \begin{pmatrix}
\gamma & -\beta \gamma & 0 & 0 \\
-\beta \gamma & \gamma & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix}
\]

with rapidity \( \xi \) defined via \( \tanh \xi = \beta \).

In addition to a contravariant vector \( x^{\mu} \) we introduce a covariant vector \( x_{\mu} \) as

\[
x_{\mu} = g_{\mu \nu} x^{\nu} = (ct, -\mathbf{r})
\]  

(5.6)

with the inverse operation

\[
x^{\mu} = g^{\mu \nu} x_{\nu}.
\]  

(5.7)

Thus a multiplication with \( g^{\mu \nu} \) or \( g_{\mu \nu} \) allows raising or lowering of indices. One of the advantages of this is an integration of the metric into a vector and thus a more compact notation. For the Euclidean metric it is \( g_{\mu \nu} = \delta_{\mu \nu} \), where \( \delta_{\mu \nu} \) is the Kronecker delta, and thus there is no difference between contravariant and covariant vectors.

The consistency of Eq. (5.6) and (5.7) is guaranteed via

\[
g_{\mu \rho} g^{\rho \nu} = \delta_{\mu \nu}.
\]

(5.8)

For the Lorentz transformation \( \Lambda \) we define in the same way:

\[
\Lambda^{\mu}_{\nu} = g_{\mu \lambda} \Lambda^{\lambda}_{\rho} g^{\rho \nu} = \Lambda_{\mu \rho} g^{\rho \nu} = g_{\mu \lambda} \Lambda^{\lambda}_{\nu},
\]  

(5.8)

which is generally true for order-2 tensors.

The term “contravariant” and “covariant” reflects the different transformation behavior of the corresponding vectors under Lorentz transformation. Contravariant vectors transform according to Eq. (5.4). On the contrary, covariant vectors transform as

\[
\Lambda^{\mu}_{\nu} x_{\nu} = g_{\mu \lambda} \Lambda^{\lambda}_{\rho} g^{\rho \nu} x_{\nu} = g_{\mu \lambda} \Lambda^{\lambda}_{\rho} x^{\rho} = g_{\mu \lambda} x^{\lambda} = x^{\prime \mu},
\]

where we have used Eqs. (5.8), (5.6) and (5.4).
We became familiar with the behaviour of position vectors under Lorentz transformations. All other four-vectors behave in the same way. Thus we define:

A **contravariant four-vector** $a^\mu$ transforms as

$$a'^\mu = \Lambda^\mu_\nu a^\nu$$  \hspace{1cm} (5.9)

and a **covariant four-vector** $a_\mu$ transforms as

$$a'_\mu = \Lambda^\mu_\nu a_\nu.$$ \hspace{1cm} (5.10)

How do four-gradients transform? We define four-gradients as

$$\frac{\partial}{\partial x^\mu} = \left( \frac{1}{c} \frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) = \left( \frac{\partial}{\partial ct}, \nabla \right) = \partial_\mu$$

and

$$\frac{\partial}{\partial x'_\mu} = \left( \frac{1}{c} \frac{\partial}{\partial t'}, -\frac{\partial}{\partial x'}, -\frac{\partial}{\partial y'}, -\frac{\partial}{\partial z'} \right) = \left( \frac{\partial}{\partial ct'}, -\nabla \right) = \partial'^\mu.$$  \hspace{1cm} (5.11)

As indicated by the notation, the vectors $\partial_\mu$ and $\partial'^\mu$ transform covariantly and contravariantly, respectively, just oppositely to the position vectors used in the derivative.

**Proof:** We multiply Eq. (5.4) with $g_\mu\lambda \Lambda^\lambda_\rho$:

$$g_\mu\lambda \Lambda^\lambda_\rho x'^\mu = g_\mu\lambda \Lambda^\lambda_\rho x^\nu$$

and obtain

$$x_\rho = \Lambda^\lambda_\rho x'_\lambda$$ \hspace{1cm} (5.11)

using Eq. (5.5). Using the chain rule we get

$$\frac{\partial}{\partial x'_\mu} = \frac{\partial x_\nu}{\partial x'_\mu} \frac{\partial}{\partial x_\nu} = \Lambda^\mu_\nu \frac{\partial}{\partial x_\nu}$$

and thus the contravariance of $\partial^\mu$ is evident. The covariance of $\partial_\mu$ can be shown in an analogous way.

Multiplying Eq. (5.11) with $\Lambda^\rho_\mu$ we get

$$x'_\mu = \Lambda^\rho_\mu x_\rho = \Lambda^\rho_\mu \Lambda^\lambda_\rho x'_\lambda$$

and thus

$$\Lambda^\rho_\mu \Lambda^\lambda_\rho = \delta^\lambda_\mu.$$  \hspace{1cm} (5.11)

This means that the transformation matrices of covariant and contravariant vectors are essentially inverse to one another. In matrix representation:

- **Contravariant**: $x' = \Lambda x$
- **Covariant**: $x' = \left( \Lambda^{-1} \right)^T x$.  

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It is useful to know that the scalar product
\[ a_\mu b^\mu = g_{\mu\nu} a^\nu b_\mu \]
of two four-vectors \( a_\mu \) and \( b^\mu \) is invariant under Lorentz transformations and thus the d’Alembertian
\[ \Box = \partial_\mu \partial^\mu = \frac{1}{c^2} \partial^2_{tt} - \nabla^2 \]
is also an invariant scalar.

We consider an electromagnetic field with a scalar potential \( \varphi(r, t) \) and a vector potential \( A(r, t) \) and combine them into a single four-vector
\[ A^\mu = (\varphi, A) \, . \]
The electric and magnetic fields associated with these four-potentials are
\[ E = -\nabla \varphi - \frac{1}{c} \frac{\partial A}{\partial t} \quad \text{and} \quad B = \nabla \times A \, . \]

Next, we consider a particle with a rest mass \( m_0 \) and an electric charge \( e \).
The contravariant four-momentum of a particle with a relativistic energy \( E \) and a three-momentum \( P = \gamma m_0 v \), where \( v \) is the particle’s three-velocity and \( \gamma \) the Lorentz factor, is
\[ P^\mu = \left( \frac{E}{c}, P \right) = (\gamma m_0 c, \gamma m_0 v) \, . \]
The squared length of \( P^\mu \) is a Lorentz invariant quantity:
\[ P_\mu P^\mu = \frac{E^2}{c^2} - P^2 = \gamma^2 m_0^2 c^2 - \gamma^2 m_0^2 v^2 = m_0^2 c^2 \]
If the particle is exposed to an electromagnetic field with a four-potential \( A^\mu \) the canonical four-momentum \( p^\mu \) reads as
\[ p^\mu = P^\mu + e c A^\mu = \left( \frac{E}{c}, P \right) \]
with
\[ E = \gamma m_0 c^2 + e \varphi \quad \text{and} \quad p = P + \frac{e}{c} A \, . \]
In lowest order \( (v \ll c) \) the energy yields the non-relativistic expression:
\[ E = m_0 c^2 + \frac{m_0}{2} v^2 + e \varphi + O\left( \frac{v^2}{c^2} \right) \, . \]
The dynamics of the classical relativistic mechanics follows from the Hamiltonian
\[ \mathcal{H}(r, p) = e \varphi + \sqrt{m_0^2 c^4 + c^2 \left( p - \frac{e}{c} A \right)^2} \, . \quad (5.12) \]

From Hamilton’s equations
\[ \frac{dr}{dt} = \frac{\partial \mathcal{H}}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial \mathcal{H}}{\partial r} \]
one can derive the Lorentz force
\[ \frac{dr}{dt} = v, \quad \frac{dP}{dt} = e \left( E + \frac{v}{c} \times B \right) \, . \]


5.3 Klein-Gordon equation

We try to derive a relativistic analogue to the Schrödinger equation. Correspondence principle reads as

\[ E \rightarrow i\hbar \frac{\partial}{\partial t}, \quad p \rightarrow -i\hbar \nabla \]

or as a four-vector

\[ p^\mu = \left( \frac{E}{c}, \mathbf{p} \right) \rightarrow i\hbar \left( \frac{\partial}{\partial ct} - \nabla \right) = i\hbar \partial^\mu. \]

This leads in case of a non-relativistic free particle with an energy \( E = H = \frac{p^2}{2m} \) to the Schrödinger equation.

As a first try we apply the correspondence principle to the Hamiltonian (5.12) of a relativistic charged particle in an electromagnetic field and obtain

\[ i\hbar \frac{\partial}{\partial t} \psi(r,t) = \left[ e\varphi + \sqrt{m_0^2 c^4 + c^2 \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)} \right] \psi(r,t). \quad (5.13) \]

An expansion in \( \frac{1}{c^2} \) leads to

\[ \sqrt{m_0^2 c^4 + c^2 \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2} \approx m_0 c^2 + \frac{1}{2m_0} \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2 + \mathcal{O} \left( \frac{1}{c^4} \right) \]

and the contribution due to the rest energy \( m_0 c^2 \) vanish using the transformation

\[ \psi(r,t) = e^{-\frac{i\hbar m_0 ct}{2}} \phi(r,t). \quad (5.14) \]

Thus we end up with a classical Schrödinger equation for \( \phi \)

\[ i\hbar \frac{\partial}{\partial t} \phi(r,t) = \left[ e\varphi + \frac{1}{2m_0} \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A} \right)^2 \right] \phi(r,t). \]

Problems with the relativistic equation (5.13):

a) The asymmetry of space and time derivatives masks the relativistic invariance.

b) The square root of a differential operator can be defined via a series expansion. This may lead to problems with the convergence. Moreover, in an expansion, arbitrary powers of the differential operator occur. This corresponds to a nonlocal theory since the whole shape of the wave function gets important.

A possible way out is to start with the square of the energy:

\[ (E - e\varphi)^2 = m_0^2 c^4 + c^2 \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2. \quad (5.15) \]

As a consequence, two solutions

\[ E = e\varphi \pm \sqrt{m_0^2 c^4 + c^2 \left( \mathbf{p} - \frac{e}{c} \mathbf{A} \right)^2} \]

are possible. In particular, a solution with a negative energy exists.
Quantization of Eq. (5.15) gives the Klein-Gordon equation:
\[
\left[ \left( \frac{i\hbar}{\partial t} - e\varphi \right)^2 - c^2 \left( \frac{\hbar}{i} \nabla - \frac{e}{c} A \right)^2 \right] \psi(r, t) = m_0^2 c^4 \psi(r, t)
\]
or using four-vectors
\[
\left[ \left( \partial_\mu + \frac{ie}{\hbar c} A_\mu \right) \left( \partial^\mu + \frac{ie}{\hbar c} A^\mu \right) + \frac{m_0^2 c^2}{\hbar^2} \right] \psi(r, t) = \left( D_\mu D^\mu + \frac{m_0^2 c^2}{\hbar^2} \right) \psi(r, t) = 0 \tag{5.16}
\]
The Klein-Gordon equation is relativistically invariant, because the scalar product \(D_\mu D^\mu\) is invariant under Lorentz transformations.

The Klein-Gordon equation for a free particle
\[
\left( \partial_\mu \partial^\mu + \frac{m_0^2 c^2}{\hbar^2} \right) \psi(r, t) = 0 \tag{5.17}
\]
corresponds to a classical wave equation with an additional mass term. Their solutions are plane waves
\[
\psi(r, t) = \psi_0 \exp \left[ -\frac{i}{\hbar} p_\mu x^\mu \right] = \psi_0 \exp \left[ -\frac{i}{\hbar} (Et - p \cdot r) \right],
\]
with a dispersion relation
\[
\frac{E^2}{c^2} - p^2 = m_0^2 c^2.
\]
As expected, there are solutions with positive and negative energy
\[
E = \pm c \sqrt{m_0^2 c^2 + p^2}
\]
separated by an energy gap, i.e. states with energies between \(m_0 c^2\) and \(-m_0 c^2\) do not exist. Furthermore, the energy spectrum is not bounded from below, which leads to stability problems. A way out is to interpret states of negative energy as antiparticles.

### 5.3.1 Continuity equation and interpretation of the wave function

How to interpret the wave functions that evolve according to the Klein-Gordon equation? The Schrödinger equation obeys a continuity equation
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot j = 0,
\]
where
\[
\rho(r, t) = |\psi(r, t)|^2 \geq 0 \tag{5.18}
\]
can be interpreted as a probability density. The corresponding probability current is given by
\[
j = \frac{\hbar}{2mi} (\psi^* \nabla \psi - \psi \nabla \psi^*) \tag{5.19}
\]
For a relativistic theory we expect a similar continuity equation to hold. Written in a covariant form
\[ \partial_{\mu}j^{\mu} = 0 \] (5.20)
with a four-current
\[ j^{\mu} = (c\rho, j). \]

We multiply Eq. (5.17) with \( \psi^* \) and subtract the complex conjugate:
\[
0 = \psi^* \left( \partial_{\mu} \partial^{\mu} + \frac{m^{2}c^{2}}{\hbar^{2}} \right) \psi - \psi \left( \partial_{\mu} \partial^{\mu} + \frac{m^{2}c^{2}}{\hbar^{2}} \right) \psi^*
= \partial_{\mu} (\psi^* \partial^{\mu} \psi - \psi \partial^{\mu} \psi^*).
\]

Thus the continuity equation (5.20) with the four-current
\[ j^{\mu} = \frac{i\hbar}{2m_{0}} (\psi^* \partial^{\mu} \psi - \psi \partial^{\mu} \psi^*) \]
is fulfilled.
The current-component \( j \) of \( j^{\mu} = (c\rho, j) \),
\[ j = \frac{\hbar}{2m_{0}c} (\psi^* \nabla \psi - \psi \nabla \psi^*), \]
equals the expression (5.19) of the non-relativistic quantum mechanics.
In contrast to (5.18), the density-component
\[ \rho = \frac{i\hbar}{2m_{0}c^{2}} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) \]
is not positive definite and therefore cannot be interpreted as a probability density. That’s because Klein-Gordon equation is second-order in time.

Let’s consider the non-relativistic limit. Using the transformation (5.14) one obtains
\[ \frac{\partial \psi}{\partial t} \approx -i \frac{m_{0}c^{2}}{\hbar} \psi \]
and thus a probability density
\[ \rho \approx |\psi|^{2}. \]

### 5.3.2 Problems of the Klein-Gordon equation

Problems of the Klein-Gordon (KG) equation:

a) Solutions with negative energy exists and the energy spectrum of free particles is not bounded from below.

b) The wave function \( \psi \) cannot be interpreted as a probability amplitude.

c) \( \psi \) depends only on \( r \) and \( t \), and it is not possible to incorporate internal degrees of freedom, e.g. a spin.
Problem c) makes a further search for a relativistic equation, that could describe electrons (spin-$\frac{1}{2}$), necessary. At the date of the discovery (1926) the physical relevance of the KG equation was unclear, because at that time only particles with spin-$\frac{1}{2}$ (electrons, protons and neutrons) were known. Later it turned our that KG equation can describe spinless scalar particles, like pions (or pi mesons) discovered in 1947. The fact that KG equation is a field equation for spin-0 particles can be seen from its non-relativistic limit, which is the spinless Schrödinger equation, and from the behavior of the wave function under Lorentz transformations.

With regard to problem b), the question arises: Can we interpret $\rho$ and $j$ in a different way? Yes, for that we switch to the charge density

$$j'^\mu = ej^\mu = \frac{i\hbar}{2m_0} (\psi^* \partial^\mu \psi - \psi \partial^\mu \psi^*) ,$$

where $e$ is an electric charge. $\rho'$ is now a charge density and can have either positive or negative values. $j'$ is the corresponding current density. Below we will see that this interpretation of $j'^\mu$ is compatible with the interpretation of states with $E < 0$ as antiparticles.

We illustrate this with the free particle. Inserting an ansatz

$$\psi = A \exp \left[ \frac{i}{\hbar} (p \cdot r - Et) \right]$$

into KG equation leads to the condition

$$E^2 = c^2 \left( p^2 + m_0^2 c^2 \right)$$

and thus to two solutions

$$\psi_\pm = A_\pm \exp \left[ \frac{i}{\hbar} (p \cdot r \mp E_p t) \right] ,$$

with energies

$$E_p = c \sqrt{p^2 + m_0^2 c^2} .$$

The corresponding charge density (5.21) reads as

$$\rho'_\pm = \pm \frac{eE_p}{m_0 c^2} |\psi_\pm|^2 .$$

This suggests the following interpretation of $\psi$: $\psi_+$ describes a particle with charge $+e$ and $\psi_-$ a particle with the same mass $m_0$, however, with an opposite charge $-e$.

In order to obtain a normalized wave function we consider a particle in a box with an edge length $L$. From periodic boundary conditions we get

$$\psi^{(n)}_\pm = A^{(n)}_\pm \exp \left[ \frac{i}{\hbar} (p_n \cdot r \mp E_n t) \right]$$

with the momentum

$$p_n = \frac{2\pi}{L} n \quad \text{with} \quad n = (n_x, n_y, n_z) \in \mathbb{N}^3$$

and the corresponding energy $E_n = E_{pn}$.
The normalization condition
\[ \pm e = \int_{L^3} d^3 r' \rho_\pm' (r) = \pm \frac{eE_n}{m_0 c^2} \frac{1}{A_\pm} \left( \int_{L^3} d^3 r' \right)^2 \]
yields the normalized wave function
\[ \psi_\pm^{(n)} = \sqrt{\frac{m_0 c^2}{E_n L^3}} \exp \left[ \frac{i}{\hbar} (p_n \cdot r \mp E_n t) \right]. \]

Both solutions have the same normalization constant and they differ only in the time factor \( \exp \left( \mp \frac{i}{\hbar} E_n t \right) \). Thus the general solution for positive and negative spin-0 particles, respectively, reads as
\[
\psi_+ = \sum_n A_n \psi_+^{(n)} = \sum_n A_n \sqrt{\frac{m_0 c^2}{E_n L^3}} \exp \left[ \frac{i}{\hbar} (p_n \cdot r - E_n t) \right],
\]
\[
\psi_- = \sum_n B_n \psi_-^{(n)} = \sum_n B_n \sqrt{\frac{m_0 c^2}{E_n L^3}} \exp \left[ \frac{i}{\hbar} (p_n \cdot r + E_n t) \right].
\]

Is it possible to describe a neutral particle? From
\[
\rho' = \frac{ie\hbar}{2m_0 c^2} \left( \psi^* \frac{\partial \psi}{\partial t} - \psi \frac{\partial \psi^*}{\partial t} \right) = -\frac{e\hbar}{m_0 c^2} \text{Im} \left( \psi^* \frac{\partial \psi}{\partial t} \right) \tag{5.22}
\]
it follows that \( \psi \) must be real in this case. Thus we obtain the general wave function of a neutral particle as
\[
\psi_0^{(n)} = \frac{1}{\sqrt{2}} \left[ \psi_+^{(n)} (p_n) + \psi_-^{(n)} (-p_n) \right] = \sqrt{\frac{m_0 c^2}{E_n L^3}} 2 \cos \left( \frac{p_n \cdot r - E_n t}{\hbar} \right).
\]

Note that \( \psi_-^{(n)} \) contributes with an opposite momentum \(-p_n\), therefore \( (\psi_0^{(n)})^* = \psi_0^{(n)} \) and the charge density (5.22) vanishes, i.e. \( \rho' = 0 \). However, the current density also disappears, \( j' = 0 \), and the continuity equation becomes a trivial identity.

In summary, for the relativistic motion of a free spinless particle there are three solutions of the Klein Gordon equation corresponding to the electric charges \((+, -, 0)\) at each momentum \( p \). Moreover, wave functions \( \psi \) and \( \psi^* \) describe opposite charges.
Chapter 6

The Dirac equation

6.1 The Dirac equation

The Dirac equation, in contrast to the Klein-Gordon equation, is of first order and only valid in the case of spin-$\frac{1}{2}$ particles. Due to the fact that the Klein-Gordon equation (KGE) expresses nothing more than the relativistic relation between energy, momentum and mass, it must be valid for particles of arbitrary spin.

The Dirac equation has a completely different origin and can be derived from the transformation properties of a spinor under the Lorentz group. We will address this later on – first we want to understand Dirac’s original line of thinking.

The KGE suffers from two flaws: The probability density is not defined positive and states with an negative energy appear. For theses reasons, the KGE was (historically) initially discarded and Dirac was looking for a replacement of it, namely a relativistic invariant equation of a field function $\hat{\psi}(x)$, which should describe free electrons.

In the case of non-relativistic electrons, Pauli (1927) found the correct description: Within the framework of the Schrödinger picture, an non-relativistic electron is described by a wave function with two components:

$$\psi(x, t) = \begin{pmatrix} \psi_1(x, t) \\ \psi_2(x, t) \end{pmatrix}.$$ 

Here $|\psi_i(x, t)|^2 d\mathbf{x}$, $(i = 1, 2)$ are the probability densities of finding the electron with a spin in positive $(i = 1)$ or negative $(i = 2)$ 2-direction within the volume element $d\mathbf{x}$ around the position $\mathbf{x}$.

Total angular momentum operator:

$$\hat{\mathbf{J}} = \hat{\mathbf{L}} + \frac{\hbar}{2} \hat{\mathbf{\sigma}},$$

where

$$\hat{\mathbf{L}} = \mathbf{x} \times \frac{\hbar}{i} \nabla$$

and

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Pauli spin-matrices
ψ(x, t) (respectively every component of it) should satisfy the Schrödinger equation

\[ i \frac{\partial}{\partial t} \psi(x, t) = -\frac{\hbar^2}{2m} \Delta \psi(x, t) \]

This equation is certainly not relativistic invariant, because only one temporal but two spacial derivations appear.

For reasons which would not seem mandatory today, Dirac was looking for a field equation to be linear in temporal and spatial derivations. We will view this as a heuristic principle and make the general linear ansatz

\[ (\gamma^\mu \partial_\mu - a) \psi(x) = 0, \quad (6.1) \]

where the number of components of ψ, the nature of the coefficients γ^μ and the constant a are still completely undefined.

Applying again the operator \((i\gamma^\mu \partial_\mu)\) to (6.1) gives

\[
\left[ - (\gamma^\mu \partial_\mu)(\gamma^\nu \partial_\nu) - i(\gamma^\mu \partial_\mu)a \right] \psi = 0
\]

resp.

\[
(\gamma^\nu \gamma^\mu \partial_\nu + a^2) \psi = 0
\]

Because of \(\partial_\mu \partial_\nu = \partial_\nu \partial_\mu\) one can replace \(\gamma^\mu \gamma^\nu\) with the symmetric combination

\[
\frac{1}{2} \left( \gamma^\mu \gamma^\nu + \gamma^\nu \gamma^\mu \right) =: \frac{1}{2} \{\gamma^\mu, \gamma^\nu\}
\]

and arrives at

\[
\frac{1}{2} \{\gamma^\mu, \gamma^\nu\} \partial_\mu \partial_\nu + a^2 \psi = 0
\]

On the other hand demands the principle of relativity that the energy-momentum-mass relation is satisfied, i.e. that every component of ψ satisfies the KGE

\[
\left( \Box + m^2 \right) \psi(x) = 0
\]

From this we derive that \(a = m\) and that the coefficient of \(\partial_\mu \partial_\nu\) in (6.2) has to be \(g^{\mu\nu}\)

\[
a = m \quad \text{and} \quad \{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \quad (6.3)
\]

This relation must be satisfied for the coefficients.

With \(\mu = \nu = 0, \quad \mu = \nu = i\) and \(\mu \neq \nu\) follows successively

\[
\left( \gamma^0 \right)^2 = 1, \quad \left( \gamma^i \right)^2 = -1, \quad \gamma^\mu \gamma^\nu = -\gamma^\nu \gamma^\mu \quad (\mu \neq \nu)
\]

These conditions can neither be satisfies by complex numbers nor 2 × 2-matrices as choice for \(\gamma^\mu\). However it is possible with 4 × 4-matrices, e.g.:

\[
\gamma^0 = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \gamma^j = \begin{pmatrix} 0 & +\sigma^j \\ -\sigma^j & 0 \end{pmatrix}, \quad j = 1, 2, 3
\]

Obviously this is not the only possible choice: \(\gamma^\mu = S \gamma^\mu S^{-1}\) with an arbitrary unitary 4 × 4-matrix \(S\) will also satisfy (6.2). The Dirac equation is then satisfied with \(\psi' = S\psi\).
CHAPTER 6. THE DIRAC EQUATION

The 1928 postulated equation of Dirac was

\( \left( i\gamma^\mu \partial_\mu - m \right) \psi(x) = 0, \quad (6.4) \)

with

\[ \psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \\ \psi_4(x) \end{pmatrix}, \]

where \( \psi(x) \) is a 4-component field function, a so called Dirac spinor.

Our goal is now to construct a (probability-)current \( j^\mu \) (like in the KGE case) and check if the density is positive.

Proceeding form the Dirac equation

\( \left( i\gamma^0 \partial_0 + i\gamma^j \partial_j - m \right) \psi = 0 \)

we consider the Hermitian conjugate equation \( \left( \gamma^0 \right)^\dagger = \gamma^0; \quad \left( \gamma^j \right)^\dagger = -\gamma^j \)

\[ \psi^{\dagger} \left( -i\gamma^0 \partial_0 + i\gamma^j \partial_j - m \right) = 0, \]

where \( \psi^{\dagger} = \partial_\mu \psi^{\dagger} \), \( \psi^{\dagger} = (\psi_1^*, \psi_2^*, \psi_3^*, \psi_4^*) \).

Multiplication from the right with \( \gamma_0 \) (and \( \gamma^j \gamma_\mu = -\gamma_0 \gamma^j \)) leads to

\[ \bar{\psi} \left( i\gamma^\mu \gamma_\mu + m \right) = 0, \quad (6.5) \]

where \( \bar{\psi} := \psi^{\dagger} \gamma^0 \) represents the adjunct spinor of \( \psi \).

With (6.5) and the Dirac equation (6.4) one can show now that the current

\[ j^\mu := \bar{\psi} \gamma^\mu \psi \]

is conserved:

\[ \partial_\mu j^\mu = \left( \partial_\mu \bar{\psi} \right) \gamma^\mu \psi + \bar{\psi} \gamma^\mu \left( \partial_\mu \psi \right) \]
\[ = \left( i m \bar{\psi} \right) \psi + \bar{\psi} \left( -i m \psi \right) \]
\[ = 0 \]

Therefore the density \( j^0 \) is given by

\[ j^0 = \bar{\psi} \gamma^0 \psi = \bar{\psi}^{\dagger} \psi = |\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + |\psi_4|^2 \]

and this expression is positive. \( j^0 \) can therefore serve as probability density for the particles described by the Dirac equation.

The difficulty with the KGE concerned states of negative energy. A Dirac particle at rest obeys \( (\psi \propto e^{ip_0 t}; \quad p_j = 0) \)

\[ \gamma^0 p_0 \psi = m \psi \quad \text{resp.} \quad p_0 \psi = m \gamma^0 \psi. \]
The eigenvalues of $\gamma^0$ are $+1$ (doubly degenerate) and $-1$ (doubly degenerate), therefore there exist two solutions with positive energy $+m$ and two solutions with negative energy $-m$. Actually it is easy to see (by writing out the four components of the Dirac equation in full), that the eigenvalues are given by

$$E = \pm \left( m^2 + p^2 \right)^{1/2}$$

For every $p$ exist two solutions with $E > 0$, corresponding to the two states of a spin-$\frac{1}{2}$ particle, and two solutions with $E < 0$.

An electron in a state with $E > 0$ can therefore (by interacting with other particles or fields) jump in a state with $E < 0$ and then cascade downwards to $E = -\infty$ while emitting an infinite amount of radiation.

**Dirac’s solution** of this problem: The electrons possess spin-$\frac{1}{2}$, therefore they satisfy the Pauli exclusion principle. Dirac assumed, that states with negative energy are already completely occupied, the Pauli principle prohibits that further electrons fall in the sea with $E < 0$.

**Remark:**
This “Dirac sea” is the vacuum. The vacuum is therefore by no means “empty”. Important postulate of this theory: antiparticles.

Assuming there exists a vacancy (“blank position”) within the electron sea – a “hole” with energy $-|E|$.

Then an electron with energy $E$ is able to fill this hole by emitting the energy $2E$ and only leaving a vacuum:

$$e^- + \text{hole} \rightarrow \text{energy}$$

Thus the “hole” possesses an effective charge $+e$ and a positive energy. Dirac’s theory postulated the existence of antiparticles for all particles with spin-$\frac{1}{2}$, and over time $e^+, \bar{p}, \bar{n}, \bar{\gamma}$ and others were all found. It became apparent that bosons also possess antiparticles (see quantized complex Klein-Gordon field).

**Remark:**
Despite the successful resolution of the negative energy problem does the Dirac equation no longer represent a single particle equation! It describes particles and antiparticles. The only consistent philosophy is to treat the spinor $\psi$ as a field and $|\psi|^2$ as a measure of the amount of particles present at a certain point. This field is naturally a quantum field.

### 6.2 Solution of the Dirac equation

We choose plane waves as an ansatz for a solution: $\psi(x) \propto e^{-ipx} = e^{-i(p^0t - \mathbf{p} \cdot \mathbf{x})}$.

Furthermore $\psi(x)$ must satisfy the KGE, which demands $p^0 = \sqrt{p^2 + m^2}$. Therefore

$$\psi(x) = e^{-ipx} u(p),$$

where $u(p)$ is a spinor to be determined.
Substituting in the Dirac equation (6.4) leads to

\[
(\not{p} - m) u(p) = 0,
\]

where \( \not{p} \equiv p^\alpha \gamma_\alpha \) represents a \( 4 \times 4 \)-matrix.

First consider \( p = 0 \), respectively

\[
p = p_R = \begin{pmatrix} m \\ 0 \\ 0 \\ 0 \end{pmatrix}
\]

We will see that this case corresponds to an electron at rest, hence the index “R”.

Calculating the zeroth component we find

\[
p^0 \gamma_0 - m = \begin{pmatrix} p^0 - m \\ p^0 - m \\ -p^0 - m \\ -p^0 - m \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ -2m \\ -2m \end{pmatrix}
\]

\((p^0 \gamma_0 - m) u(p_R) = 0\) has two linear independent solutions.

\[
u_s(p_R) = \sqrt{2m} \begin{pmatrix} \chi_s \\ 0 \end{pmatrix},
\]

where \( s = \pm \frac{1}{2} \) and

\[
\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}
\]

are two-spinors.

**Remark:** Here we use the normalization \( \sqrt{2m} \) of the spinor \( u_s(p) \). Other normalizations are possible, e.g. 1 (see Schwabl, exercise).

We combine the two upper and the two lower components of the Dirac spinor each to a two-spinor. For an arbitrary four-vector we make the ansatz

\[
u(p) = \begin{pmatrix} \xi \\ \eta \end{pmatrix},
\]

where \( \xi \) and \( \eta \) are spinors with two components.

From \((p^0 \gamma^0 - p \gamma - m) u(p) = 0\) follows

\[
\begin{pmatrix} p^0 - m & -p \cdot \sigma \\ p \cdot \sigma & -p^0 - m \end{pmatrix} \begin{pmatrix} \xi \\ \eta \end{pmatrix} = 0.
\]

Writing above expression out in full we have

\[
\begin{pmatrix}
0 & p^0 - m & -p^3 & -p^1 + ip^2 \\
p^0 - m & 0 & -p^1 - ip^2 & p^3 \\
p^3 & p^1 - ip^2 & -p^0 - m & 0 \\
p^1 + ip^2 & -p^3 & 0 & -p^0 - m
\end{pmatrix}
\begin{pmatrix}
\xi_1 \\
\xi_2 \\
\eta_1 \\
\eta_2
\end{pmatrix} = 0.
\]
and further

\[(p^0 - m) \xi - (p \cdot \sigma) \eta = 0 \quad (a)\]
\[(p \cdot \sigma) \xi - (p^0 + m) \eta = 0 \quad (b)\]

which leads to the relation

\[\eta = \frac{p \cdot \sigma}{p^0 + m}. \quad (b)\]

Checking (a):

\[\left( p^0 - m - \frac{(p \cdot \sigma)^2}{p^0 + m} \right) \xi = \left( p^0 - m - \frac{p^2}{p^0 + m} \right) \xi = \frac{(p^0)^2 - m^2 - p^2}{p^0 + m} \xi = 0\]

The two-component spinor \(\xi\) is therefore completely arbitrary. In the case of a general four-momentum \(p\) we obtain two linear independent solutions of negative frequency as well, which we want to normalize in the following way:

\[u_s(p) = \sqrt{p^0 + m} \left( \frac{\chi_s}{p^0 + m} \right) \quad s = \pm \frac{1}{2}\]

**Remark:** Note again, that the spinor is normalized to \(\sqrt{2p^0}\) – other choices, like 1, are also commonly used (Schwabl, exercise).

Analogously, we get the solutions for positive frequencies via:

**Ansatz:** \(\psi(x) = e^{ipx} v(p), v(p)\) the to be determined spinor.

Substitution in the Dirac-Equation gives:

\[\left( \not{p} + m \right) v(p) = 0\]

We again choose two linear independent solutions \(\forall p\)

\[v_s(p) = -\sqrt{p^0 + m} \left( \frac{p \sigma}{p^0 + m} \right) \epsilon \chi_s \quad s = \pm \frac{1}{2}, \epsilon = \left( \begin{array}{cc} 0 & 1 \\ -1 & 0 \end{array} \right)\]

Due to the linearity of the Dirac equation, the general solution is given by a superposition in the form of a Fourier integral:

\[\psi(x) = \int \frac{dp}{(2\pi)^3} \frac{1}{2p^0} \sum_{s=\pm \frac{1}{2}} \left\{ e^{ipx} v_s(p) \beta_s^\alpha(p) + e^{-ipx} u_s(p) \alpha_s(p) \right\}\]

Here \(\alpha_s(p)\) and \(\beta_s^\alpha(p)\) represent two arbitrary complex valued functions.
6.3 Non-relativistic limiting case and the magnetic moment of the electron

Particles with a spin possess an “inner” magnetic moment. A charge $e$, which is moving on an closed circular orbit, interacts with a magnetic field and possess an effective magnetic moment.

$$\mu = \frac{e}{2m} L$$

Would nature be “simple”, the control of proportionality between electron spin $S = \frac{1}{2} \hbar \sigma$ and it’s magnetic moment $e/2m$, such that the inner magnetic moment would assume the value $(e/2m) \cdot |S| = e\hbar/4m$.

The resulting shift in frequencies of the spectral lines would correspond to the “normal” Zeeman effect. However experiments show an “anomalous” Zeeman effect – the proportionality constant is $2$ times the one of the circular orbit motion, i.e. the magnetic moment of the electron is $-\mu$

where

$$\mu = 2 \frac{e}{2m} S = \frac{e}{m} S = \frac{e\hbar}{2m} \sigma$$

The factor $2$ is often called Landé factor, $g_s = 2$. This is an immediate result of the Dirac equation. To derive this we have to consider the equation in the case of an electron in presence of an electromagnetic field.

We use the scheme of “minimal coupling” (The reason will later on become clear when looking at gauge theories, but is in this case analogous to classical mechanics).

$$p^\mu \rightarrow p^\mu - e A^\mu,$$

where $p^\mu = (E, p)$ the momentum four-vector, $A^\mu = (\phi, A)$ the usual vector potential – and $\phi$ the electric potential, i.e.

$$E \rightarrow E - e\phi, \quad p \rightarrow p - eA$$

The Dirac equation then reads

$$\gamma^0 (E - e\phi)\psi - \gamma \cdot (p - eA)\psi = m\psi.$$

In standard representation, matrices and spinor are given by

$$\gamma^0 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \gamma = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix}, \quad \psi = \begin{pmatrix} u \\ v \end{pmatrix}$$

We find:

$$(E - e\phi) - \sigma \cdot (p - eA) = mu \quad (*)$$

$$-(E - e\phi) + \sigma \cdot (p - eA) = mv \quad (**)$$

The second equation gives $v = (E + m - e\phi)^{-1} \sigma \cdot (p - eA) u$ (note that the order of the factors is of importance because $p$ and $\phi$ do not commute).

In the non-relativistic limiting case we find $E + m - e\phi \approx 2m$ and $p \approx mv$ ($v$ the velocity). Therefore

$$\therefore \quad v \approx \frac{1}{2m} \sigma \cdot (p - eA) u = \mathcal{O} \left( \frac{\nu}{c} \right) u,$$
i.e. the two lower components of $\psi$ are much smaller as the upper ones.

Substituting this into (*) we arrive at

$$ Eu = \frac{1}{2m} \sigma \cdot \pi \sigma \cdot \pi u + m u + e\phi u, $$

with $\pi := p - eA$. If $E = m + W$, then

$$ Wu = \left( \frac{1}{2m} \sigma \cdot \pi \sigma \cdot \pi + e\phi \right) u. $$

Because of $\sigma_i \sigma_j = \delta_{ij} + \varepsilon_{ijk} \sigma_k$ it follows $(\sigma \cdot A)(\sigma \cdot B) = A \cdot B + i\sigma \cdot (A \times B)$, from what follows

$$ (\sigma \cdot \pi)^2 = \pi \cdot \pi + i\sigma \cdot (\pi \times \pi) $$

$$ = (p - eA)^2 + i\sigma \frac{(p - eA) \times (p - eA)}{-e(p \times A \cdot A + p)} = eh\nabla \times A = eB $$

By identifying $Wu = H u$, we find

$$ \mathcal{H} = \frac{1}{2m} (p - eA)^2 + e\phi - \frac{e\hbar}{2m} \sigma \cdot B $$

We arrive at the Pauli equation $\mathcal{H} u = Eu$, from which one can derive $g_s = 2$.

Note: Through quantum electrodynamics (QED) one actually finds that $g_s$ is slightly bigger than 2.

To derive the relativistic correction of the Pauli equation, we again consider (**) for the case $A = 0$, i.e. $\pi = p$:

$$ v = (E + m - e\phi)^{-1} \sigma \cdot p u $$

$$ = \left( \frac{\sigma \cdot p}{2m} - \frac{1}{2m}(E - m - e\phi) \frac{\sigma \cdot p}{2m} \right) u $$

(b.c. $\frac{1}{E + m - e\phi} = \frac{1}{2m} - \frac{E - m - e\phi}{(2m)^2}$)

Inserting this in (*) gives

$$ Eu = (e\phi + m) u + \sigma \cdot p \left( \frac{\sigma \cdot p}{2m} - \frac{1}{2m}(E - m - e\phi) \frac{\sigma \cdot p}{2m} \right) u $$

$$ = \left\{ \begin{array}{l} \frac{(\sigma \cdot p)}{2m} + e\phi + m - \frac{(\sigma \cdot p)}{2m} \frac{E - m - e\phi}{2m} \frac{\sigma \cdot p}{2m} \end{array} \right\} u $$

$$ = \mathcal{H}_2 u $$

Because in leading order $v = \frac{\sigma \cdot p}{2m} u$, the Dirac spinor $\psi = \begin{pmatrix} u \\ v \end{pmatrix}$ is correctly normalized to 1, if we instead of $u$ choose $\tilde{u} = (1 + \frac{p^2}{8m}) u$, because then

$$ 1 = \int d\mathbf{r} \tilde{\psi} \tilde{\psi} = \int d\mathbf{r} \begin{pmatrix} u^\dagger \\ v^\dagger \end{pmatrix} \gamma^0 \begin{pmatrix} u \\ v \end{pmatrix} = \int d\mathbf{r} \begin{pmatrix} u^\dagger u - v^\dagger v \end{pmatrix} $$

$$ = \int d\mathbf{r} u^\dagger \left( 1 - \left( \frac{\sigma \cdot p}{2m} \right)^2 \right) u, $$
i.e. with

\[
\tilde{u} = \left(1 - \frac{p^2}{4m^2}\right)^{-1/2} u \approx \left(1 - \frac{p^2}{8m^2}\right)^{-1} u
\]

\[
\psi = \left(\begin{array}{c} u \\ v \end{array}\right)
\]

is correctly normalized.

We will now rewrite \(\mathcal{H}_2 u = E u\) using \(\tilde{u}\):

\[
u = \Omega^{-1} \tilde{u} = \left(1 + \frac{p^2}{8m^2}\right)^{-1} u \approx \left(1 - \frac{p^2}{8m^2}\right) \tilde{u}.
\]

Therefore

\[
(E - m)\Omega^{-1} \tilde{u} = (\mathcal{H}_2 - m)\Omega^{-1} \tilde{u}
\]

\[
\Omega^{-2} E' \tilde{u} = \Omega^{-1} (\mathcal{H}_2 - m)\Omega^{-1} \text{ where } E' := E - m
\]

i.e.

\[
\left(1 - \frac{p^2}{4m^2}\right) E' \tilde{u} = \left\{ \left(1 - \frac{p^2}{8m^2}\right) \left(\frac{p^2}{2m} + e\phi - \frac{\sigma \cdot p}{2m} E' - e\phi \frac{\sigma \cdot p}{2m} \right) \left(1 - \frac{p^2}{8m^2}\right) \right\} \tilde{u}
\]

\[
\approx \left\{ \frac{p^2}{2m} + e\phi - \frac{\sigma \cdot p}{2m} E' - e\phi \frac{\sigma \cdot p}{2m} - \frac{p^2}{8m^2} \left(\frac{p^2}{2m} + e\phi\right) - \left(\frac{p^2}{2m} + e\phi\right) \frac{p^2}{8m^2} \right\} \tilde{u}
\]

\[
\Rightarrow \quad E' \tilde{u} = \left\{ \frac{p^2}{2m} + e\phi - \frac{\sigma \cdot p}{8m^3} + \frac{p^2}{4m^2} E' - e\phi \frac{\sigma \cdot p}{8m^3} \frac{E' - e\phi}{2m} \frac{\sigma \cdot p}{2m} \right\} \tilde{u}
\]

\[
\text{Because } (\sigma \cdot p)^2 = p^2 \text{ one is able to write}
\]

\[
E' \tilde{u} = \left\{ \frac{p^2}{2m} + e\phi - \frac{p^4}{8m^3} + \frac{\sigma \cdot p}{2m} E' - e\phi \frac{\sigma \cdot p}{2m} \right\} \tilde{u}
\]

\[
(\ast \ast \ast) = A^2 B + BA^2 - 2ABA
\]

\[
= A(AB - BA) - (AB - BA)A = [A, [A, B]]
\]

\[
= \frac{1}{8m^2} \left[ \sigma \cdot p, \left[ \sigma \cdot p, E' - e\phi \right] \right]
\]

\[
= -ie\hbar \sigma \cdot \nabla \phi
\]

\[
= \sigma_i \sigma_j [p_i, \nabla \phi_j] + \sigma_i [p_i, \nabla \phi_j] + \sigma_i \sigma_j \nabla \phi_j + \sigma_i [\sigma_i, \nabla \phi_j] p_i + [\sigma_i, \sigma_j] \nabla \phi_j p_i
\]

\[
= \hbar \Delta \phi + 2i \sigma \cdot (\nabla \phi \times p)
\]
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\[ E' \hat{u} = \left\{ \begin{array}{c}
\frac{p^2}{2m} + e\phi - \frac{p^4}{8m^3} \\
p^4\text{-term}
\end{array} \right. + \left\{ \begin{array}{c}
\frac{\hbar^2}{8m^2} \Delta \phi \\
\text{Darwin-term}
\end{array} \right. + \left\{ \begin{array}{c}
\frac{e}{4m^2} \sigma \cdot (\nabla \phi \times p) \\
\text{LS coupling}
\end{array} \right. \hat{u} \]

These are the leading relativistic corrections of the Pauli equation. Corrections of higher order in \( \nu/c \) can systematically be calculated by using the Foldy-Wouthuysen transformation.

If \( A \neq 0 \) one has to replace \( p \) through \( p - eA \) as well as adding the additional term \( g_s e^2 \frac{e}{2m} S \) to the Hamiltonian.

The meaning and implications of the single additional terms was already discussed in Quantum Mechanics I:

- The **Darwin term** only has an effect for \( s \)-states when considering a Coulomb potential, because \( \Delta \frac{1}{r} = 4\pi \delta(r) \).

- The **\( p^4 \)**-term follows from
  \[ E = m \sqrt{1 + \frac{p^2}{m^2}} \approx m \left( 1 + \frac{p^2}{2m^2} - \frac{1}{8} \left( \frac{p^2}{m^2} \right)^2 \right) = m + \frac{p^2}{2m} - \frac{p^4}{8m^3} \]

- **LS coupling** refers to spin-orbit coupling: For a central potential we have \( \nabla \phi = \frac{\xi}{r} \phi' \), therefore:
  \[ \frac{\hbar}{4m^2} \sigma \cdot (\nabla \phi \times p) = \frac{\hbar}{4m^2} \frac{1}{r} e\phi'(r) \sigma \cdot (r \times p) \]
  \[ = \frac{\hbar}{4m^2} \frac{e\phi'}{r} \sigma \cdot L, \quad L : \text{Orbital angular momentum} \]

6.4 Lorentz covariance of the Dirac equation

**Lorentz covariance and the transformation of spinors**

The *principle of relativity* states that the laws of nature are identical in every inertial reference frame.

We consider two inertial frames \( I \) and \( I' \) with the space-time coordinates \( x \) and \( x' \). Let the wave function of a particle in these two frames be \( \psi \) and \( \psi' \), respectively. We write the Poincaré transformation between \( I \) and \( I' \) as

\[ x' = \Lambda x + a. \quad (6.7) \]

It must be possible to construct the wave function \( \psi' \) from \( \psi \). This means that there must be a local relationship between \( \psi' \) and \( \psi \):

\[ \psi'(x') = F(\psi(x)) = F(\psi(\Lambda^{-1}(x' - a))). \quad (6.8) \]

The principle of relativity together with the functional relation (6.8) necessarily leads to the requirement of **Lorentz covariance**: The Dirac equation in \( I \) is transformed by (6.7) and (6.8) into a Dirac equation in \( I' \). (The Dirac equation is form invariant with respect to Poincaré
In order that both \( \psi \) and \( \psi' \) may satisfy the linear Dirac equation, their functional relationship must be linear, i.e.

\[
\psi'(x') = S(\Lambda) \psi(x) = S(\Lambda) \psi(\Lambda^{-1}(x' - a)).
\] (6.9a)

Here, \( S(\Lambda) \) is a \( 4 \times 4 \)-matrix, with which the spinor \( \psi \) is to be multiplied. We will determine \( S(\Lambda) \) below. In components, the transformation reads:

\[
\psi'_\alpha(x') = \sum_{\beta=1}^{4} S_{\alpha\beta}(\Lambda) \psi_\beta(\Lambda^{-1}(x' - a)).
\] (6.9b)

The Lorentz covariance of the Dirac equation requires that \( \psi' \) obey the equation

\[
(-i\gamma^\mu \partial'_\mu + m) \psi'(x') = 0, \quad (c = 1, \ h = 1)
\] (6.10)

where

\[
\partial'_\mu = \frac{\partial}{\partial x'^\mu}.
\]

The \( \gamma \)-matrices are unchanged under the Lorentz transformations. In order to determine \( S \), we need to convert the Dirac equation in the primed and unprimed coordinate system into one another. The Dirac equation in the unprimed coordinate system

\[
(-i\gamma^\mu \partial_\mu + m) \psi(x) = 0
\] (6.11)

can by means of the relation

\[
\frac{\partial}{\partial x'^\mu} = \frac{\partial x'^\nu}{\partial x^\mu} \frac{\partial}{\partial x'^\nu} = \Lambda^\nu_{\mu} \partial'_\nu
\]

and

\[
S^{-1} \psi'(x') = \psi(x),
\]

be brought into the form

\[
(-i\gamma^\mu \Lambda^\nu_{\mu} \partial'_\nu + m) S^{-1}(\Lambda) \psi'(x') = 0.
\] (6.12a)

After multiplying from the left by \( S \), one obtains

\[
-i S \Lambda^\nu_{\mu} \gamma^\mu S^{-1}(\Lambda) \partial'_\nu \psi'(x') + m \psi'(x') = 0.
\] (6.12b)

From a comparison of (6.12b) with (6.10), it follows that the Dirac equation is form invariant under Lorentz transformations, provided \( S(\Lambda) \) satisfies the following condition:

\[
S(\Lambda)^{-1} \gamma^\nu S(\Lambda) = \Lambda^\nu_{\mu} \gamma^\mu.
\] (6.13)

It is possible to show (see next section) that this equation has nonsingular solutions for \( S(\Lambda) \). A wave function that transforms under a Lorentz transformation according to \( \psi' = S\psi \) is known as a four-component Lorentz spinor.
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Determination of the representation $S(\Lambda)$

Infinite Lorentz transformations

We first consider infinitesimal (proper, orthochronous) Lorentz transformations

$$\Lambda^\nu_\mu = g^\nu_\mu + \Delta \omega^\nu_\mu$$

with infinitesimal and antisymmetric $\Delta \omega^\nu_\mu$

$$\Delta \omega^\nu_\mu = -\Delta \omega^\mu_\nu.$$  \hspace{1cm} (6.14b)

This equation implies that $\Delta \omega^\nu_\mu$ can have only 6 independent nonvanishing elements. These transformations satisfy the defining relation for Lorentz transformations

$$\Lambda^\lambda_\mu g^\mu_\nu \Lambda^\rho_\nu = g^\lambda_\rho,$$  \hspace{1cm} (6.15)

as can be seen by inserting (6.14) into this equation:

$$g^\lambda_\mu g^\mu_\nu g^\rho_\nu + \Delta \omega^\lambda_\rho + \Delta \omega^\rho_\lambda + O((\Delta \omega)^2) = g^\lambda_\rho.$$  \hspace{1cm} (6.16)

Each of the 6 independent elements of $\Delta \omega^\mu_\nu$ generates an infinitesimal Lorentz transformation. We consider some typical special cases:

$$\Delta \omega^0_1 = -\Delta \omega^0_1 = -\Delta \beta : \text{ Transformation onto a coordinate system moving with velocity } c\Delta \beta \text{ in the } x \text{ direction}$$  \hspace{1cm} (6.17)

$$\Delta \omega^1_2 = -\Delta \omega^1_2 = \Delta \varphi : \text{ Transformation onto a coordinate system that is rotated by an angle } \Delta \varphi \text{ about the axis (see Fig. 6.1).}$$  \hspace{1cm} (6.18)

The spatial components are transformed under this passive transformation as follows:

$$x'^1 = x^1 + \Delta \varphi x^2$$

$$x'^2 = -\Delta \varphi x^1 + x^2 \text{ or } x' = x + \begin{pmatrix} 0 \\ 0 \\ -\Delta \varphi \end{pmatrix} x = x + \begin{pmatrix} e_1 & e_2 & e_3 \\ 0 & 0 & -\Delta \varphi \\ x^1 & x^2 & x^3 \end{pmatrix}$$  \hspace{1cm} (6.19)

It must be possible to expand $S$ as a power series in $\Delta \omega^{\mu\nu}$. We write

$$S = 1 + \tau, \quad S^{-1} = 1 - \tau,$$  \hspace{1cm} (6.20)

where $\tau$ is likewise infinitesimal, meaning of order $O(\omega^{\mu\nu})$. We insert (6.20) into the equation for $S$, namely $S^{-1} \gamma^\mu S = \Lambda^\mu_\nu \gamma^\nu$, and get

$$(1 - \tau) \gamma^\mu (1 + \tau) = \gamma^\mu + \gamma^\mu \tau - \tau \gamma^\mu = \gamma^\mu + \Delta \omega^{\mu_\nu} \gamma^\nu,$$  \hspace{1cm} (6.21a)

from which the equation determining $\tau$ follows as

$$\gamma^\mu \tau - \tau \gamma^\mu = \Delta \omega^{\mu_\nu} \gamma^\nu.$$  \hspace{1cm} (6.21b)

To within an additive multiple of $1$, this unambiguously determines $\tau$. If there were two solutions, then the difference between them would commute with all $\gamma^\mu$, and thus be proportional to $1$. 

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Due to the invariance of the norm, the determinant of $S$ must be unity, and thus, to first order in $\Gamma \omega^{\mu\nu}$, we have

$$\det(S) = \det(\mathbb{1} + \tau) = \det(\mathbb{1}) + \text{Tr}(\tau) = 1 + \text{Tr}(\tau) = 1.$$  (6.22)

It thus follows that

$$\text{Tr}(\tau) = 0.$$  (6.23)

Equations (6.21b) and (6.23) have the solution

$$\tau = \frac{1}{8} \Delta \omega^{\mu\nu}(\gamma_\mu \gamma_\nu - \gamma_\nu \gamma_\mu) = -\frac{1}{4} \Delta \omega^{\mu\nu} \sigma_{\mu\nu},$$  (6.24)

where we have introduced the definition

$$\sigma_{\mu\nu} = \frac{i}{2} [\gamma_\mu, \gamma_\nu].$$  (6.25)

Equation (6.24) can be derived by calculating the commutator of $\tau$ with $\gamma^\mu$; the vanishing of the trace is guaranteed by the general properties of the $\gamma$ matrices.

**Rotation about the $z$ axis**

We first consider the rotation $R_3$ about the $z$ axis as given by (6.18). According to (6.18) and (6.24),

$$\tau(R_3) = \frac{i}{2} \Delta \varphi \sigma_{12},$$

and with

$$\sigma^{12} = \sigma_{12} = \frac{i}{2} [\gamma_1, \gamma_2] = i\gamma_1 \gamma_2 = i \begin{pmatrix} 0 & \sigma^1 \\ -\sigma^1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma^2 \\ -\sigma^2 & 0 \end{pmatrix} = \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}.$$  (6.26)
it follows that
\[ S = 1 + \frac{i}{2} \Delta \varphi \sigma^{12} = 1 + \frac{i}{2} \Delta \varphi \begin{pmatrix} \sigma^3 & 0 \\ 0 & -\sigma^3 \end{pmatrix}. \] (6.27)

By a succession of infinitesimal rotations we can construct the transformation matrix \( S \) for a finite rotation through an angle \( \vartheta \). This is achieved by decomposing the finite rotation into a sequence of \( N \) steps \( \vartheta/N \):

\[
\psi'(x') = S\psi(x) = \lim_{N \to \infty} \left( 1 + \frac{i}{2N} \vartheta \sigma^{12} \right)^N \psi(x) \\
= e^{\frac{i}{2} \vartheta \sigma^{12}} \psi \\
= \left( \cos \frac{\vartheta}{2} + i \sigma^{12} \sin \frac{\vartheta}{2} \right) \psi(x).
\] (6.28)

For the coordinates and the four-vectors, this succession of transformations implies that

\[
x' = \lim_{N \to \infty} \left( 1 + \frac{\vartheta}{N} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \right) \cdots \left( 1 + \frac{\vartheta}{N} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \right) x \\
= \exp \left[ \vartheta \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \right] x = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \vartheta & \sin \vartheta & 0 \\ 0 & -\sin \vartheta & \cos \vartheta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} x,
\] (6.29)

and is thus identical to the usual rotation matrix for rotation through an angle \( \vartheta \). The transformation \( S \) for rotations (6.28) is unitary \((S^{-1} = S^\dagger)\). From (6.28), one sees that
\[
S(2\pi) = -\mathbb{1} \quad (6.30a) \\
S(4\pi) = \mathbb{1}.
\] (6.30b)

This means that spinors do not regain their initial value after a rotation through \( 2\pi \), but only after a rotation through \( 4\pi \), a fact that is also confirmed by neutron scattering experiments. We draw attention here to the analogy with the transformation of Pauli spinors with respect to rotations:

\[
\varphi'(x') = e^{\frac{i}{2} \omega \cdot \sigma} \varphi(x).
\] (6.31)

\section*{Lorentz Transformation Along the \( x^1 \) Direction}

According to (6.17),
\[
\Delta \omega^{01} = \Delta \beta
\] (6.32)
and (6.24) becomes
\[
\tau(L_1) = \frac{1}{2} \Delta \beta \gamma_0 \gamma_1 = \frac{1}{2} \Delta \alpha_1.
\] (6.33)
We may now determine $S$ for a finite Lorentz transformation along the $x^1$ axis. For the velocity $v/c$, we have $\tanh \eta = \frac{v}{c}$.

The decomposition of $\eta$ into $N$ steps of $\frac{\eta}{N}$ leads to the following transformation of the coordinates and other four-vectors:

\[
x'^\mu = \lim_{N \to \infty} \left( g + \frac{\eta}{N} I \right)^\mu_\nu \left( g + \frac{\eta}{N} I \right)^\nu_1 \cdots \left( g + \frac{\eta}{N} I \right)^\nu_{N-1} x^\nu
\]

\[
g^\mu_\nu = \delta^\mu_\nu,
\]

\[
I \equiv I^\nu_\mu = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad I^2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad I^3 = I
\]

\[
x' = e^{\eta I} x = \left( 1 + \eta I + \frac{1}{2!} \eta^2 I^2 + \frac{1}{3!} \eta^3 I + \frac{1}{4!} I^2 \cdots \right) x
\]

\[
x'^\mu = \left( 1 - I^2 + I^2 \cosh \eta + I \sinh \eta \right)^\mu_\nu x^\nu
\]

\[
= \begin{pmatrix} \cosh \eta & - \sinh \eta & 0 & 0 \\ - \sinh \eta & \cosh \eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x^0 \\ x^1 \\ x^2 \\ x^3 \end{pmatrix}.
\]

The $N$-fold application of the infinitesimal Lorentz transformation

\[
L_1 \left( \frac{\eta}{N} \right) = 1 + \frac{\eta}{N} I
\]

then leads, in the limit of large $N$, to the Lorentz transformation

\[
L_1(\eta) = e^{\eta I} = \begin{pmatrix} \cosh \eta & - \sinh \eta & 0 & 0 \\ - \sinh \eta & \cosh \eta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.
\]

We note that the $N$ infinitesimal steps of $\frac{\eta}{N}$ add up to $\eta$. However, this does not imply a simple addition of velocities.

We now calculate the corresponding spinor transformation

\[
S(L_1) = \lim_{N \to \infty} \left( 1 + \frac{\eta}{2 N} \alpha_1 \right)^N = e^{\frac{\eta}{2} \alpha_1}
\]

\[
= 1 \cosh \frac{\eta}{2} + \alpha_1 \sinh \frac{\eta}{2}.
\]

Note: $\alpha_i = \gamma_0 \gamma_i$.

For homogeneous restricted Lorentz transformations, $S$ is hermitian ($S(L_1)^\dagger = S(L_1)$).

For general infinitesimal transformations, characterized by infinitesimal antisymmetric $\Delta \omega^{\mu\nu}$, equation (6.24) implies that

\[
S(\Lambda) = 1 - \frac{i}{4} \sigma_{\mu\nu} \Delta \omega^{\mu\nu}.
\]

This yields the finite transformation

\[
S(\Lambda) = e^{-\frac{i}{4} \sigma_{\mu\nu} \omega^{\mu\nu}}
\]
with $\omega^{\mu\nu} = -\omega^{\nu\mu}$ and the Lorentz transformation reads $\Lambda = e^{\omega}$, where the matrix elements of $\omega$ are equal to $\omega^{\mu\nu}$. For example, one can represent a rotation through an angle $\vartheta$ about an arbitrary axis $\hat{n}$ as

$$S = e^{\frac{i}{2}\vartheta \hat{n} \cdot \Sigma}, \tag{6.36c}$$

where

$$\Sigma = \begin{pmatrix} \sigma & 0 \\ 0 & \sigma \end{pmatrix}. \tag{6.36d}$$

Summary:

**Rotation group**

Rotations about the three axes $x^1, x^2, x^3$ are described by

$$R_i(\theta) = e^{i\theta D^i}$$

where

$$D^1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \end{pmatrix}, \quad D^2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad D^3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

The generator $D^i$ satisfy the $su(2)$-algebra

$$[D^i, D^j] = i\epsilon^{ijk}D^k = i\epsilon_{ijk}D^k.$$

**Boosts**

Boosts along the three axes $x^1, x^2, x^3$ are described by

$$L_i(\eta) = e^{-i\eta I^i}$$

where

$$I^1 = \begin{pmatrix} 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad I^2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad I^3 = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix}.$$

The generators $I^i$ do not form a closed algebra and the Lorentz boosts also do not formu a subset of the Lorentz group. Instead we have

$$[I^i, I^j] = -i\epsilon^{ijk}D^k = -i\epsilon_{ijk}D^k.$$
Lorentz algebra

A general infinitesimal Lorentz transformation in the restricted Lorentz group $L^\dagger = \lambda^\mu_\nu + \Delta\omega^\mu_\nu$
can be expressed via the generators of rotations and boosts

\[ \Delta\omega = i\Delta\theta^i D^i - i\Delta\eta^i I^i. \]

The generators form an algebra with

\[ [D^i, D^j] = i\epsilon_{ijk} D^k, \quad [I^i, I^j] = -i\epsilon_{ijk} D^k, \quad [D^i, I^j] = i\epsilon_{ijk} I^k. \]

One gets a finite transformations by exponentiation of the infinitesimal transformations

\[ R_i(\theta) = e^{i\theta D^i}, \quad L_i(\eta) = e^{-i\eta I^i}. \]

Spatial Reflection, Parity

The Lorentz transformation corresponding to a spatial reflection is represented by

\[ \Lambda^\mu_\nu = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \] (6.37)

The associated $S$ is determined, according to (6.13), from

\[ S^{-1}\gamma^\mu S = \Lambda^\mu_\nu\gamma^\nu = \sum_{\nu=1}^{4} g^{\mu\nu}\gamma^\nu = g^{\mu\mu}\gamma^\mu, \] (6.38)

where no summation over $\mu$ is implied. One immediately sees that the solution of (6.38), which we shall denote in this case by $P$, is given by

\[ S = P = e^{i\varphi\gamma^0}. \] (6.39)

Here, $e^{i\varphi}$ is an unobservable phase factor. This is conventionally taken to have one of the four values $\pm 1, \pm i$; four reflections then yield the identity $1$. The spinors transform under a spatial reflection according to

\[ \psi'(x') = \psi'(x', t) = \psi'(-x, t) = e^{i\varphi\gamma^0}\psi(x) = e^{i\varphi\gamma^0}\psi(-x', t). \] (6.40)

The complete spatial reflection (parity) transformation for spinors is denoted by

\[ P = e^{i\varphi\gamma^0}P^{(0)}, \] (6.40')

where $P^{(0)}$ causes the spatial reflection $x \to -x$.  

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From the relationship \( \gamma^0 \equiv \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \) one sees in the rest frame of the particle, spinors of positive and negative energy that are eigenstates of \( P \) - with opposite eigenvalues, i.e., opposite parity. This means that the intrinsic parities of particles and antiparticles are opposite.

**Further Properties of \( S \)**

For the calculation of the transformation of bilinear forms such as \( j^\mu(x) \), we need to establish a relationship between the adjoint transformations \( S^\dagger \) and \( S^{-1} \).

**Assertion:**

\[
S^\dagger \gamma^0 = b \gamma^0 S^{-1},
\]

where

\[
b = \pm 1 \quad \text{for} \quad \Lambda^{00} \begin{cases} \geq +1 \\ \leq -1 \end{cases}.
\]

**Proof:** We take as our starting point Eq. (6.13)

\[
S^{-1} \gamma^\mu S = \Lambda^{\mu \nu} \gamma^\nu, \quad \Lambda^{\mu \nu} \quad \text{real},
\]

and write the adjoint relation

\[
(\Lambda^{\mu \nu} \gamma^\nu)^\dagger = S^\dagger \gamma^\mu S^{\dagger -1}.
\]

The hermitian adjoint matrix can be expressed most concisely as

\[
\gamma^{\mu \dagger} = \gamma^0 \gamma^\mu \gamma^0.
\]

By means of the anticommutation relations, one easily checks that (6.44) is in accord with \( \gamma^{0 \dagger} = \gamma^0 \), \( \gamma^{k \dagger} = -\gamma^k \). We insert this into the left- and the right-hand sides of (6.43) and then multiply by \( \gamma^0 \) from the left- and right-hand side to gain

\[
\begin{align*}
\gamma^0 \Lambda^{\mu \nu} \gamma^\nu \gamma^0 \gamma^0 &= \gamma^0 S^\dagger \gamma^0 \gamma^\mu \gamma^0 S^{\dagger -1} \gamma^0 \\
\Lambda^{\mu \nu} \gamma^{\nu} &= S^{-1} \gamma^\mu S = \gamma^0 S^\dagger \gamma^0 \gamma^\mu (\gamma^0 S^\dagger \gamma^0)^{-1},
\end{align*}
\]

since \( (\gamma^0)^{-1} = \gamma^0 \). Furthermore, on the left-hand side we have made the substitution \( \Lambda^{\mu \nu} \gamma^\nu = S^{-1} \gamma^\mu S \). We now multiply by \( S \) and \( S^{-1} \):

\[
\gamma^\mu = S \gamma^0 S^\dagger \gamma^0 \gamma^\mu (\gamma^0 S^\dagger \gamma^0)^{-1} \gamma^0 S^{-1} \equiv (S \gamma^0 S^\dagger \gamma^0) \gamma^\mu (S \gamma^0 S^\dagger \gamma^0)^{-1}.
\]

Thus, \( S \gamma^0 S^\dagger \gamma^0 \) commutes with all \( \gamma^\mu \) and is therefore a multiple of the unit matrix

\[
S \gamma^0 S^\dagger = b \mathbb{1},
\]

which also implies that

\[
S \gamma^0 S^\dagger = b \gamma^0
\]
and yields the relation we are seeking
\[ S^\dagger \gamma^0 = b(S\gamma^0)^{-1} = b\gamma^0 S^{-1}. \tag{6.41a} \]
Since \((\gamma^0)^\dagger = \gamma^0\) and \(S\gamma^0 S^\dagger\) are hermitian, by taking the adjoint of (6.46) one obtains \(S\gamma^0 S^\dagger = b^*\gamma^0\), from which it follows that
\[ b^* = b \tag{6.47} \]
and thus \(b\) is real. Making use of the fact that the normalization of \(S\) is fixed by \(\det S = 1\), on calculating the determinant of (6.46), one obtains \(b^4 = 1\). This, together with (6.47), yields:
\[ b = \pm 1. \tag{6.48} \]
The significance of the sign in (6.48) becomes apparent when one considers
\[ S^\dagger S = S^\dagger \gamma^0 \gamma^0 S = b\gamma^0 S^{-1}\gamma^0 S = b\gamma^0 \Lambda^0 \gamma^\nu \]
\[ = b\Lambda^0_{00} + \sum_{k=1}^{3} b\Lambda^0_{0k} \gamma^{0k}_{\alpha} \gamma^\nu_{\alpha}. \tag{6.49} \]
\(S^\dagger S\) has positive definite eigenvalues, as can be seen from the following. Firstly, \(\det S^\dagger S = 1\) is equal to the product of all the eigenvalues, and these must therefore all be nonzero. Furthermore, \(S^\dagger S\) is hermitian and its eigenfunctions satisfy \(S^\dagger S\psi_a = a\psi_a\), whence
\[ a\psi^\dagger_a \psi_a = \psi^\dagger_a S^\dagger S\psi_a = (S\psi_a)^\dagger S\psi_a > 0 \]
and thus \(a > 0\). Since the trace of \(S^\dagger S\) is equal to the sum of all the eigenvalues, we have, in view of (6.49) and using \(\text{Tr} \alpha^k = 0\),
\[ 0 < \text{Tr}(S^\dagger S) = 4b\Lambda^0_{00}. \]
Thus \(b\Lambda^0_{00} > 0\). Hence, we have the following relationship between the signs of \(\Lambda^0_{00}\) and \(b\):
\[ \Lambda^0_{00} \geq 1 \quad \text{for} \quad b = 1 \]
\[ \Lambda^0_{00} \leq -1 \quad \text{for} \quad b = -1. \tag{6.41b} \]
For Lorentz transformations that do not change the direction of time, we have \(b = 1\); while those that do cause time reversal have \(b = -1\).

**Transformation of Bilinear Forms**

The *adjoint* spinor is defined by
\[ \bar{\psi} = \psi^\dagger \gamma^0. \tag{6.50} \]
We recall that \(\psi^\dagger\) is referred to as a hermitian adjoint spinor. The additional introduction of \(\bar{\psi}\) is useful because it allows quantities such as the current density to be written in a concise form. We obtain the following transformation behaviour under a Lorentz transformation:
\[ \psi' = S\psi \implies \psi'^\dagger = \psi^\dagger S^\dagger \implies \bar{\psi}' = \psi^\dagger S^\dagger \gamma^0 = b\psi^\dagger \gamma^0 S^{-1}, \tag{6.51} \]

\(^1\)Note: For the Lorentz transformation \(L^+\) (restricted L.T. and rotations) and for spatial reflections, one can derive this relation with \(b = 1\) from the explicit representations.
thus,
\[
\psi' = b \bar{\psi} S^{-1}.
\] (6.52)

Given the above definition, the current density reads:
\[
j^\mu = c \psi^\dagger \gamma^0 \gamma^\mu \psi = c \bar{\psi} \gamma^\mu \psi
\] (6.53)

and thus transforms as
\[
j^\mu' = cb \bar{\psi} S^{-1} \gamma^\mu S \psi = \Lambda^\mu_\nu cb \bar{\psi} \gamma^\nu \psi = b \Lambda^\mu_\nu j^\nu.
\] (6.54)

Hence, \(j^\mu\) transforms in the same way as a vector for Lorentz transformations without time reflection. In the same way one immediately sees, using (6.9a) and (6.52), that \(\bar{\psi}(x)\psi(x)\) transforms as a scalar:
\[
\bar{\psi}'(x')\psi'(x') = b \bar{\psi}(x') S^{-1} S \psi(x') = b \bar{\psi}(x) \psi(x).
\] (6.55a)

We now summarize the transformation behaviour of the most important bilinear quantities under \textit{orthochronous Lorentz transformations}, i.e., transformations that \textit{do not reverse the direction of time}:

\[
\begin{align*}
\bar{\psi}'(x')\psi'(x') &= \bar{\psi}(x)\psi(x) \quad \text{scalar} \\
nu' \bar{\psi}'(x') \gamma^\mu \psi'(x') &= \Lambda^\mu_\nu \bar{\psi}(x) \gamma^\mu \psi(x) \quad \text{vector} \\
nu' \bar{\psi}'(x') \sigma^{\mu\nu} \psi'(x') &= \Lambda^\mu_\rho \Lambda^\nu_\sigma \bar{\psi}(x) \sigma^{\rho\sigma} \psi(x) \quad \text{antisymmetric tensor} \\
nu' \bar{\psi}'(x') \gamma_5 \gamma^\mu \psi'(x') &= (\det \Lambda) \Lambda^\mu_\nu \bar{\psi}(x) \gamma_5 \gamma^\nu \psi(x) \quad \text{pseudovector} \\
nu' \bar{\psi}'(x') \gamma_5 \gamma_5 \psi'(x') &= (\det \Lambda) \bar{\psi}(x) \gamma_5 \psi(x) \quad \text{pseudoscalar},
\end{align*}
\] (6.55a)

where \(\gamma_5 = i \gamma^0 \gamma^1 \gamma^2 \gamma^3\). We recall that \(\det \Lambda = \pm 1\); for spatial reflections the sign is \(-1\).
Appendix A

Correlation Functions, Scattering, and Response

A.1 Scattering and Response

If a time-dependent field $E e^{i(kr-\omega t)}$ is applied to many-particle system (solid, liquid, or gas), this induces a “polarization”:

$$P(k, \omega) e^{i(kr-\omega t)} + P(k, 2\omega) e^{i(2kr-2\omega t)} + P(2k, \omega) e^{i(2kr-\omega t)} + \ldots$$

periodicity as the applied field

nonlinear effects

Linear susceptibility is a property of the unperturbed sample:

$$\chi(k, \omega) := \lim_{E \to 0} \frac{P(k, \omega)}{E}$$

Scattering experiments with particles:

The wavelength of the particles must be similar to the scale of the structure that one wants to resolve.

Energy must be comparable to the excitation energies of the quasiparticles.

For example, neutron scattering with thermal neutrons from nuclear reactors. ($\lambda \approx 0.18 \text{ nm for } E = 25 \text{ meV } \approx 290 \text{ K}$).

Inelastic scattering cross-section

$H_0$: Hamiltonian of a many-particle system (sample)

$x_\alpha$: Coordinates of the particles of the sample (position and other degrees of freedom)

$m, r, m_s$: mass, position and spin of the incident particle.

$$H = H_0 + \frac{p^2}{2m} + W(\{x_\alpha\}, r)$$

with the kinetic energy of the incident particle $p^2/2m$ and the interaction between the sample and the incident particle $W(\{x_\alpha\}, r)$. 

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In second quantization

\[ H = H_0 + \frac{\hbar^2}{2m} \sum_{k,k',\sigma'\sigma''} a_{k'\sigma'}^\dagger a_{k\sigma''} \frac{1}{V} \int d^3r e^{-i(k' - k)r} W_{\sigma'\sigma''} \{x_\alpha, r\} \]

\[ = H_0 + \frac{\hbar^2}{2m} \sum_{k,k',\sigma'\sigma''} a_{k'\sigma'}^\dagger a_{k\sigma''} W_{k'k\sigma'\sigma''} \{x_\alpha\} \]

\(a_{k'\sigma'}\) creates a incident particle with \(k', \sigma'\)
\(a_{k\sigma''}\) annihilates a incident particle with \(k', \sigma''\)

Eigenstates of \(H_0\):

\[ H_0|n\rangle = E_n|n\rangle \]

Initial state \(|k_1, m_{s_1}, n_1\rangle\) \((|n_1\rangle \text{ initial state of the sample})\)
Final state \(|k_2, m_{s_2}, n_2\rangle\) \((|n_2\rangle \text{ final state of the sample})\)

The transition probability per unit time (Fermi’s golden rule):

\[ \Gamma(k_1, m_{s_1}, n_1 \rightarrow k_2, m_{s_2}, n_2) = \frac{2\pi}{\hbar} |\langle k_2, m_{s_2}, n_2|W|k_2, m_{s_1}, n_1\rangle|^2 \delta(E_{n_1} - E_{n_2} + \hbar\omega) \]

where \(\langle k_2, m_{s_2}, n_2|W|k_2, m_{s_1}, n_1\rangle = W_{k_2-k_1}^{m_{s_2}m_{s_1}}\{x_\alpha\}\) and \(\hbar\omega = \frac{\hbar^2}{2m}(k_1^2 - k_2^2)\).

The distribution of initial states of the sample \(|n_1\rangle\) is \(p(n_1) \geq 0\) with \(\sum_{n_1} p(n_1) = 1\)

The distribution of the spin states of the incident particle \(m_{s_1}\) is \(p_s(m_{s_1})\) with \(\sum_{m_{s_1}} p_s(m_{s_1}) = 1\)

If only \(k_2\) (and not \(m_{s_1}\)) is measured:

\[ \Gamma(k_1 \rightarrow k_2) = \sum_{n_2, n_1} \sum_{m_{s_1}, m_{s_2}} p(n_1) p_s(m_{s_1}) \Gamma(k_1, m_{s_1}, n_1 \rightarrow k_2, m_{s_2}, n_2) \]

The differential scattering cross-section per atom:

\[ \frac{d^2\sigma}{d\Omega de} d\Omega de = \frac{\text{probability of transition into } d\Omega de/s}{\text{number of scatterers} \times \text{flux of incident particles}} \]

The element of the solid angle into which is scattered is \(d\Omega\), the flux of incident particles is equal to the magnitude of their current density, the number of scatterers is \(N\), the normalization volume is \(L^3\).

The states of the incident particles are \(\psi_{k_1}(r) = \frac{1}{L^{3/2}} e^{i k_1 r}\), thus the current density is \(j(r) = -\frac{i\hbar}{2m}(\psi^* \nabla \psi - (\nabla \psi^*) \psi) = \frac{\hbar k_1}{mL^3}\) and \(\frac{d^2\sigma}{d\Omega de} d\Omega de = \frac{1}{N \hbar k_1} \Gamma(k_1 \rightarrow k_2) \left(\frac{L}{2\pi}\right)^3 d^3k_2\)
The number of final states, i.e., the number of $k^2$ values in the interval $d^3k_2$ is $\left(\frac{3L^2}{2\pi}\right)^3 d^3k_2$

**Remark:** Systems in equilibrium: $p(n_1) = e^{-\beta E_{n_1}} Z$ (from density matrix $\rho = e^{-\beta H_0} Z$).

Due to $\delta(\omega) = \int \frac{dt}{2\pi} e^{i\omega t}$ the scattering cross-section contains the factor

$$\frac{1}{\hbar} \int \frac{dt}{2\pi} e^{i(E_{n_1} - E_{n_2} + \hbar\omega)/\hbar} \langle n_1 | e^{-ikx_\alpha} | n_2 \rangle$$

$$= \frac{1}{2\pi\hbar} \int dt e^{i\omega t} \langle n_1 | e^{iH_0 t/\hbar} e^{-ikx_\alpha} e^{-iH_0 t/\hbar} | n_2 \rangle$$

$$= \frac{1}{2\pi\hbar} \int dt e^{i\omega t} \langle n_1 | e^{-ikx_\alpha(t)} | n_2 \rangle$$

$$\Rightarrow S_{coh}(k,\omega) = \int \frac{dt}{2\pi\hbar} e^{i\omega t} \frac{1}{N} \sum_{\alpha\beta} \langle e^{-ikx_\alpha(t)} e^{ikx_\beta(0)} \rangle \left( \frac{1}{\delta_{\alpha\beta}} \right)$$

where the index coh or inc refers to coherent or incoherent dynamical structure function, respectively. Both contain an elastic ($\omega = 0$) and an inelastic ($\omega \neq 0$) component.

The thermal average of an operator $O$ is defined by $\langle O \rangle = \sum_n \frac{e^{-\beta E_n}}{Z} \langle n | O | n \rangle = \text{Tr}(\rho O)$.

Density operator of the target system (sample):

$$\rho(x, t) = \sum_{\alpha=1}^N \delta(x - x_\alpha(t))$$

and its Fourier transform:

$$\rho_k(t) = \frac{1}{\sqrt{V}} \int d^3x e^{-ikx} \rho(x, t) = \frac{1}{\sqrt{V}} \sum_{\alpha=1}^N e^{-ikx_\alpha(t)}$$

$$\Rightarrow S_{coh}(k,\omega) = \int \frac{dt}{2\pi\hbar} e^{i\omega t} \frac{V}{N} \langle \rho_k(t) \rho_{-k}(0) \rangle$$

with the density-density correlation function $\langle \rho_k(t) \rho_{-k}(0) \rangle$, the momentum $\hbar k$ and the energy transfer $\hbar \omega$ from the scattered particles to the target system.

Application: scattering from solids to determine the lattice dynamics.

The one-phonon scattering: resonances at $\pm \omega t_1(k)$ and $\pm \omega t_2(k)$ (two transverse phonons), and at $\pm \omega l(k)$ (longitudinal phonons)

The width of the resonances: lifetime of the phonons.

The background intensity is due to multiphonon scattering.

The intensity of the resonances depends on the scattering geometry via the scalar product of $k$ with the polarization vector of the phonons and via the Debye-Waller factor.

Scattering cross-section $\leftrightarrow$ correlation functions of the many-particle system

In the following: correlation functions $\leftrightarrow$ response function
With \( \epsilon = \frac{\hbar^2 k^2}{2m} \), it follows that \( d\epsilon = \frac{\hbar^2 k^2}{m} \) and \( d^3k = \frac{m}{\pi^2 k^2} \) \( d\epsilon \) \( \Rightarrow \)

\[
\frac{d^2 \sigma}{d\Omega d\epsilon} = \left( \frac{m}{2\pi\hbar^2} \right)^2 \frac{k^2 L^6}{k_1 N} \sum_{n_1:n_2 \atop m_1:m_2} p(n_1)p(m_{s_1})|\langle k_1, m_{s_1}, n_1|W|k_2, m_{s_2}, n_2 \rangle|^2 \delta(E_{n_1} - E_{n_2} + \hbar\omega)
\]

**Special case: neutron scattering** (neutral particle)

\( \Rightarrow \) Scattering solely by nuclei.

The range of the nuclear force: \( R \approx 10^{-12} \text{ cm} \) \( \Rightarrow \) \( k_1 R \approx 10^{-4} \ll 1 \) \( \Rightarrow \) only s-wave scattering.

\( \Rightarrow \) The interaction can be represented by an effective pseudopotential.

\[
W(x) = \frac{2\pi\hbar^2}{m} \sum_{\alpha=1}^N a_\alpha \delta(x_{\alpha} - x)
\]

where \( a_\alpha \) is the scattering lengths of the nuclei (Born approximation).

\( \Rightarrow \) independent of the spin \( m_{s_1} \)!

\[
\Rightarrow \frac{d^2 \sigma}{d\Omega d\epsilon} = \frac{k_2}{k_1} \frac{1}{N} \sum_{n_1:n_2} p(n_1) \left| \sum_{\alpha=1}^N a_\alpha |e^{ikx_{\alpha}}|n_2 \rangle \right|^2 \delta(E_{n_1} - E_{n_2} + \hbar\omega)
\]

We have used

\[
|\langle k_1|W|k_2 \rangle| = \frac{2\pi\hbar^2}{mL^3} \int d^3x \ e^{-ik_1x} \sum_{\alpha} a_\alpha \delta(x - x_{\alpha}) e^{ik_2x}
\]

\[
= \frac{2\pi\hbar^2}{mL^3} \sum_{\alpha} a_\alpha e^{-i(k_1 - k_2)x_{\alpha}}
\]

and

\[
\left| \sum_{\alpha=1}^N a_\alpha |e^{ikx_{\alpha}}|n_2 \rangle \right|^2 = \sum_{\alpha,\beta} a_\alpha a_\beta |\langle n_1|e^{-ikx_\alpha}|n_2 \rangle \langle n_2|e^{ikx_\beta}|n_1 \rangle \delta(E_{n_1} - E_{n_2} + k\omega)\]

Averaging over the various isotopes with different scattering lengths.

Assumption: positions of the isotopes are randomly distributed:

\[
a_{\alpha}a_{\beta} = \begin{cases} a^2 & \text{for } \alpha \neq \beta \\ a^2 & \text{for } \alpha = \beta \end{cases} \quad \text{with} \quad a = \frac{1}{N} \sum_{\alpha=1}^N a_\alpha \quad \text{and} \quad a^2 = \frac{1}{N} \sum_{\alpha=1}^N a_\alpha^2
\]

\( \Rightarrow \) Decomposition of the scattering cross-section into a **coherent** and an **incoherent** part

\[
\frac{d^2 \sigma}{d\Omega d\epsilon} = A_{\text{coh}} S_{\text{coh}}(k, \omega) + A_{\text{inc}} S_{\text{inc}}(k, \omega)
\]

With

\[
A_{\text{coh}} = a^2 k_2 \frac{k_2}{k_1}, \quad A_{\text{inc}} = (a^2 - a^2) k_2 \frac{k_2}{k_1}\quad \text{amplitudes superpose, interference}
\]

\[
S_{\text{coh}} = \frac{1}{N} \sum_{\alpha,\beta} \sum_{n_1:n_2} p(n_1) \langle n_1|e^{-ikx_\alpha}|n_2 \rangle \langle n_2|e^{ikx_\beta}|n_1 \rangle \delta(E_{n_1} - E_{n_2} + \hbar\omega)
\]

\[
S_{\text{inc}} = \frac{1}{N} \sum_{\alpha} \sum_{n_1:n_2} p(n_1) |\langle n_1|e^{-ikx_\alpha}|n_2 \rangle|^2 \delta(E_{n_1} - E_{n_2} + \hbar\omega)
\]

intensities superpose, no interference
APPENDIX A. CORRELATION FUNCTIONS, SCATTERING, AND RESPONSE

\( S_{\text{coh}} \) contains information about the correlations between different atoms. 
\( S_{\text{inc}} \) contains information about the correlation of each atom with itself.

### A.2 Correlation and response functions

\( H_0 \): time independent Hamiltonian of a many-particle system

Schrödinger equation: 
\[ i\hbar \frac{\partial}{\partial t} |\psi, t\rangle = H_0 |\psi, t\rangle \]

Formal solution:
\[ |\psi, t\rangle = e^{-iH_0(t-t_0)/\hbar} |\psi, t_0\rangle =: U(t, t_0) |\psi, t_0\rangle \]

Heisenberg representation:

- State \( |\psi_H\rangle = |\psi, t_0\rangle \) is time-independent,
- Operator \( A(t) = U_0^\dagger(t, t_0) A U_0(t, t_0) \) is time-dependent

Heisenberg equation of motion 
\[ \frac{d}{dt} A(t) = \frac{1}{\hbar} [H_0, A(t)] \]

Density matrix:

\[ \rho = e^{-\beta H_0} \] with \( Z = \text{Tr} e^{-\beta H_0} \)
\[ \rho_G = \frac{e^{-\beta(H_0-\mu N)}}{Z_G} \] with \( Z_G = \text{Tr} e^{-\beta(H_0-\mu N)} \)

Mean values: 
\[ \langle O \rangle = \text{Tr} (\rho O) \]

Correlation function:
\[ C_{AB}(t, t') : = \langle A(t) B(t') \rangle = \text{Tr} (\rho e^{iH_0 t/\hbar} A e^{-iH_0 t/\hbar} e^{iH_0 t'/\hbar} B e^{-iH_0 t'/\hbar}) = \text{Tr} (\rho e^{iH_0(t-t')/\hbar} A e^{-iH_0(t-t')/\hbar} B) = C_{AB}(t-t', 0) \Rightarrow \text{temporal translational invariance} \]

Definition:

\[
\begin{align*}
G^>_AB(t) : & = \langle A(t) B(0) \rangle \\
G^<_AB(t) : & = \langle B(0) A(t) \rangle \\
\end{align*}
\]  
\( \rightarrow \) Fourier transform: 
\[ G^>_AB(\omega) = \int dt e^{i\omega t} G^>_AB(t) \]

\( \rightarrow G^>_AB(\omega) = \int dt e^{i\omega t} \text{Tr} (\rho e^{iH_0 t/\hbar} A e^{-iH_0 t/\hbar} B) \]
\[ = \int dt e^{i\omega t} \sum_{n,m} \langle n | e^{-\beta H_0} e^{iH_0 t/\hbar} A|m\rangle \langle m | e^{-iH_0 t/\hbar} A|n\rangle e^{iE_m t/\hbar} \langle m | B|n\rangle \]
\[ = \frac{1}{Z} \sum_{n,m} e^{\beta E_n} e^{iE_n t/\hbar} \langle n | A|m\rangle \langle m | B|n\rangle \int dt e^{i(t(E_n-E_m)/\hbar + \omega)} \]

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\( \Rightarrow G^>_{AB}(\omega) = \frac{2\pi}{Z} \sum_{n,m} e^{-\beta E_n} \langle n | A | m \rangle \langle m | B | n \rangle \delta \left( \frac{E_n - E_m}{\hbar} + \omega \right) \)  
(A.1)

and \( G^<_{AB}(\omega) = \frac{2\pi}{Z} \sum_{n,m} e^{-\beta E_n} \langle n | B | m \rangle \langle m | A | n \rangle \delta \left( \frac{E_m - E_n}{\hbar} + \omega \right) \)  
(A.2)

\( \Rightarrow G^>_{AB}(-\omega) = G^<_{BA}(\omega) \)

\( G^<_{AB}(\omega) = e^{-\beta \hbar \omega} G^>_{AB}(\omega) \)  
(A.3)

\( \Rightarrow m \leftrightarrow n \)

\( \Rightarrow E_m = E_n + \hbar \omega \)  
(A.5)

For example:

\[ A = \rho_k \quad \text{and} \quad B = \rho_{-k} \]

with the Fourier transform \( \rho_k(r) = \frac{1}{\sqrt{V}} \int d^3 r e^{-i k r} \rho(r, t) = \frac{1}{\sqrt{V}} \sum_{\alpha=1}^{N} e^{-i k r_{\alpha}(t)} \)

of the density operator \( \rho(r, t) = \sum_{\alpha=1}^{N} \delta(r - r_{\alpha}(t)) \)

Density-density correlation function \( \langle \rho_k(t) \rho_{-k}(t) \rangle \)

Coherent scattering cross-section \( S_{\text{coh}}(k, \omega) = \int \frac{dt}{2\pi \hbar} e^{i \omega t} \frac{V}{N} \langle \rho_k(t) \rho_{-k}(t) \rangle \)

Due to (A.3) follows:

\[ S_{\text{coh}}(k, -\omega) = e^{-\beta \hbar \omega} S_{\text{coh}}(-k, \omega) \]

\[ = e^{-\beta \hbar \omega} S_{\text{coh}}(k, \omega) \] \( \text{for systems with inversion symmetry} \)

\( \Rightarrow \) Anti-Stokes lines (energy loss by the sample) are weaker by a factor \( e^{-\beta \hbar \omega} \) than the Stokes lines (energy gain).

For \( T \to 0 \) \( S_{\text{coh}}(k, \omega < 0) \to 0 \)

(system is then in the ground cannot transfer any energy to the scattered particle).

### A.3 Dynamical Susceptibility

Consider a many-particle system influenced by an external force \( F(t) \) which couples to the operator \( B \):

\[ H = H_0 + H'(t) \quad ; \quad H'(t) = - \frac{F(t)}{c\text{-number}} \cdot B \]  
(A.6)

For \( t \leq t_0 \): \( F(t) = 0 \) (the system is in equilibrium).

How does the system response to the perturbation (A.6)?
The mean value of $A$ at time $t$:

$$
\overline{A(t)} = \text{Tr}(\rho_S(t) A) = \text{Tr}(U(t, t_0) \rho_S(t_0) U^\dagger(t, t_0) A)
$$

$$
= \text{Tr}(\rho_S(t_0) U^\dagger(t, t_0) A U(t, t_0))
$$

$$
= \text{Tr} \left( \frac{e^{-\beta H_0}}{Z} U^\dagger(t, t_0) A U(t, t_0) \right) = \langle U^\dagger(t, t_0) A U(t, t_0) \rangle_0
$$

The system is in equilibrium at $t_0$, thus $\rho_S(t_0) = e^{-\beta H_0} / Z$.

$U(t, t_0)$ can be determined perturbation theoretically in the interaction representation.

Equation of motion: $i \hbar \frac{d}{dt} U(t, t_0) = H U(t, t_0)$

**Ansatz:**

$$
U(t, t_0) = e^{-iH_0(t-t_0)/\hbar} U'(t, t_0)
$$

$$
\Rightarrow i \hbar \frac{d}{dt} U'(t, t_0) = e^{iH_0(t-t_0)/\hbar} \left( -H_0 + H \right) U = H'(t)
$$

Thus $i \hbar \frac{d}{dt} U'(t, t_0) = H'_1(t) U'(t, t_0)$

$$
H'_1(t) = e^{iH_0(t-t_0)/\hbar} H'(t) e^{-iH_0(t-t_0)/\hbar}
$$

“Interaction representation of $H'$”.

$$
\Rightarrow U'(t, t_0) = 1 + \frac{1}{i \hbar} \int_{t_0}^{t} dt' \ H'_1(t') U'(t', t_0)
$$

$$
= 1 + \frac{1}{i \hbar} \int_{t_0}^{t} dt' H'_1(t') + \frac{1}{(i \hbar)^2} \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' H'_1(t') H'_1(t'') + \ldots \quad (A.7)
$$

$$
= \mathcal{T} \exp \left\{ \frac{1}{i \hbar} \int_{t_0}^{t} dt' \ H'_1(t') \right\}
$$

with the time-ordering operator $\mathcal{T}$.

For the **linear** response, we need only the first two terms in (A.7).

$$
\sim \langle A(t) \rangle = \langle U'^\dagger(t, t_0) e^{iH_0(t-t_0)/\hbar} A e^{-iH_0(t-t_0)/\hbar} U'(t, t_0) \rangle_0
$$

$$
= \langle \left( 1 - \frac{1}{i \hbar} \int_{t_0}^{t} dt' H'_1(t') \right) e^{iH_0(t-t_0)/\hbar} A e^{-iH_0(t-t_0)/\hbar} \left( 1 + \frac{1}{i \hbar} \int_{t_0}^{t} dt' H'_1(t') \right) \rangle_0
$$

$$
= \text{Tr} \left( \frac{e^{-\beta H_0}}{Z} \left( 1 - \frac{1}{i \hbar} \int_{t_0}^{t} dt' H'_1(t') \right) e^{iH_0(t-t_0)/\hbar} A e^{-iH_0(t-t_0)/\hbar} \right) \langle A \rangle_0
$$

$$
+ \frac{1}{i \hbar} \int_{t_0}^{t} dt' \left[ e^{iH_0(t-t_0)/\hbar} A e^{-iH_0(t-t_0)/\hbar} H'_1(t') \right]_0
$$

$$
= e^{iH_0(t-t_0)/\hbar} H' e^{-iH_0(t-t_0)/\hbar} = -B(t') \cdot F(t')
$$
⇒ \langle A(t) \rangle = \langle A \rangle_0 - \frac{1}{i\hbar} \int_{t_0}^{t} dt' \langle [A(t), B(t')] \rangle_0 F(t')

Initially \( t_0 \to -\infty \) the system is in equilibrium and \( F(t') \) is switched on at a later instant. ⇒

\[
\Delta \langle A(t) \rangle = \langle A(t) \rangle - \langle A \rangle_0 = \int_{-\infty}^{\infty} dt' \chi_{AB}(t - t') F(t')
\]

with \( \chi_{AB}(t - t') = \frac{i}{\hbar} \Theta(t - t') \langle [A(t), B(t')] \rangle_0 \)

with dynamical susceptibility or linear response function \( \chi_{AB} \) and the step function

\[
\Theta(x) = \begin{cases} 
1 & x \geq 0 \\
0 & x < 0 
\end{cases}
\]

which ensures causality.

Fourier transform of the dynamical susceptibility

\[
\chi_{AB}(z) = \int_{-\infty}^{\infty} dt e^{izt} \chi_{AB}(t)
\]

Consider a very slowly switched on periodic perturbation \( (\epsilon \to 0, \epsilon > 0) \)

\[
H' = - \left( B F_\omega e^{-i\omega t'} + B^\dagger F_\omega^* e^{i\omega t'} \right) e^{\epsilon t'}
\]

\[
\Rightarrow \Delta \langle A(t) \rangle = \int_{-\infty}^{\infty} dt' \left( \chi_{AB}(t - t') F_\omega e^{-i\omega t'} + \chi_{AB}^*(t - t') F_\omega^* e^{i\omega t'} \right) e^{\epsilon t'} \xrightarrow{\epsilon \to 0} \chi_{AB}(\omega) F_\omega e^{-i\omega t} + \chi_{AB}^*( -\omega) F_\omega^* e^{i\omega t}
\]

The effect of the periodic perturbation on \( \Delta \langle A(t) \rangle \) is proportional to the force.

Resonances in the susceptibility: strong reaction to forces at the corresponding frequency.

### A.4 Dispersion Relations

Causality ⇒ \( \chi_{AB}(t) = 0 \) for \( t < 0 \)
⇒ \( \chi_{AB}(z) \) is analytical in the upper half plane (due to \( e^{-\text{Im} zt} \) in the Fourier transform)
⇒ \( \chi_{AB}(z) = \frac{1}{2\pi i} \int_{\gamma} dz' \frac{\chi_{AB}(z')}{z' - z} \) (Cauchy’s integral theorem)
The semicircular part of the integration path does not contribute if $\chi_{AB}(z')$ is sufficiently small at infinity.

\[
\Rightarrow \chi_{AB}(z) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} dx' \frac{\chi_{AB}(x')}{x' - z}
\]

\[
\rightarrow \chi_{AB}(x) = \lim_{\epsilon \to 0} \chi_{AB}(x + i\epsilon) = \lim_{\epsilon \to 0} \int_{-\infty}^{\infty} dx' \frac{\chi_{AB}(x')}{2\pi i} \frac{1}{x' - x - i\epsilon}
\]

\[
\lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} \frac{dx'}{2\pi i} \frac{f(x')}{x' - x - i\epsilon} = \lim_{\epsilon \to 0} \left( \int_{-\infty}^{x-\epsilon} \frac{dx'}{2\pi i} + \int_{x+\epsilon}^{+\infty} \frac{dx'}{2\pi i} \right) \frac{f(x')}{x' - x} + \frac{1}{2} \int \frac{dz}{2\pi i} \frac{f(z)}{z - x} = f(x)
\]

\[
= P \int \frac{dx'}{2\pi i} \frac{f(x')}{x' - x} + \int \frac{dx'}{2} f(x') \delta(x' - x),
\]

with the Cauchy principal value defined as

\[
P \int \frac{dx'}{x' - x} = \lim_{\epsilon \to 0} \left( \int_{-\infty}^{x-\epsilon} dx' + \int_{x+\epsilon}^{+\infty} dx' \right) \frac{f(x')}{x' - x}
\]

Or formal:

\[
\frac{1}{x' - x - i\epsilon} = P \left( \frac{1}{x' - x} \right) + \pi i \delta(x' - x)
\]

i.e.

\[
\chi_{AB}(x) = P \int \frac{dx'}{2\pi i} \frac{\chi_{AB}(x')}{x' - x} + \frac{1}{2} \chi_{AB}(x)
\]

\[
\Rightarrow \chi_{AB}(x) = \frac{1}{\pi i} P \int dx' \frac{\chi_{AB}(x')}{x' - x}
\]

i.e.

\[
\Re \chi_{AB}(x) = \Re \left\{ \frac{1}{\pi i} P \int dx' \frac{\Im \chi_{AB}(x') + \Re \chi_{AB}(x')}{x' - x} \right\}
\]

\[
= \frac{1}{\pi} P \int dx' \frac{\Im \chi_{AB}(x')}{x' - x}
\]

\[
\Im \chi_{AB}(x) = -\frac{1}{\pi} P \int dx' \frac{\Re \chi_{AB}(x')}{x' - x}
\]
A.5 Spectral Representation

Definition: Dissipative response $\chi''_{AB}(t) = \frac{1}{2\hbar} \langle [A(t), B(0)] \rangle$,

Fourier transform: $\chi''_{AB}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} \chi''_{AB}(t)$.

Due to $\Theta(t) = \lim_{\epsilon \to 0} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \frac{i \chi''_{AB}(t)}{\omega + i\epsilon}$ we get

$$\chi_{AB}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} \Theta(t) 2i \chi''_{AB}(t)$$

(A.8)

$$= \frac{1}{\pi} \int_{-\infty}^{+\infty} d\omega' \frac{\chi''_{AB}(\omega')}{\omega' - \omega - i\epsilon}$$

(A.9)

$$= \frac{1}{\pi} P \int_{-\infty}^{+\infty} d\omega' \frac{\chi''_{AB}(\omega')}{\omega' - \omega} + i \chi''_{AB}(\omega)$$

(A.10)

$$= \chi'_{AB}(\omega) + i \chi''_{AB}(\omega)$$

(A.11)

Decomposition into real and imaginary parts if $\chi''_{AB}(\omega)$ is real.

A.6 Fluctuation-Dissipation Theorem

Due to $\chi''_{AB}(t) = \frac{1}{2\hbar} \{ \langle A(t)B(0) \rangle - \langle B(0)A(t) \rangle \}$

it is $\chi''_{AB}(\omega) = \frac{1}{2\hbar} \{ \overline{G^>_{AB}(\omega)} - \overline{G^<_{AB}(\omega)} \}$

thus

$$\chi''_{AB}(\omega) = \frac{1}{2\hbar} \overline{G^>_{AB}(\omega)} (1 - e^{-\beta\hbar\omega})$$

is the so-called fluctuation-dissipation theorem

or with (A.9)

$$\chi_{AB}(\omega) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} d\omega' \overline{G^>_{AB}(\omega') \frac{(1 - e^{-\beta\hbar\omega'})}{\omega' - \omega - i\epsilon}}$$

(A.12)

Classical limit: $\beta\hbar\omega \ll 1$ (left frequency and temperature region)

$\Rightarrow \chi''_{AB}(\omega) = \frac{\beta \omega}{2} \overline{G^>_{AB}(\omega)}$
APPENDIX A. CORRELATION FUNCTIONS, SCATTERING, AND RESPONSE

\[ \chi_{AB}(\omega = 0) = \beta \int \frac{d\omega'}{2\pi} G_{AB}^>(\omega') = \beta G_{AB}^>(t = 0), \]

where \( \chi_{AB}(\omega = 0) \) is the static susceptibility and \( G_{AB}^>(t = 0) \) is the equal-time correlation function of \( A \) and \( B \).

The name fluctuation-dissipation theorem is appropriate since \( G_{AB}(\omega) \) is a measure of the correlation between fluctuations of \( A \) and \( B \), whilst \( \chi''_{AB} \) describes the dissipation.

That \( \chi''_{AB} \) has to do with dissipation can be seen as follows: Consider a perturbation of the form

\[ H' = \Theta(t)(A^\dagger F e^{-i\omega t} + AF^* e^{i\omega t}), \]

where \( F \) is complex. The golden rule gives a transition rate per unit time from the state \( n \) into the state \( m \):

\[ \Gamma_{n \rightarrow m} = \frac{2\pi}{\hbar} \left\{ \delta(E_m - E_n - \hbar \omega) |\langle m | A^\dagger F | n \rangle|^2 + \delta(E_m - E_n + \hbar \omega) |\langle m | AF^* | n \rangle|^2 \right\} \]

\( \Rightarrow \) The power of the external force (= the energy absorbed per unit time)

\[ W = \sum_{n,m} \frac{e^{-\beta E_n}}{Z} \Gamma_{n \rightarrow m}(E_m - E_n) \]

\[ = \frac{2\pi}{Z} \left\{ \sum_{n,m} e^{-\beta E_n} \langle n | A | m \rangle \langle m | A^\dagger | n \rangle |F|^2 \delta(E_m - E_n - \hbar \omega) \cdot \frac{E_m - E_n}{\hbar} \right\} \]

\[ + \sum_{n,m} e^{-\beta E_n} \langle n | A^\dagger | m \rangle \langle m | A | n \rangle |F|^2 \delta(E_m - E_n + \hbar \omega) \cdot \frac{E_m - E_n}{\hbar} \right\} \]

\[ = \frac{\omega}{\hbar} \left\{ G_{AB}^>(\omega) - G_{AB}^<(-\omega) \right\} |F|^2 = 2\omega \chi''_{AA^\dagger}(\omega) \cdot |F|^2 \]

A.7 Example of Application: Harmonic crystal

Assumption: a Bravais lattice, i.e., a lattice with one atom per unit cell.

Index \( n = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} \) and equilibrium position of an atom \( a_n = \begin{pmatrix} n_x \cdot a_x \\ n_y \cdot a_y \\ n_z \cdot a_z \end{pmatrix} \)

with \( n_{x,y,z} = 1, \ldots, N_{x,y,z} \) and the number of lattice points \( N = N_x \cdot N_y \cdot N_z \).

Displacement from the equilibrium position \( u_n = x_n - a_n \)

Harmonic approximation of the Hamiltonian (Taylor expansion of the potential energy around the equilibrium position):
\[ \hat{H} = \sum_n \frac{\hat{p}_n^2}{2M} + \sum_{n,n'} \hat{u}_n D_{n,n'} \hat{u}_{n'} \quad \text{with} \quad \hat{p}_n = -i\hbar \nabla u_n \]

Normal coordinates \( Q \) diagonalize the potential energy in the harmonic approximation.

\[ \hat{u}_n = \frac{1}{\sqrt{NM}} \sum_{k,\lambda} e^{ik\cdot a_n} \epsilon(k, \lambda) \hat{Q}_{k,\lambda} , \quad (A.13) \]

where \( \epsilon(k, \lambda) \) are the three polarization vectors \( (\lambda = 1, 2, 3) \) and \( k \) is the wave vector with components \( k_i = n_i \frac{2\pi}{Na_i} \) due to periodic boundary conditions. Thus

\[ \hat{H} = -\sum_{k,\lambda} \frac{\hbar^2}{2M} \Delta Q + \sum_{k,\lambda} \omega_{k,\lambda}^2 Q_{k,\lambda}^2 \]

Define a creation and annihilation operators like for the harmonic oscillator:

\[ \hat{Q}_{k,\lambda} = \sqrt{\frac{\hbar}{2\omega_{k,\lambda}}} \left( a_{k,\lambda} + a_{k,\lambda}^\dagger \right) \quad (A.14) \]

Thus

\[ \hat{H} = \sum_{k,\lambda} \hbar \omega_{k,\lambda} \left( a_{k,\lambda}^\dagger a_{k,\lambda} + \frac{1}{2} \right) \]

Commutation relations: \( [a_{k,\lambda}, a_{k',\lambda'}^\dagger] = \delta_{\lambda\lambda'}\delta_{kk'} \) and \( [a_{k,\lambda}, a_{k',\lambda'}] = [a_{k',\lambda}, a_{k',\lambda'}^\dagger] = 0 \)

Dynamical susceptibility for the displacements:

\[ \chi^{ij}(n - n', t) = \frac{i}{\hbar} \Theta(t) \langle [u_n^i(t), u_{n'}^j(0)] \rangle \quad (A.15) \]

or \[ \chi^{mij}(n - n', t) = \frac{1}{2\hbar} \langle [u_n^i(t), u_{n'}^j(0)] \rangle \quad (A.16) \]

Thus

\[ \chi^{ij}(n - n', t) = 2i\Theta(t) \chi^{mij}(n - n', t) \]

Remark: \( n - n' \) instead of \( n, n' \) due to translational invariance.

Phonon correlation function:

\[ D^{ij}(n - n', t) = \langle u_n^i(t) u_{n'}^j(0) \rangle \]
APPENDIX A. CORRELATION FUNCTIONS, SCATTERING, AND RESPONSE

Insert (A.14) into (A.13), and use this (ū expressed in terms of a, a†) in (A.16):

\[ \chi^{mij}(\mathbf{n} - \mathbf{n}', t) = \frac{1}{2\hbar} \frac{1}{NM} \sum_{k, \lambda \ k', \lambda'} e^{ikn + ik'n'} e^i(k, \lambda) e^j(k', \lambda') \]

\[ \times \frac{\hbar}{\sqrt{4\omega_{k, \lambda}\omega_{k', \lambda'}}} \langle \left[ a_{k, \lambda}(t) + a^\dagger_{-k, \lambda}(t) , (a_{k', \lambda'}(0) + a^\dagger_{-k', \lambda'}(0)) \right] \rangle \]

with \( a_{k, \lambda}(t) = e^{-i\omega_{k, \lambda}t} a_{k, \lambda}(0) \)

Auxiliary calculation: For \( H = \hbar \omega a^\dagger a \) it is \( a(t) = e^{+i\omega t} a e^{-i\omega t}, \) thus

\[ \langle n|a(t)|m \rangle = e^{+i\omega(n-m)t} \langle n|a|m \rangle = e^{-i\omega t} \langle n|a|m \rangle \]

Thus

\[ \left[ a_{k, \lambda}(t) + a^\dagger_{-k, \lambda}(t) , (a_{k', \lambda'}(0) + a^\dagger_{-k', \lambda'}(0)) \right] = \left[ a^\dagger_{-k, \lambda}(t), a_{k', \lambda'}(0) \right] + \left[ a_{k, \lambda}(t), a^\dagger_{-k', \lambda'}(0) \right] = -e^{-i\omega_{k, \lambda}t} \delta_{k, k'} \delta_{\lambda, \lambda'} + e^{i\omega_{k, \lambda}t} \delta_{k, -k'} \delta_{\lambda, \lambda'} \]

\[ \Rightarrow \chi^{mij}(\mathbf{n} - \mathbf{n}', t) = \frac{1}{4NM} \sum_{k, \lambda} e^{ik(n - n') - \lambda} e^i(k, \lambda) e^j(k, \lambda) \frac{1}{\omega_{k, \lambda}} (e^{-i\omega_{k, \lambda}t} - e^{i\omega_{k, \lambda}t}) \]

The polarization vectors for Bravais lattices are real, thus

\[ \chi^{mij}(\mathbf{n} - \mathbf{n}', t) = \frac{-i}{2NM} \sum_{k, \lambda} e^{ik(n - n')} e^i(k, \lambda) e^j(k, \lambda) \frac{1}{\omega_{k, \lambda}} \sin(\omega_{k, \lambda}t) \]

It is \( \chi^{ij}(\mathbf{n} - \mathbf{n}', t) = 2i \Theta(t) \chi^{mij}(\mathbf{n} - \mathbf{n}', t) \), thus

\[ \chi^{ij}(\mathbf{n} - \mathbf{n}', t) = \frac{1}{NM} \sum_{k, \lambda} e^{ik(n - n')} e^i(k, \lambda) e^j(k, \lambda) \frac{1}{\omega_{k, \lambda}} \sin(\omega_{k, \lambda}t) \Theta(t) \]

or \( \chi^{ij}(\mathbf{n} - \mathbf{n}', \omega) = \frac{1}{NM} \sum_{k, \lambda} e^{ik(n - n')} e^i(k, \lambda) e^j(k, \lambda) \frac{1}{\omega_{k, \lambda}} \int_0^\infty dt e^{i\omega t} \sin(\omega_{k, \lambda}t) \]

Auxiliary calculation:

\[ \frac{1}{i} \int_0^\infty dt e^{i\omega t} = \lim_{\epsilon \to 0} \frac{1}{i} \int_0^\infty dt e^{i\omega t} e^{-\epsilon t} = \lim_{\epsilon \to 0} \frac{1}{i} \frac{1}{i\omega - \epsilon} = \lim_{\epsilon \to 0} \frac{1}{\omega + i\epsilon} \]

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Spatial Fourier transform:

\[ \chi^{ij}(q, \omega) = \sum_n e^{-i\mathbf{q}n} \chi^{ij}(n, \omega) \]

\[ = \frac{1}{2NM} \sum_{k, \lambda} \sum_n e^{-i\mathbf{a}_n(k-q)} \frac{\epsilon^i(k, \lambda)\epsilon^j(k, \lambda)}{\omega_{k, \lambda}} \left\{ \frac{1}{\omega + \omega_{k, \lambda} + i\epsilon} - \frac{1}{\omega - \omega_{k, \lambda} + i\epsilon} \right\} \]

\[ = \frac{1}{2M} \sum_\lambda \frac{\epsilon^i(q, \lambda)\epsilon^j(q, \lambda)}{\omega_{q, \lambda}} \left\{ \frac{1}{\omega + \omega_{q, \lambda} + i\epsilon} - \frac{1}{\omega - \omega_{q, \lambda} + i\epsilon} \right\} \]

For the decompositions

\[ \chi^{ij}(n - n', \omega) = \chi^{nij}(n - n', \omega) + i \chi^{nij}(n - n', \omega) \]

this leads to

\[ \chi^{nij}(n - n', \omega) = \frac{1}{2NM} \sum_{k, \lambda} e^{i\mathbf{k}(\mathbf{a}_n - \mathbf{a}_{n'})} \frac{\epsilon^i(k, \lambda)\epsilon^j(k, \lambda)}{\omega_{k, \lambda}} \times \left\{ P \left( \frac{1}{\omega + \omega_{k, \lambda}} \right) - P \left( \frac{1}{\omega - \omega_{k, \lambda}} \right) \right\} \]

\[ \chi^{nij}(n - n', \omega) = \frac{\pi}{2NM} \sum_{k, \lambda} e^{i\mathbf{k}(\mathbf{a}_n - \mathbf{a}_{n'})} \frac{\epsilon^i(k, \lambda)\epsilon^j(k, \lambda)}{\omega_{k, \lambda}} \times \{ \delta(\omega - \omega_{k, \lambda}) - \delta(\omega + \omega_{k, \lambda}) \} \]

or

\[ \chi^{nij}(q, \omega) = \frac{1}{2M} \sum_\lambda \frac{\epsilon^i(q, \lambda)\epsilon^j(q, \lambda)}{\omega_{q, \lambda}} \times \left\{ P \left( \frac{1}{\omega + \omega_{q, \lambda}} \right) - P \left( \frac{1}{\omega - \omega_{q, \lambda}} \right) \right\} \]

\[ \chi^{nij}(q, \omega) = \frac{\pi}{2M} \sum_\lambda \frac{\epsilon^i(q, \lambda)\epsilon^j(q, \lambda)}{\omega_{q, \lambda}} \times \{ \delta(\omega - \omega_{q, \lambda}) - \delta(\omega + \omega_{q, \lambda}) \} \]

The phonon correlation function can be either calculated directly, or determined with the help of the fluctuation-dissipation theorem from \( \chi^{nij}(n - n', \omega) \):

\[ D^{ij}(n - n', \omega) = 2\hbar \frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega} - 1} \chi^{nij}(n - n', \omega) \]

\[ = 2\hbar (1 + n(\omega)) \chi^{nij}(n - n', \omega) \]

\[ = \frac{\pi \hbar}{NM} \sum_{k, \lambda} e^{i\mathbf{k}(\mathbf{a}_n - \mathbf{a}_{n'})} \frac{\epsilon^i(k, \lambda)\epsilon^j(k, \lambda)}{\omega_{k, \lambda}} \times \{ (1 + n_{k, \lambda})\delta(\omega - \omega_{k, \lambda}) - n_{k, \lambda}\delta(\omega + \omega_{k, \lambda}) \} \]

or

\[ D^{ij}(q, \omega) = 2\hbar (1 + n(\omega)) \chi^{nij}(q, \omega) \]

\[ = \frac{\pi \hbar}{M} \sum_\lambda \frac{\epsilon^i(q, \lambda)\epsilon^j(q, \lambda)}{\omega_{q, \lambda}} \{ (1 + n_{q, \lambda})\delta(\omega - \omega_{q, \lambda}) - n_{q, \lambda}\delta(\omega + \omega_{q, \lambda}) \} \]
with \( n_{q,\lambda} = \langle a_{q,\lambda}^\dagger a_{q,\lambda} \rangle = \frac{1}{e^{\beta \hbar \omega_{q,\lambda}} - 1} \) the average thermal occupation number for phonons of wave vector \( q \) and polarization \( \lambda \).

The phonon resonances in \( D_{ij}(q,\omega) \) for a particular \( q \) are sharp \( \delta \)-function-like peaks at the positions \( \pm \omega_{q,\lambda} \).

The expansion of the density-density correlation function, which determines the inelastic neutron scattering cross-section, contains the phonon correlation function \( D_{ij}(q,\omega) \).

\[ \rightarrow \] The excitations of the many-particle system (in this case the phonons) express themselves as resonances in the scattering cross-section.

In reality, the phonons interact with one another and also with other excitations of the system, e.g., with the electrons in a metal. \[ \rightarrow \] Damping of the phonons.

Replace \( \epsilon \) by a finite damping constant. \[ \rightarrow \] The phonon resonances then acquire a finite width.