Chapter 3

Many-particle Quantum Systems

Many physical systems consist of a very large number of particles. Often, the particle number is even variable:

- The relativistic formulation of quantum mechanics had led us to the concept of particles and antiparticles. It had shown that the quantum mechanics of a single particle is inconsistent in itself, because particle - antiparticle pairs can be created in scattering processes.

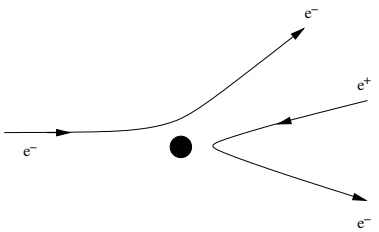


Figure 3.1: Klein paradoxon

- Systems with extremely large particle numbers exist in condensed matter systems, e.g. the electron system in metals ($\sim 10^{23}$ particles!).

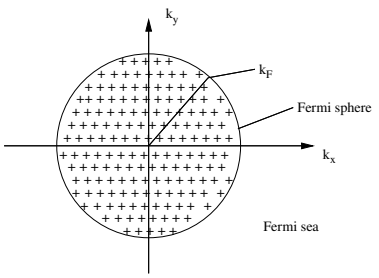


Figure 3.2:

The particle number can be variable through the coupling to a reservoir with particle exchange.

This calls for an efficient method to describe many-particle systems as well as the creation and destruction of particles. This method will be provided by the *"Second quantization"*.

Remark:

The combination of the many-particle formulation and of the relativistic formulation of quantum mechanics will also lead to the understanding of the connection between the spin of a particle species and the symmetry of the wave function under particle exchange.

3.1 Second quantization

3.1.1 Many-particle states (wave functions)

The quantum state of a many-particle system (particle number N) is given by specifying a complete set of quantum numbers ($\equiv$ set of eigenvalues of commuting observables) for all particles, e.g., in position representation the wave function depending on the coordinates $\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N$ (and spin $\sigma_1, \sigma_2, \ldots, \sigma_N$) of all N particles:

$$\psi(x_1, \ldots, x_N) \qquad N \approx 10^{23} \tag{3.1}$$

$$x_i = (\vec{x}_i, t_i, \sigma_i, \ldots) \qquad \text{collective coordinate} \tag{3.2}$$

Constructing a basis set for many-particle states:

- For an *interacting* system the Hamiltonian reads

$$H(x_1 \ldots x_N) = \sum_{i=1}^{N} H^{(1)}(x_i) + \sum_{(i,j),i\neq j} H^{(2)}(x_i, x_j) \tag{3.3}$$

single-particle H:

$$H^{(1)}(x_i) = T(x_i) = -i\frac{\hbar^2}{2m}\frac{\partial^2}{\vec{x}_i^2} + U(\vec{x}_i) \tag{3.4}$$

(e.g. kinetic energy, single-particle potential)

two-particle H:

$$H^{(2)}(x_i, x_j) = V(\vec{x}_i - \vec{x}_j) = \frac{e^2}{|\vec{x}_i - \vec{x}_j|} \tag{3.5}$$

(e.g. interaction potential between two particles)

If $H^{(2)} \neq 0$ the eigenstates do, in general, not factorize into a product of single-particle eigenstates. In this case, it is not possible to specify the state of a single particle in the system alone.

- Only if the system is non-interacting

$$H(x_1 \dots x_N) \equiv H_0(x_1 \dots x_N) = \sum_{i=1}^{N} H^{(1)}(x_i) \tag{3.6}$$

the eigenstates can be written as a product of single-particle states:

$$H_0|\alpha_1^{(k_1)}, \dots, \alpha_N^{(k_N)}\rangle = E|\alpha_1^{(k_1)}, \dots, \alpha_N^{(k_N)}\rangle, \quad \text{where} \tag{3.7}$$

$$|\alpha_1^{(k_1)}, \dots, \alpha_N^{(k_N)}\rangle = |\alpha_1^{(k_1)}\rangle|\alpha_2^{(k_2)}\rangle \dots |\alpha_N^{(k_N)}\rangle \tag{3.8}$$

(non-interacting) many-particle eigenstate with

$$H^{(1)}(x_i)|\alpha_i^{(k_i)}\rangle = E|\alpha_i^{(k_i)}\rangle, \; E = \sum_{i=1}^{N} E_i \tag{3.9}$$

$|\alpha_i^{(k_i)}\rangle$ is the single-particle eigenstate of the i-th particle with quantum numbers $\alpha_i^{(k_i)}$ and eigenenergy E_i.

Proof:

$$
\begin{aligned}
H_0|\alpha_1 \dots \alpha_N\rangle &= \left[\sum_i H^{(1)}(x_i)\right] |\alpha_1\rangle \dots |\alpha_N\rangle && (3.10)\\
&= \left(H^{(1)}(x_1)|\alpha_1\rangle\right) |\alpha_2\rangle \dots |\alpha_n\rangle + |\alpha_1\rangle && (3.11)\\
&\quad \times \left(H^{(1)}(x_2)|\alpha_2\rangle\right) |\alpha_3\rangle \dots |\alpha_N\rangle + \dots \\
&\quad + |\alpha_1\rangle \dots |\alpha_{N-1}\rangle \left(H^{(1)}(x_N)|\alpha_N\rangle\right) \\
&= \sum_{i=1}^{N} \left\{|\alpha_1\rangle \dots \left(H^{(1)}(x_i)|\alpha_i\rangle\right) \dots |\alpha_N\rangle\right\} && (3.12)\\
&= \sum_{i=1}^{N} \left\{|\alpha_1\rangle \dots (E_i|\alpha_i\rangle) \dots |\alpha_n\rangle\right\} && (3.13)\\
&= \underbrace{\left(\sum_{i=1}^{N} E_i\right)}_{E} |\alpha_1\rangle \dots |\alpha_N\rangle && (3.14)
\end{aligned}
$$

□

For a *non-interacting* system, the single-particle energies are additive. This is in general *not* true for interacting systems.

Identical particles:

Quantum mechanical particles (of the same species) are indistinguishable. This introduces another constraint on the form of the state (wave function):

It must have definite parity $\mathcal{P} = \pm 1$ with respect to the interchange of 2 particles:

$$|\alpha_1^{(k_1)} \dots \alpha_i^{(k_i)} \dots \alpha_j^{(k_j)} \dots \alpha_n^{(k_N)}\rangle = \pm |\alpha_1^{(k_1)} \dots \alpha_j^{(k_j)} \dots \alpha_i^{(k_i)} \dots \alpha_n^{(k_N)}\rangle \qquad \forall i, j \tag{3.15}$$

$\alpha_i^{(k_i)}$ is the quantum number of the i-th particle

The state of a non-interacting many-particle system can be written as

$$\boxed{|\psi\rangle = |\alpha_1^{(k_1)} \dots \alpha_n^{(k_N)}\rangle = \left(\frac{n_{k_1}! n_{k_1}! \dots}{N!}\right)^{1/2} \sum_P (\pm 1)^P |\alpha_{P(1)}^{(k_1)}\rangle \dots |\alpha_{P(N)}^{(k_N)}\rangle} \tag{3.16}$$

The sum runs over all permutations of $1, 2, 3, \ldots, N$. $+$ is for bosons and - for fermions. For fermions the totally antisymmetry sum of products of single-particle states can be written as a determinant (*Slater determinant*):

$$|\psi\rangle = \frac{1}{N!} \begin{vmatrix} |\alpha_1^{(k_1)}\rangle & |\alpha_1^{(k_2)}\rangle & \ldots & |\alpha_1^{(k_N)}\rangle \\ \vdots & \vdots & & \vdots \\ |\alpha_N^{(K_1)}\rangle & |\alpha_N^{(k_2)}\rangle & \ldots & |\alpha_N^{(k_N)}\rangle \end{vmatrix} \tag{3.17}$$

Fermions: Total antisymmetry of state $\Rightarrow$
Any single-particle state $\alpha^{(k)}$can be at most singly occupied.

Proof:

$$\begin{aligned} |\psi\rangle|\alpha_1^{(k_1)} \ldots \alpha_i^{(k)} \ldots \alpha_j^{(k)} \ldots \alpha_n^{(k_N)}\rangle &\overset{(*)}{=} -|\alpha_1^{(k_1)} \ldots \alpha_j^{(k)} \ldots \alpha_i^{(k)} \ldots \alpha_n^{(k_N)}\rangle \\ &\overset{(**)}{=} |\alpha_1^{(k_1)} \ldots \alpha_i^{(k)} \ldots \alpha_j^{(k)} \ldots \alpha_n^{(k_N)}\rangle \\ \Rightarrow |\psi\rangle &= 0 \end{aligned}$$

□

The i-th and j-th particle have the same upper index because they are in the same state $\alpha^(k)$. In $(*)$ we have used the antisymmetry of fermions and in $(**)$ we could exchange $i \leftrightarrow j$ because they map onto the same state.

Basis set of the many-particle Hilbert space:

Since $B^{(1)} = |\alpha^{(k)}\rangle \Big| k = 1, 2, \ldots$ is a complete basis of the single-particle Hilbert space, the set of states with definite parity

$$B^{(N)} = |\alpha_1^{(k_1)} \ldots \alpha_N^{(k_N)}\rangle \Big| k_i = 1, 2, \ldots; i = 1, \ldots, N \tag{3.18}$$

is a complete basis of the N-particle Hilbert space.

$\rightarrow$ Any N-particle state (e.g. eigenstate of an interacting system) can be written as a linear combination of the $|\alpha_1^{(k_1)} \ldots \alpha_N^{(k_N)}\rangle$'s.

In real systems, the total particle number N can be variable.

Definition:

The Hilbert space of all states with particle number $N = 0, 1, 2, \ldots$ spanned by the basis set

$$|\alpha_1^{(k_1)} \ldots \alpha_N^{(k_N)}\rangle \Big| k_i = 1, 2, \ldots; i = 1, \ldots, N; N = 0, 1, 2, \ldots \tag{3.19}$$

is called *Fock space*.

3.1.2 Particle number representation: Creation and destruction operators

In $|\alpha_1^{(k_1)} \ldots \alpha_N^{(k_N)}\rangle$ each basis state is specified by specifying for each particle $i = 1, \ldots, N$ the state $\alpha^{(k_i)}$ it is in. Alternatively, each basis state can be specified by giving, for each single-particle state α^k the occupation number n_k of that state, i.e. the number of particles which are in that state.

Particle number representation:

1. Choose a basis of single-particle states, e.g. momentum eigenstates $|\vec{k}\rangle$.
2. A basis state (not necessarily eigenstate of an interacting system) if the N-particle system is specified uniquely by giving the occupation numbers $n_k, k = 1, 2, \ldots$ for each single-particle state.
3. In this way the occupation numbers n_k and the total particle number $N = \sum_k n_k$ are introduced as new *quantum numbers* of the system. They specify a many-particle basis state uniquely, once the underlying single-particle basis has been chosen.

$$|\alpha_1^{(k_1)} \ldots \alpha_N^{(k_N)}\rangle \equiv |n_{k_1}, n_{k_2}, \ldots, n_{k_i}, \ldots\rangle \tag{3.20}$$

The *orthonormality* of the N-particle basis sates follows from the orthonormality of the single-particle basis states:

$$\langle m_1 m_2 \ldots m_k \ldots | n_1 n_2 \ldots n_k \ldots\rangle = \delta_{m_1 n_1} \cdot \delta_{m_2 n_2} \ldots = \prod_{k=1}^{\infty} \delta_{m_k n_k} \tag{3.21}$$

Shorthand notation:
$k = 1, 2, 3, \ldots$ labels the single-particle eigenstates.

Creation and destruction operators

It is useful to introduce operators which *reduce* or *increase* the new quantum numbers n_k by one unit.

1. **Bosons:**

   (a) **Definition:**

$$\boxed{a_k|\ldots n_k\ldots\rangle = \sqrt{n_k}|\ldots(n_k-1)\ldots\rangle} \tag{3.22}$$

   Definition of the *destruction operator* a_k.
   The prefactor f_k in the action of a_k has to fulfill the condition that $a_k|\ldots n_k \equiv 0\ldots\rangle = 0$. Hence, it is *defined* as $f_k := \sqrt{n_k}$. The square root is chosen for convenience (see below) and in analogy to the destruction operator for the harmonic oscillator.

   Creation and particle number operators:

   To find the action of the the hermitean conjugate operator $a_k^\dagger$, we consider (n_k not bounded from above)

$$|\psi_k\rangle := a_k|\ldots n_k\ldots\rangle = \sqrt{n_k}|\ldots(n_k-1)\ldots\rangle \tag{3.23}$$

$$\langle\psi_k|\psi_k\rangle = \langle\ldots n_k\ldots|a_k^\dagger a_k|\ldots n_k\ldots\rangle \tag{3.24}$$

$$= \sqrt{n_k}^2 = n_k \tag{3.25}$$

   (b) Orthonormality $\Rightarrow$

$$a_k^\dagger a_k|\ldots n_k\ldots\rangle \propto |\ldots n_k\ldots\rangle \tag{3.26}$$

   with eigenvalue n_k:

$$\boxed{\begin{array}{l} a_k^\dagger a_k|\ldots n_k\ldots\rangle = n_k|\ldots n_k\ldots\rangle \\ \widehat{n_k} = a_k^\dagger a_k \quad \text{particle number operator in single-particle state k} \\ n_k \geq 0, \text{ integer} \end{array}}$$

It follows, in particular, that the eigenvalue spectrum of $a_k^\dagger a_k$ is positive semidefinite, $\mathbb{N}$.

(c)

$$\begin{aligned} a_k^\dagger a_k |\ldots n_k \ldots\rangle &= \sqrt{n_k}\, a_k^\dagger |\ldots (n_k-1)\ldots\rangle && (3.27)\\ &= n_k |\ldots n_k \ldots\rangle && (3.28)\\ \Rightarrow a_k^\dagger |\ldots (n_k-1)\ldots\rangle &= \sqrt{n_k}\, |\ldots n_k \ldots\rangle \qquad \text{or} \quad n_k - 1 \ (3.29) \end{aligned}$$

The square root of n_k is specific for bosons.

$$\boxed{a_k^\dagger |\ldots n_k \ldots\rangle = \sqrt{n_k+1}\, |\ldots (n_k{+}1)\ldots\rangle}$$

$a_k^\dagger$ is the *creation operator* for a particle in single-particle state k.

(d) Commutation relations for $a_k, a_k^\dagger$:

$$\begin{aligned} a_k a_k^\dagger |\ldots n_k \ldots\rangle &= \sqrt{n_k+1}\, a_k |\ldots (n_k+1)\ldots\rangle && (3.30)\\ &= (n_k+1) |\ldots n_k \ldots\rangle && (3.31)\\ a_k^\dagger a_k |\ldots n_k \ldots\rangle &= n_k |\ldots n_k \ldots\rangle \qquad \forall n_k && (3.32)\\ \Leftrightarrow a_k a_k^\dagger - a_k^\dagger a_k &= 1 && (3.33) \end{aligned}$$

Similarly:

$$\boxed{\begin{aligned} \left[a_k, a_k^\dagger\right] &= 1 \\ \left[a_k, a_{k'}^\dagger\right] &= 0 \qquad k' = k \\ [a_k, a_{k'}] &= 0 \qquad \forall k, k' \end{aligned}} \qquad (3.34)$$

2. **Fermions:**

In addition, the occupation number is limited to not more than 1. This has profound consequences for the action of $a^\dagger$ (not for a_k) and hence for the commutation relations.

(a) **Definition:**

$$\boxed{\begin{aligned} &c_k |n_1 \ldots n_k \ldots\rangle = n_k |n_1 \ldots (n_k-1)\ldots\rangle \\ &n_k = 0, 1 \qquad \text{(at most single occupation of state k)} \end{aligned}} \qquad (3.35)$$

As for bosons, the prefactor n_k is chosen such that a_k annihilates the states with $n_k = 0$. Since $n_k = 0, 1$ only, the square root can be omitted here.

Action of $c_k^\dagger$:

$$\begin{aligned} |\phi_k\rangle &:= c_k|\ldots n_k \ldots\rangle && (3.36)\\ &= n_k|\ldots (n_k-1)\ldots\rangle && (3.37)\\ \langle\phi_k|\phi_k\rangle &= \langle\ldots n_k \ldots|c_k^\dagger c_k|\ldots n_k\ldots\rangle && (3.38)\\ &= n_k^2 = n_k \qquad (n_k = 0,1) && (3.39) \end{aligned}$$

(b)

$$\begin{aligned} c_k^\dagger c_k|\ldots n_k\ldots\rangle &= n_k|\ldots n_k\ldots\rangle\\ \widehat{n_k} &= c_k^\dagger c_k \end{aligned}$$

particle number operator with positive semidefinite eigenvalue spectrum (0,1)

(c) Orthonormality

$$\begin{aligned} c_k^\dagger c_k|\ldots n_k\ldots\rangle &= n_k \cdot c_k^\dagger|\ldots (n_k-1)\ldots\rangle && (3.40)\\ &\propto n_k|\ldots n_k\ldots\rangle && (3.41)\\ \Rightarrow c_k^\dagger|\ldots n_k'\ldots\rangle &= f_k|\ldots n_k'+1\ldots\rangle && (3.42) \end{aligned}$$

where

$$f_k = \begin{cases} 1 & n_k' = 0\\ 0 & n_k' = 1 \quad \text{(no double occupancy!)} \end{cases} \tag{3.43}$$

$$c_k^\dagger|\ldots n_k\ldots\rangle = (1-n_k)|\ldots (n_k+1)\ldots\rangle, \quad n_k = 0,1 \tag{3.44}$$

$c_k^\dagger$ is *creation operator* for particle in state k.

(d) Commutation relations

$$
\begin{aligned}
c_k^\dagger c_k|\ldots n_k\ldots\rangle &= n_k|\ldots n_k\ldots\rangle && (3.45)\\
c_k c_k^\dagger|\ldots n_k\ldots\rangle &= (1+n_k)(1-n_k)|\ldots n_k\ldots\rangle && (3.46)\\
&= (1-n_k^2)|\ldots n_k\ldots\rangle && (3.47)\\
&\overset{n_k=0,1}{=} (1-n_k)|\ldots n_k\ldots\rangle, \qquad \forall n_i=0,1 && (3.48)\\
c_k c_k^\dagger + c_k^\dagger c_k &= 1 && (3.49)\\
c_k c_k &= 0 && (3.50)\\
c_k^\dagger c_k^\dagger &= 0 \qquad (\text{since } n_k = 0,1 \text{ only}) && (3.51)
\end{aligned}
$$

Antisymmetry of state wrt. interchange of particles

$$
\begin{aligned}
c_k c_{k'} &= -c_{k'} c_k && (3.52)\\
c_k c_{k'}^\dagger &= -c_{k'}^\dagger c_k && (3.53)
\end{aligned}
$$

$$
\boxed{
\begin{aligned}
\{c_k, c_k^\dagger\} &= 1\\
\{c_k, c_{k'}\} &= \{c_k^\dagger, c_{k'}^\dagger\} = 0 \qquad \forall k, k'\\
\{c_k, c_{k'}^\dagger\} &= 0 \qquad k \neq k'
\end{aligned}
} \qquad (3.54)
$$

3.1.3 Momentum and position representation: field operators

Let $\{|\vec{k}\rangle\}$ be the single-particle momentum basis $\langle\vec{x}|\vec{k}\rangle = \frac{e^{i\vec{k}\vec{x}}}{(2\pi)^{3/2}}$.

$\left.\begin{matrix} a_{\vec{k}}, a_{\vec{k}}^\dagger \\ c_{\vec{k}}, c_{\vec{k}}^\dagger \end{matrix}\right\}$ destruction/ creation operators for $\left\{\begin{matrix} \text{bosons} \\ \text{fermions} \end{matrix}\right.$

We define the Fourier transform of $a_{\vec{k}}$ as

$$
\begin{aligned}
\widehat{\psi}(\vec{x}) &= \int \frac{d^3k}{(2\pi)^{3/2}} a_{\vec{k}} e^{i\vec{k}\vec{x}} && (3.55)\\
\widehat{\psi}^\dagger(\vec{x}) &= \int \frac{d^3k}{(2\pi)^{3/2}} a_{\vec{k}}^\dagger e^{-i\vec{k}\vec{x}} && (3.56)
\end{aligned}
$$

Action of $\widehat{\psi}(\vec{x})$ on an N-particle position eigenstate

$$|\vec{y}_1 \dots \vec{y}_N\rangle = \int d^3k_1 \dots \int d^3k_N \underbrace{|\vec{k}_1 \dots \vec{k}_N\rangle}_{k_i \text{ each one singly occupied}} \times \underbrace{\langle \vec{k}_1 \dots \vec{k}_N | \vec{y}_1 \dots \vec{y}_N \rangle}_{\left(\frac{1}{(2\pi)^{3/2}}\right)^N e^{-i\vec{k}_1\vec{y}_1} \dots e^{-i\vec{k}_N\vec{y}_N}} \tag{3.57}$$

$$\widehat{\psi}(\vec{x})|\vec{y}_1 \dots \vec{y}_N\rangle = \int \frac{d^3k}{(2\pi)^{3/2}} \int \frac{d^3k_1}{(2\pi)^{3/2}} \dots \int \frac{d^3k_N}{(2\pi)^{3/2}} e^{i\vec{k}\vec{x}} e^{-i\vec{k}_1\vec{y}_1} \times \dots e^{-i\vec{k}_N\vec{y}_N} \underbrace{a_{\vec{k}}|\vec{k}_1 \dots \vec{k}_N\rangle}_{=\sum_{j=1}^N \delta^3(\vec{k}-\vec{k}_j)|\vec{k}_1 \dots \cancel{\vec{k}_j} \dots \vec{k}_N\rangle} \tag{3.58}$$

$$= \sum_{j=1}^N \frac{1}{(2\pi)^{3/2}} \int \frac{d^3k_1}{(2\pi)^{3/2}} \dots \int \frac{d^3k_j}{(2\pi)^{3/2}} \dots \times \int \frac{d^3k_N}{(2\pi)^{3/2}} e^{-i\vec{k}_1\vec{y}_1} \dots \cancel{e^{-i\vec{k}_j(\vec{y}_j-\vec{x})}} \dots e^{-i\vec{k}_N\vec{y}_N} |\vec{k}_1 \dots \cancel{\vec{k}_j} \dots \vec{k}_N\rangle \tag{3.59}$$

$$= \sum_{j=1}^N |\vec{y}_1 \dots \cancel{\vec{y}_j} \dots \vec{y}_N\rangle \delta^3(\vec{x} - \vec{y}_j) \tag{3.60}$$

Hence, $\widehat{\psi}(\vec{x})$ is the destruction operator for a particle at position $\vec{x}$. *"Field operator"*

Since $\widehat{\psi}(\vec{x})$ is analogous to the wave function but appears in particle number representation as an operator, this representation is also called *2nd quantization*. From the definition of $\psi, \psi^\dagger$ (linear relation to $a, a^\dagger$) it follows that $\psi, \psi^\dagger$ obey the same commutation relations as $a, a^\dagger$.

3.1.4 2nd quantized representation of operators

An operator can be given in the occupation number representation by calculating its matrix elements in the occupation number basis $\{|n_1, \dots, n_k, \dots\rangle\}$.

1. **Single-particle operators:**

$$H^{(1)} = \sum_{i=1}^N H^{(1)}(x_i) \tag{3.61}$$

$H^{(1)}$ acting on $|n_1, \ldots, n_k, \ldots\rangle$ can at most change the state $|\alpha^{(k_i)}\rangle$ of any one of the N particles (but not the states of two or more particles), since each term in $H^{(1)}$ depends only on a single coordinate.
Hence, the matrix elements of $H^{(1)}$ in the occupation number representation are of the form

$$\left[H^{(1)}\right]_{n_i,n_j}^{n_i-\delta,n_j+\delta} := \langle n_1, \ldots, n_i-\delta, \ldots, n_j+\delta, \ldots | H^{(1)} | n_1, \ldots, n_i, \ldots, n_j, \ldots\rangle \tag{3.62}$$

where $\delta = \begin{cases} 0 \text{ for diagonal elements (no change of occupation numbers)} \\ \delta = \pm 1 \text{ for off-diagonal elements} \end{cases}$

and i, j arbitrary. n_i is the occupation number of a single-particle in the state i.

$$\begin{aligned}
& \left[H^{(1)}\right]_{n_i,n_j}^{n_i-\delta,n_j+\delta} && (3.63)\\
= & \sum_{l=1}^{N} \langle \alpha_1^{(k_1)}, \ldots, \alpha_l^{(j)}, \ldots, \alpha_N^{(k_N)} | H^{(1)}(x_l) && (3.64)\\
& \times | \alpha_1^{(k_1)}, \ldots, \alpha_l^{(i)}, \ldots, \alpha_n^{(k_N)} \rangle \\
= & \langle \alpha^{(j)} | H^{(1)}(x) | \alpha^{(i)} \rangle \sqrt{n_j}\sqrt{n_i} && (3.65)\\
= & \underbrace{\int d^3x\, \phi^{(j)}(\vec{x})^* H^{(1)}(\vec{x}) \phi^{(i)}(\vec{x})}_{H_{ji}^{(1)}} \sqrt{n_j}\sqrt{n_i} && (3.66)\\
= & H_{ji}^{(1)} \sqrt{n_j}\sqrt{n_i} && (3.67)
\end{aligned}$$

with $\phi^{(i)}(\vec{x}) = \langle \vec{x} | \alpha^{(i)} \rangle$.

With the definition of $a_i, a_i^\dagger$ or $c_i, c_i^\dagger$, $H^{(1)}$ can, hence, be written in occupation number representation

$$\boxed{\begin{aligned} H^{(1)} &= \sum_{ij} H_{ji}^{(1)} a_j^\dagger a_i \\ H_{ji}^{(1)} &= \int d^3x\, \phi^{(j)}(\vec{x})^* H^{(1)}(\vec{x}) \phi^{(i)}(\vec{x}) \end{aligned}} \tag{3.68}$$

and similar for fermions: $a_i \to c_i, \quad a_i^\dagger \to c_i^\dagger$

2. **Two-particle operators:**

$$H^{(2)} = \sum_{(i,j),i\neq j} H^{(2)}(\vec{x}_i, \vec{x}_j) \tag{3.69}$$

$H^{(2)}$ acting on a many-particle product state can change the states of at most 2 particles, i.e. in occupation number representation, it can change, at most, the occupation numbers of 2 different single-particle states.

One obtains, in analogy to $H^{(1)}$:

$$\boxed{\begin{aligned} H^{(2)} &= \sum_{iklm} H^{(2)}_{ik,lm} a_i^\dagger a_k^\dagger a_l a_m \\ H^{(2)}_{ik,lm} &= \int d^3x \int d^3x' \, \phi^{(i)}(\vec{x})^* \phi^{(k)}(\vec{x}')^* H^{(2)}(\vec{x}, \vec{x}') \phi^{(l)}(\vec{x}') \phi^{(m)}(\vec{x}) \end{aligned}} \tag{3.70}$$

3. **Particle density operator:**

$$\widehat{\rho}(\vec{x}) = \psi^\dagger(\vec{x})\psi(\vec{x}) \tag{3.71}$$

Proof: Total particle number:

$$\widehat{N} = \int d^3x \psi^\dagger(\vec{x})\psi(\vec{x}) \tag{3.72}$$

$$= \int d^3x \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} a_{\vec{k}}^\dagger a_{\vec{k}'} e^{-i(\vec{k}-\vec{k}')\vec{x}} \tag{3.73}$$

$$= \int \frac{d^3k}{(2\pi)^3} a_{\vec{k}}^\dagger a_{\vec{k}'} \tag{3.74}$$

$$= \int \frac{d^3k}{(2\pi)^3} \widehat{n}_{\vec{k}} \tag{3.75}$$

where we have used $\int d^3x \, e^{-i(\vec{k}-\vec{k}')\vec{x}} = \delta^3(\vec{k}-\vec{k}') \cdot (2\pi)^3$.

General rule to calculate operator $\widehat{A}$ in 2nd quantization representation:

- Take expectation value of operator

$$\langle A \rangle = \int d^3x \psi^\dagger(\vec{x}) \widehat{A} \psi(\vec{x}) \tag{3.76}$$

- Replace $\psi(\vec{x}) \to \widehat{\psi}(\vec{x})$ and $\psi^*(\vec{x}) \to \psi^\dagger(\vec{x})$
- Equations of motion of creation/ destruction operator in Heisenberg picture:

$$H = \sum_{\vec{k}} \varepsilon_{\vec{k}} a^\dagger_{\vec{k}} a_{\vec{k}} \tag{3.77}$$

$$i\hbar \frac{\partial}{\partial t} a_{\vec{k}} = [a_{\vec{k}}, H] = \varepsilon_{\vec{k}} a_{\vec{k}} \tag{3.78}$$

$$a_{\vec{k}} = a_{\vec{k}}(0) e^{-i\frac{\varepsilon_{\vec{k}}}{\hbar}t} \tag{3.79}$$

$$a^\dagger_{\vec{k}} = a^\dagger_{\vec{k}}(0) e^{i\frac{\varepsilon_{\vec{k}}}{\hbar}t} \tag{3.80}$$

3.2 The spin-statistics theorem

In chapter 1 we had seen that the relativistic formulation of quantum mechanics necessarily leads to

1. an eigenvalue spectrum of the energy which is not bounded from below (negative energy eigenvalues E for free particles). The $E < 0$ solutions cannot be discarded, because they appear necessarily as parts of the solutions of physical problems:
   - relativistic scattering (Klein paradoxon)
   - (Gaussian) wave packet of finite temporal extension
   - $\to$ no stable ground state
2. a many-particle theory through the creation of particle-antiparticle pairs.

Therefore, *relativistic single-particle* quantum mechanics is inconsistent in itself. (The stability problem was partially solved by the concept of the Dirac sea for spin-$\frac{1}{2}$ particles, but not for particles with integer spin.) In section 3.1 we had developed efficient techniques to treat many-particle systems with even variable

number of particles: *field theory*
The fact that quantum mechanical particles are indistinguishable had implied a definite parity ± 1 of the state wrt. interchange of particles, i.e. commutation/anticommutation rules for creation/destruction operators.
In this section we will see that both of the inconsistencies above are remedied by combining the relativistic theory with the many-body description, i.e. by a field theoretic description of relativistic quantum mechanics.
This will at the same time lead to a definite relation between the spin of a particle (integer or half-integer) and the parity of its many-body wave function under particle interchange ($\rightarrow$ statistics).
We will restrict ourselves to the explicit treatment of spin-0 and spin-1/2 particles, although a general group theoretic treatment, based on the different behavior of integer/half-integer spin particles under Lorentz transformations is possible.

1. **Spin-0 particles**

   The Klein-Gordon equation

   $$((i\hbar c)^2 \underbrace{\partial_\mu \partial^\mu}_{\frac{\partial^2}{\partial(ct)^2}-\vec{\nabla}^2} -(mc^2)^2)\psi(\underline{x}) = 0 \tag{3.81}$$

   implies the continuity equation

   $$\partial_\mu j^\mu = 0, \qquad \frac{\partial}{\partial t}\frac{1}{c}j^0 + \vec{\nabla}\cdot\vec{j} = 0 \tag{3.82}$$

   with

   $$j^0 = \frac{i\hbar}{2c}\left(\psi^*\left(\frac{\partial}{\partial t}\psi\right) - \left(\frac{\partial}{\partial t}\psi^*\right)\psi\right) = j_0 \tag{3.83}$$

   $$\vec{j} = \frac{i\hbar}{2}\left(\psi^*\left(\vec{\nabla}\psi\right) - \left(\vec{\nabla}\psi^*\right)\psi\right) = (\vec{j}^\mu) = -(\vec{j}_\mu) \tag{3.84}$$

   $$\text{or} \qquad j_\mu = \frac{i\hbar}{2}\left(\psi^*\left(\frac{\partial}{\partial x^\mu}\psi\right) - \left(\frac{\partial}{\partial x^\mu}\psi^*\right)\psi\right) \tag{3.85}$$

   Since $i\hbar\frac{\partial}{\partial t}$ is the energy operator, j^0 had been interpreted in a preliminary way as an energy density. This assumes implicitly that $\psi^*(\underline{x})\psi(\underline{x})$ has the dimension of a particle density, as in the non-relativistic case (i.e. $\int d^3x\, \psi^*\psi$ =particle number, dimensionless). However, this interpretation is inconsistent, because:

- j^0 is not positive definite: negative energies?
- The interpretation of $\psi^*(\underline{x})\psi(\underline{x})$ as a particle density is not relativistically covariant, because, by this interpretation, the particle number $N = \int d^3x\, \psi^*(\underline{x})\psi(\underline{x})$ is not relativistically invariant (as it should!) (only the 3-dimensional integral).

→ How should we define the field amplitude to obtain a relativistically invariant particle number?

The quantity $N = \int d^4x\, \psi^*(\underline{x})\psi(\underline{x})$ is explicitly invariant, where

$$\psi(\underline{x}) = \int \frac{d^4k}{(2\pi)^3}\psi(\underline{k})e^{i\underline{k}\underline{x}}\sqrt{N(\underline{k})} \tag{3.86}$$

and $\sqrt{N(\underline{k})}$ is a normalization factor for plane wave states determined below. $N = \int d^4x\, \psi^*\psi$ is written as a 3-dimensional integral over a *density* by observing that the plane wave states must obey the relativistic dispersion

$$E^2 = \vec{p}^2c^2 + (mc^2)^2 \qquad \text{or} \tag{3.87}$$

$$(k^0)^2 = \underbrace{\vec{k}^2 + \left(\frac{mc}{\hbar}\right)^2}_{\varepsilon_{\vec{k}}^2} \tag{3.88}$$

$$\underline{k} = \begin{pmatrix} \frac{\omega}{c} \\ \vec{k} \end{pmatrix} \tag{3.89}$$

$$\underline{p} = \hbar\underline{k} \tag{3.90}$$

Hence:

$$N = \int d^4x \int \frac{d^4k}{(2\pi)^4} \int \frac{d^4k'}{(2\pi)^4}\psi^*(\underline{k})\psi(\underline{k'})e^{-i(\vec{k}\vec{x}-k^0t)}e^{i(\vec{k'}\vec{x}-k^{0\prime}t)} \tag{3.91}$$

$$= \int d^3x \int \frac{d^4k}{(2\pi)^4} \int \frac{d^3k'}{(2\pi)^3}\psi^*(\vec{k},k^0)\psi(\vec{k'},k^{0\prime})\delta(k^{0\,2} - \varepsilon_{\vec{k}}^2) \tag{3.92}$$

$$\times\delta(k^{0\prime 2} - \varepsilon_{\vec{k'}}^2)\delta(|\vec{k}| - |\vec{k'}|)e^{-i\vec{k}\vec{x}}e^{i\vec{k'}\vec{x}} \qquad \underbrace{\delta(k^{0\,2} - \varepsilon_{\vec{k}}^2)}_{=\frac{1}{2|\varepsilon_{\vec{k}}|}(\delta(k^0-\varepsilon_{\vec{k}})+\delta(k^0+\varepsilon_{\vec{k}}))}$$

$$= \int d^3x \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3}e^{-i\vec{k}\vec{x}}e^{i\vec{k'}\vec{x}}\delta(|\vec{k}| - |\vec{k'}|)\frac{1}{(2\pi)}\frac{1}{2|\varepsilon_{\vec{k}}|} \tag{3.93}$$

$$\times[\psi^*(\vec{k},\varepsilon_{\vec{k}})\psi(\vec{k'},\varepsilon_{\vec{k'}}) + \psi^*(\vec{k},-\varepsilon_{\vec{k}})\psi(\vec{k'},-\varepsilon_{\vec{k'}})] \tag{3.94}$$

$\Rightarrow$ A relativistically covariant density is obtained, if we define the plane wave amplitudes with the normalization factor $\frac{1}{\sqrt{2\varepsilon_{\vec{k}}}}\frac{1}{\sqrt{V}}$.

$$\psi_{\underline{k}}(\underline{x}) = \frac{1}{\sqrt{V}}\frac{1}{\sqrt{2\varepsilon_{\vec{k}}}}e^{i\underline{k}\underline{x}} \tag{3.95}$$

However, then $|\psi_{\underline{k}}(\underline{x})|^2$ does not have dimension of a particle density any longer, and j^0 does not have dimension of an energy density.
Therefore, a rigorous definition of the energy density is needed. It will also lead to the correct interpretation of j^μ.
In classical mechanics the energy is obtained as the Hamilton function from the Lagrange and Hamilton formalism. These need to be generalized to field theory now.
Lagrange and Hamilton formalism in relativistic field theory: generalization to infinite number of degrees of freedom.

Classical mechanics	**Field theory**
Lagrange formalism	
• parameter of the motion time t	coordinates $\underline{x} = \begin{pmatrix} ct \\ \vec{x} \end{pmatrix}$
• variables $\vec{x}(t), \dot{\vec{x}}(t)$, trajectory	$\psi(\underline{x})$ field amplitude, complex (=coordinate of the field ψ at each parameter value $\underline{x}$)
• Lagrange function $L = T(\vec{x}, \dot{\vec{x}}) - V(\vec{x}, \dot{\vec{x}})$	Lagrange density $\mathcal{L}\left(\psi, \frac{\partial}{\partial x^\mu}\psi\right) = T\left(\psi, \frac{\partial}{\partial x^\mu}\psi\right) - V\left(\psi, \frac{\partial}{\partial x^\mu}\psi\right)$ The relativistic covariance requires that $\mathcal{L}$ is function of derivatives wrt. *all* 4 coordinates
• Action principle $S = \int_{t_1}^{t_2} dt\, L(\vec{x}(t), \dot{\vec{x}}(t))$ $\delta S = 0$	$S = \int_{-\infty}^{+\infty} d^4x\, \mathcal{L}\left(\psi(\underline{x}), \frac{\partial}{\partial x^\mu}\psi(\underline{x})\right)$ $\delta S = 0$
• Euler-Lagrange equation $\frac{d}{dt}\frac{\partial L}{d\dot{\vec{x}}} - \frac{\partial L}{\partial \vec{x}} = 0$	for ψ $\frac{\partial}{\partial x^\mu}\frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \psi^*}{\partial x^\mu}\right)} - \frac{\partial \mathcal{L}}{\partial \psi^*} = 0$ (and similar for ψ^*)
Hamiltonian formalism	
• variables coordinates and canonical momenta $\vec{x}, \vec{p} = \frac{\partial L}{\partial \dot{\vec{x}}}$	$\psi(\underline{x}), \Pi^\mu(\underline{x}) = \frac{\partial \mathcal{L}}{\partial\left(\frac{\partial \psi^*}{\partial x^\mu}\right)}$
• Hamilton function $H = \dot{\vec{x}} \cdot \vec{p} - \mathcal{L}$	Energy momentum tensor $T^\mu{}_\nu = \frac{\partial \psi^*}{\partial x^\nu}\Pi^\mu - \delta^\mu{}_\nu \mathcal{L}\left(\psi, \frac{\partial \psi}{\partial x^\mu}\right)$ The $T^0{}_0$ component is the energy density

We now apply the Lagrange formalism to the Klein-Gordon theory in order to obtain the rigorous expression for the energy density:

The free Klein-Gordon equation is obtained as the Euler-Lagrange equa-

tion of motion from the Lagrange density *defined* as

$$\boxed{\mathcal{L}\left(\psi, \frac{\partial}{\partial x^\mu}\psi\right) = \partial_\mu\psi^*\partial^\mu\psi - m^2\psi^*\psi} \tag{3.96}$$

(sum convention and $c = 1$)

Proof:

$$\frac{\partial\mathcal{L}}{\partial\psi^*} = -m^2 \tag{3.97}$$

$$\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi^*}{\partial x^\mu}\right)} = \partial^\mu\psi \tag{3.98}$$

$$\frac{\partial}{\partial x^\mu}\frac{\partial\mathcal{L}}{\partial\left(\frac{\partial\psi^*}{\partial x^\mu}\right)} = \partial_\mu\partial^\mu\psi \tag{3.99}$$

In Euler-Lagrange:

$$\Rightarrow \quad \partial_\mu\partial^\mu\psi + m^2\psi = 0 \qquad \text{Klein-Gordon equation} \tag{3.100}$$

From $\mathcal{L}$ we obtain now the correct energy density as:

Canonical momentum: $\Pi^\mu(\underline{x}) = \frac{\partial\mathcal{L}}{\partial(\partial_\mu\psi^*)} = \partial^\mu\psi$

$$T^\mu{}_\nu = 2\partial_\nu\psi^*\partial^\mu\psi - \delta^\mu{}_\nu((\partial_\alpha\psi^*)(\partial^\alpha\psi) - m^2\psi^*\psi) \tag{3.101}$$

$$T_{\mu\nu} = 2\partial_\mu\psi^*\partial_\mu\psi - g_{\mu\nu}(\partial_\alpha\psi^*\partial^\alpha\psi - m^2\psi^*\psi) \tag{3.102}$$

$$T_{00} = T^{00} = T^0{}_0 \tag{3.103}$$

$$= \left(\frac{\partial}{\partial(ct)}\psi^*\right)\left(\frac{\partial}{\partial(ct)}\psi\right) + (\vec{\nabla}\psi^*)(\vec{\nabla}\psi) + m^2\psi^*\psi \tag{3.104}$$

$$= \left|\frac{\partial\psi}{\partial t}\right|^2 + |\vec{\nabla}\psi|^2 + m^2|\psi|^2 \tag{3.105}$$

positive definite

Energy density of a plane wave:

$$\psi = \frac{1}{\sqrt{V}}\frac{1}{\sqrt{2\varepsilon_{\vec{k}}}}e^{i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)} \tag{3.106}$$

$$\varepsilon_{\vec{k}} = (\vec{k}^2+m^2)^{1/2}, \qquad c=\hbar=1 \tag{3.107}$$

$$T_{00} = \frac{1}{2\varepsilon_{\vec{k}}V}\Big[\varepsilon_{\vec{k}}^2 + \underbrace{\vec{k}^2+m^2}_{\varepsilon_{\vec{k}}^2}\Big] \tag{3.108}$$

$$= \frac{\varepsilon_{\vec{k}}}{V} \tag{3.109}$$

Formulation of the Klein-Gordon theory for many-particle systems

Any (single-particle) wave function $\psi(\underline{x})$ can be developed into momentum eigenstates

$$\psi(\underline{x}) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{\sqrt{2\varepsilon_{\vec{k}}}}\left[\widetilde{a}_{\vec{k}}^{(+)}(t)e^{+i\vec{k}\vec{x}} + \widetilde{a}_{\vec{k}}^{(-)}(t)e^{+i\vec{k}\vec{x}}\right] \tag{3.110}$$

where the coefficients $\widetilde{a}_{\vec{k}}^{(\pm)}(t)$ have time dependence according to $E>0$ and $E<0$ solutions, respectively:

$$\widetilde{a}_{\vec{k}}^{(\pm)}(t) = a_{\vec{k}}^{(\pm)}e^{\mp i\varepsilon_{\vec{k}}t} \qquad (\hbar=c=1) \tag{3.111}$$

with $\varepsilon_{\vec{k}} = \hbar\omega_{\vec{k}} = +\sqrt{\vec{p}^2+m^2}$,

$$\psi(\underline{x}) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{\sqrt{2\varepsilon_{\vec{k}}}}\left[a_{\vec{k}}^{(+)}e^{i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)} + a_{\vec{k}}^{(-)}e^{+i(\vec{k}\vec{x}+\varepsilon_{\vec{k}}t)}\right]. \tag{3.112}$$

The second term has t-dependence like a state with negative energy.

The stability problem is ultimately cured by the *interpretation* that each wave function $\sim e^{-i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)}$ with *negative* energy $-\varepsilon_{\vec{k}} = -\hbar\omega_{\vec{k}}$ corresponds to this $\vec{k}$-state being *unoccupied*, and thus having *more* energy than in the occupied state (which is *no* wave function present, i.e. the vacuum state).

The concept of occupancy of a state is conveniently formulated in terms of creation/annihilation operators:

From the rules of 2nd quantization, the *energy operator* of the Klein-Gordon

theory is obtained from the energy expectation value $\langle E\rangle = \int d^3x\, T_{00}$ by replacing the wave function $\psi(\underline{x})$ with the *field operator* $\widehat{\psi}(\underline{x})$

$$\psi(\underline{x}) \rightarrow \widehat{\psi}(\underline{x}) \tag{3.113}$$
$$\psi^*(\underline{x}) \rightarrow \widehat{\psi}^\dagger(\underline{x}) \tag{3.114}$$

(in the following, the tilde will be omitted).

$$\widehat{H} = \int d^3x\, \widehat{T}_{00} \tag{3.115}$$
$$= \int d^3x \left[|\partial_t\psi|^2 + |\vec{\nabla}\psi|^2 + m^2|\psi|^2\right] \tag{3.116}$$

has the dimension of energy with

$$\psi(\underline{x}) = \int \frac{d^3k}{(2\pi)^3}\frac{1}{\sqrt{2\varepsilon_{\vec{k}}}}\left[a^{(+)}_{\vec{k}}\exp\left(i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)\right) + a^{(-)}_{\vec{k}}\exp\left(-i(-\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)\right)\right] \tag{3.117}$$

. The destruction of a particle in state $(+\vec{k}, -\varepsilon_{\vec{k}})$ is interpreted as the creation of a particle in state $-\vec{k}$ with positive energy: $(-\vec{k}, +\varepsilon_{\vec{k}})$, relative to the vacuum (where the $\varepsilon_{\vec{k}}$ state is occupied).

$$\text{destruction } (+\vec{k}, -\varepsilon_{\vec{k}}) \equiv \text{creation } (-\vec{k}, \varepsilon_{\vec{k}}) = \text{antiparticle creation}$$
$$\text{creation } (+\vec{k}, -\varepsilon_{\vec{k}}) \equiv \text{destruction } (-\vec{k}, \varepsilon_{\vec{k}})$$

Therefore, we replace the annihilator of a $E < 0$ (free) particle $a^{(-)}_{\vec{k}}$ by a creation operator $a^{(-)}_{\vec{k}} \equiv b^{(+)}_{-\vec{k}}$ (and drop the $^{(+)}$ in $a^{(+)}_{\vec{k}}$).

$$\psi(\underline{x}) = \int \frac{d^3k}{(2\pi)^3}\left[a_{\vec{k}}e^{i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)} + b^{(+)}_{-\vec{k}}e^{i(-\vec{k}\vec{x}+\varepsilon_{\vec{k}}t)}\right], \tag{3.118}$$

so that all terms in $\psi(\underline{x})$ have the correct time dependence for creation/ annihilation of a $E > 0$ particle, respectively.
Destruction of particle at $\underline{x}$ has component of destruction and antiparticle creation (as seen before for strongly localized wave functions $\Delta x \lesssim \lambda_C = \frac{\hbar}{mc}$).

With this definition of the field operators $\psi(\underline{x}), \psi^\dagger(\underline{x})$ calculate the energy operator:

$$\begin{aligned}
\widehat{H} &= \int d^3x \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \frac{1}{2\sqrt{\varepsilon_{\vec{k}}}\sqrt{\varepsilon_{\vec{k}'}}} \left[i\varepsilon_{\vec{k}} a^{(+)}_{\vec{k}} e^{-i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)} - i\varepsilon_{\vec{k}} b_{-\vec{k}} e^{-i(-\vec{k}\vec{x}+\varepsilon_{\vec{k}}t)} \right] && (3.119)\\
&\times \left[-i\varepsilon_{\vec{k}'} a_{\vec{k}'} e^{+i(\vec{k}'\vec{x}-\varepsilon_{\vec{k}'}t)} + i\varepsilon_{\vec{k}'} b^{(+)}_{-\vec{k}'} e^{i(-\vec{k}'\vec{x}+\varepsilon_{\vec{k}'}t)} \right] && (3.120)\\
&+ \left[-i\vec{k} a^{(+)}_{\vec{k}} e^{-i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)} + i\vec{k} b_{-\vec{k}} e^{-i(-\vec{k}\vec{x}+\varepsilon_{\vec{k}}t)} \right] && (3.121)\\
&\times \left[i\vec{k}' a_{\vec{k}'} e^{+i(\vec{k}'\vec{x}-\varepsilon_{\vec{k}'}t)} - i\vec{k}' b^{(+)}_{-\vec{k}'} e^{i(-\vec{k}'\vec{x}+\varepsilon_{\vec{k}'}t)} \right] && (3.122)\\
&+ m^2 \left[a^{(+)}_{\vec{k}} e^{-i(\vec{k}\vec{x}-\varepsilon_{\vec{k}}t)} + b_{-\vec{k}} e^{-i(-\vec{k}\vec{x}+\varepsilon_{\vec{k}}t)} \right] && (3.123)\\
&\times \left[a_{\vec{k}'} e^{+i(\vec{k}'\vec{x}-\varepsilon_{\vec{k}'}t)} + b^{(+)}_{-\vec{k}'} e^{i(-\vec{k}'\vec{x}+\varepsilon_{\vec{k}'}t)} \right] && (3.124)
\end{aligned}$$

$$\begin{aligned}
&= \int \frac{d^3k}{(2\pi)^3} \int \frac{d^3k'}{(2\pi)^3} \frac{1}{2} \frac{1}{\sqrt{\varepsilon_{\vec{k}}}\sqrt{\varepsilon_{v\vec{k}'}}} \left[\left[\varepsilon^2_{\vec{k}} + \underbrace{\vec{k}^2 + m^2}_{\varepsilon_{\vec{k}}} \right] \left\{ a^{(+)}_{\vec{k}} a_{\vec{k}'} e^{i(\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}'})t} \delta^3(\vec{k}-\vec{k}')(2\pi)^3 \right.\right.\\
&\quad \left. + b_{-\vec{k}} b^{(+)}_{-\vec{k}'} e^{-i(\varepsilon_{\vec{k}}-\varepsilon_{\vec{k}'})t} \delta^3(\vec{k}-\vec{k}')(2\pi)^3 \right\}\\
&\quad - \left[\varepsilon^2_{\vec{k}} - \vec{k}^2 + m^2 \right] \left\{ a^{(+)}_{\vec{k}} b^{(+)}_{-\vec{k}'} e^{i(\varepsilon_{\vec{k}}+\varepsilon_{\vec{k}'})t} \delta^3(\vec{k}+\vec{k}')(2\pi)^3 \right.\\
&\quad \left.\left. + a_{\vec{k}} b_{\vec{k}} e^{-i(\varepsilon_{\vec{k}}+\varepsilon_{\vec{k}'})t} \delta^3(\vec{k}+\vec{k}')(2\pi)^3 \right\} \right]\\
&= \int \frac{d^3k}{(2\pi)^3} \varepsilon_{\vec{k}} \left(a^{(+)}_{\vec{k}} a_{\vec{k}} + b_{-\vec{k}} b^{(+)}_{-\vec{k}} \right) + \varepsilon_{\vec{k}=0} \left[a^{(+)}_0 b^{(+)}_0 e^{2i\varepsilon_{\vec{k}=0}t} + a_0 b_0 e^{-2i\varepsilon_{\vec{k}=0}t} \right]\\
\Rightarrow \widehat{H} &= \int \frac{d^3k}{(2\pi)^3} \varepsilon_{\vec{k}} \left(a^{(+)}_{\vec{k}} a_{\vec{k}} + b_{\vec{k}} b^{(+)}_{\vec{k}} \right)
\end{aligned}$$

The factors $e^{\pm i(\varepsilon_{\vec{k}}+\varepsilon_{\vec{k}'})t}\delta^3(\vec{k}+\vec{k}')$ vanish after $\int dt$ except for $\vec{k} = \vec{k}' = 0$ (Bose-Einstein condensation only).

$\widehat{H}$ is positive definite exactly if $b, b^{(+)}$ obey commutation rules of bosons:

$$[b_{\vec{k}}, b^{(+)}_{\vec{k}}] = 1 \qquad (3.125)$$

$$\widehat{H} = \int \frac{d^3k}{(2\pi)^3} \hbar\omega_{\vec{k}} \left(a^{(+)}_{\vec{k}} a_{\vec{k}} + b^{(+)}_{\vec{k}} b_{\vec{k}} + 1 \right) \qquad (3.126)$$

The 1 can be neglected because ∞ energy of occupied $E < 0$ states in the vacuum. The term $a^{(+)}_{\vec{k}} a_{\vec{k}}$ is the particle and the term $b^{(+)}_{\vec{k}} b_{\vec{k}}$ is the antiparticle number in state $\vec{k}$ (= constant shift of energy zero point).

Stability demands:

Spin-0 particles obey Bose commutation rules $[\vec{a}_{\vec{k}}, \vec{a}_{\vec{k}'}] = \delta_{\vec{k},\vec{k}'}$, etc.	(3.127)

Analogous:

$$j^0 = \int \frac{d^3k}{(2\pi)^3} (a^{(+)}_{\vec{k}} a_{\vec{k}} - b^{(+)}_{-\vec{k}} b_{\vec{k}} - \underbrace{1}_{(*)}) \tag{3.128}$$

$(*)$ ∞ particle number from occupied states

2. **Spin-$\frac{1}{2}$ particles**

We have the same decomposition of the field operators:

$$\psi_\sigma(\underline{x}) = \int \frac{d^3k}{(2\pi)^3} \left[c_{\vec{k},\sigma} u(\vec{k},\sigma) e^{i(\vec{k}\vec{x} - \varepsilon_{\vec{k}} t)} + d^{(+)}_{-\vec{k},-\sigma} v(\vec{k},\sigma) e^{+i(-\vec{k}\vec{x} + \varepsilon_{\vec{k}} t)} \right] \tag{3.129}$$

$\psi^\dagger_\sigma(\underline{x})$ analogous.

However, the energy is calculated from the Dirac Hamilton operator:

$$H = c\,\vec{\alpha} \cdot \widehat{\vec{p}} + \beta mc^2 = \begin{pmatrix} mc^2 & c\,\vec{\sigma} \cdot \widehat{\vec{p}} \\ c\,\vec{\sigma} \cdot \widehat{\vec{p}} & -mc^2 \end{pmatrix} \tag{3.130}$$

$$\langle E \rangle = \int d^3x \sum_\sigma \underbrace{\psi^\dagger_\sigma(\underline{x})}_{\text{Dirac spinors}} H \psi_\sigma(\underline{x}), \qquad \widehat{\vec{p}} = -i\hbar \frac{\partial}{\partial \vec{x}} \tag{3.131}$$

With:

$$
\begin{aligned}
u(\vec{k},\uparrow) &= \sqrt{\frac{E_{\vec{p}}+m}{2m}}\begin{pmatrix} 1 \\ 0 \\ \frac{p_z}{E_{\vec{p}}+m} \\ \frac{p_x+ip_y}{E_{\vec{p}}+m} \end{pmatrix} \\
u(\vec{k},\downarrow) &= \sqrt{\frac{E_{\vec{p}}+m}{2m}}\begin{pmatrix} 0 \\ 1 \\ \frac{p_z}{E_{\vec{p}}+m} \\ \frac{p_x+ip_y}{E_{\vec{p}}+m} \end{pmatrix} \qquad E>0 \text{ spinors} \\
v(\vec{k},\uparrow) &= \sqrt{\frac{E_{\vec{p}}+m}{2m}}\begin{pmatrix} \frac{p_z}{E_{\vec{p}}+m} \\ \frac{p_x+ip_y}{E_{\vec{p}}+m} \\ 1 \\ 0 \end{pmatrix} \\
v(\vec{k},\downarrow) &= \sqrt{\frac{E_{\vec{p}}+m}{2m}}\begin{pmatrix} \frac{p_z}{E_{\vec{p}}+m} \\ \frac{p_x+ip_y}{E_{\vec{p}}+m} \\ 0 \\ 1 \end{pmatrix} \qquad E<0 \text{ spinors} \\
H\left[u(\vec{k},\sigma)e^{i\vec{k}\vec{x}}\right] &= \varepsilon_{\vec{p}}\left[u(\vec{k},\sigma)e^{i\vec{k}\vec{x}}\right] \\
H\left[v(\vec{k},\sigma)e^{i\vec{k}\vec{x}}\right] &= -\varepsilon_{\vec{p}}\left[v(\vec{k},\sigma)e^{i\vec{k}\vec{x}}\right] \\
\varepsilon_{\vec{p}} &= \sqrt{\vec{p}^2c^2+(mc^2)^2}, \qquad \vec{p}=\hbar\vec{k}
\end{aligned}
$$

Hence, we obtain for spin-$\frac{1}{2}$ particles in 2nd quantization:

$$\widehat{H} = \int \frac{d^3k}{(2\pi)^3}\sum_\sigma E_{\vec{p}}\left(c^{(+)}_{\vec{k},\sigma}c_{\vec{k},\sigma} - d_{\vec{k},\sigma}d^{(+)}_{\vec{k},\sigma}\right) + \mathcal{O}\left(c^{(+)}d^{(+)}, dc\right) \tag{3.132}$$

(The terms $c^{(+)}_{\vec{k},\sigma}d^{(+)}_{\vec{k},\sigma}$ and $d_{\vec{k},\sigma}c_{\vec{k},\sigma}$ will vanish, since no double occupancy.)

$\widehat{H}$ positive definite exactly if $d, d^{(+)}$ obey anticommutation rules:

$$\left\{d_{\vec{k},\sigma}, d^{(+)}_{\vec{k},\sigma}\right\} = 1 \tag{3.133}$$

$$\widehat{H} = \int \frac{d^3k}{(2\pi)^3}\sum_\sigma E_{\vec{p}}\left(c^{(+)}_{\vec{k},\sigma}c_{\vec{k},\sigma} + d^{(+)}_{\vec{k},\sigma}d_{\vec{k},\sigma} - \not{1}\right) \tag{3.134}$$

Stability:

$$\boxed{\begin{array}{l}\text{Spin-}\frac{1}{2}\text{ particles obey Fermi anticommutation rules}\\ \left\{c_{\vec{k},\sigma}, c^{(+)}_{\vec{k}',\sigma'}\right\} = \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'} \qquad \text{etc.}\end{array}} \tag{3.135}$$

General:

$$\boxed{\begin{array}{ll}\text{integer spin:} & \text{bosons}\\ \text{half-integer spin:} & \text{fermions}\end{array}} \quad \textbf{Spin-statistics theorem} \tag{3.136}$$

Follows, because any integer spin particle can be composed of spin-0 and an *even* number of spin-$\frac{1}{2}$ particles, and because any half-integer spin particle can be composed of spin-0 and an *odd* number of spin-$\frac{1}{2}$ particles.

3.3 $U(1)$ gauge symmetry and particle number conservation

In the QM I course if had been discussed that the invariance under (global) $U(1)$ phase transformations implies the particle number conservation. Specifically, it had been shown that the continuity equation is valid, if ψ and ψ^* obey equations of motion (Schrödinger equations) which are complex conjugate to each other (which is only true for a $U(1)$ symmetric system).
The relation between particle number and phase can be made more explicit by means of the 2nd quantized formalism.
We consider the many-body state in "product state representation" (i.e. specifying the state of each particle):

$$|\phi(\alpha_{k_1}, \alpha_{k_2}, \ldots, \alpha_{k_N})\rangle_N = \left(\frac{n_{k_1}! n_{k_2}! \ldots}{N!}\right)^{1/2} \sum_P (\pm 1)^P |\alpha^{(k_1)}_{P(1)}\rangle \ldots |\alpha^{(k_N)}_{P(N)}\rangle \tag{3.137}$$

$U(1)$ gauge transformation transforms each single-particle state as

$$U(\varphi): \quad |\alpha_i^{(k_i)} \longmapsto e^{+i\varphi}|\alpha_i^{(k_i)}\rangle \tag{3.138}$$

Since the N particles are indistinguishable, each single-particle state in $|\phi\rangle$ transforms under U with the *same* phase factor.
This means

$$U(\varphi): \quad |\phi\rangle_N \longmapsto e^{+iN\varphi}|\phi\rangle_N \tag{3.139}$$

or for an arbitrary number of particles:

$$U(\varphi): \quad |\phi(0)\rangle \longmapsto e^{-i\varphi\widehat{N}}|\phi\rangle = |\phi(\varphi)\rangle \qquad (*) \tag{3.140}$$

where $\widehat{N}$ is the particle number operator.

$$\boxed{\widehat{N} \text{ is the generator of } U(1)} \tag{3.141}$$

Commutation relation:

Expressing $\widehat{N}$ in "product state representation":

$$|\phi(\Delta\varphi)\rangle \overset{\text{Taylor expansion}}{=} \sum_k \frac{1}{k!} \left.\frac{d^k|\phi\rangle}{d\varphi^k}\right|_{\varphi=0} (\Delta\varphi)^k \tag{3.142}$$

$$= e^{\Delta\varphi\frac{d}{d\varphi}}|\phi(\varphi=0)\rangle \tag{3.143}$$

$$= e^{i\Delta\varphi\left(-i\frac{d}{d\varphi}\right)}|\phi(\varphi=0)\rangle \tag{3.144}$$

Comparing with $(*)$ implies:

$$\boxed{\widehat{N} = -i\tfrac{d}{d\varphi}, \qquad \varphi = \text{phase}} \tag{3.145}$$

Phase and particle number are conjugate operators, analogous to position $\widehat{\vec{x}}$ and momentum $-i\hbar\frac{\partial}{\partial\vec{x}}$. It follows, in analogy:

$$\boxed{[\varphi, \widehat{N}] = i} \tag{3.146}$$

Proof:

$$\begin{aligned}
[\varphi, \widehat{N}] &= -i\left(\varphi\frac{d}{d\varphi} - \frac{d}{d\varphi}\varphi\right) \\
&= -i\left(\varphi\frac{d}{d\varphi} - \frac{d\varphi}{d\varphi} - \varphi\frac{d}{d\varphi}\right) \\
&= i
\end{aligned}$$

□

Particle number conservation:

Since $\widehat{N}$ is the generator of the Lie group $U(1)$ it is conserved, if the Hamiltonian is $U(1)$ invariant.

Proof:

$U(1)$-invariance:

$$e^{i\varphi\widehat{N}} H e^{-i\varphi\widehat{N}} = H \tag{3.147}$$

For infinitesimal φ:

$$\begin{aligned} H &= e^{i\varphi\widehat{N}} H e^{-i\varphi\widehat{N}} \\ &= (1+i\varphi\widehat{N}) H (1-i\varphi\widehat{N}) \\ &= H + i\varphi[\widehat{N}, H] \\ \Leftrightarrow [\widehat{N}, H] &= 0 \end{aligned}$$

Heisenberg equation of motion:

$$i\hbar\frac{\partial}{\partial t}\widehat{N} = [\widehat{N}, H] = 0, \quad \widehat{N} \text{ conserved} \tag{3.148}$$

Measurability of phase and particle number:

Since $\widehat{\varphi}$, and $\widehat{N}$ do not commute, they cannot be measured simultaneously with arbitrary precision. We have the uncertainty relation (analogous to $\vec{x} - \vec{p}$ uncertainty):

$$\boxed{\Delta\varphi\Delta N \lesssim \tfrac{1}{2}} \tag{3.149}$$

Consequences of the discreteness of the spectrum of $\widehat{N}$:

In contrast to $\vec{p}$, the spectrum of $\widehat{N}$ is discrete, $N = 1, 2, 3, \ldots$.
Although the commutation relation (3.56) has been proven in "product state representation", it must be valid in any representation.
In particular, in particle number representation, $\widehat{N}$ is diagonal with discrete eigenvalues $N = 1, 2, 3 \ldots$. In order to obey the commutation relation (3.56), the phase operator must be in particle number representation:

$$\widehat{\varphi} = +i\frac{d}{dN}, \qquad N = \text{particle number} \tag{3.150}$$

The derivative $\frac{d}{dN}$ is meaningful only when $N \gg 1$:

$$\frac{df}{dN} \underset{N\to\infty}{\longrightarrow} \frac{f(N+1)-f(N)}{(N+1)-N} = \frac{[f(N+1)-f(N)]/N}{1/N} \tag{3.151}$$

For a state with small particle number $N \approx 1$, the phase $\widehat{\varphi} = i\frac{d}{dN}$ not only cannot be measured precisely, but is not even defined.

Interpretation:

A plane wave state $\frac{1}{\sqrt{2\pi}} e^{i(\vec{k}\vec{x}-\omega t)}$ with fixed phase is normalized to ∞ (or a finite *density*), i.e. contains always an infinite particle number.
A state with a finite particle number, normalized to a finite number, must be localized in space and for time, i.e., by Fourier decomposition, does not have a well-defined phase.

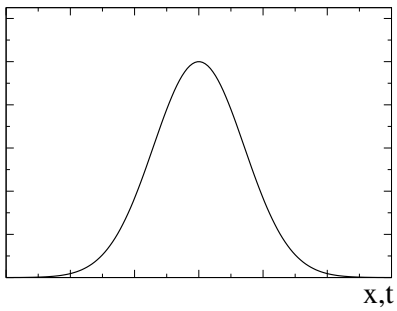


Figure 3.3:

These properties play a role in systems with many coherent particles in one state (lasers, Bose condensates).

3.4 Perturbation theory for many-particle systems: Green's functions and Feynman diagram techniques

3.4.1 Schrödinger, Heisenberg and interaction pictures (reminder)

Schrödinger picture

- Operators $\widehat{A}, H$ time independent
- State $|\psi(t)\rangle$ time dependent
- $i\hbar\frac{d}{dt}|\phi(t)\rangle = H|\phi(t)\rangle$
  Formal solution: $|\phi(t)\rangle = e^{-\frac{i}{\hbar}Ht}|\phi(0)\rangle$
- Expectation value:
  $\langle\widehat{A}\rangle = \langle\phi(t)|\widehat{A}|\phi(t)\rangle = \langle\phi(0)|\underbrace{e^{\frac{i}{\hbar}Ht}\widehat{A}e^{-\frac{i}{\hbar}Ht}}_{\widehat{A}_H(t)}|\phi(0)\rangle$

Heisenberg picture The time dependence of an expectation value $\langle A\rangle$ can be cast from $|\phi(t)\rangle$ into a time dependence of the operator A:

- $\widehat{A}_H(t) = e^{\frac{i}{\hbar}Ht}\widehat{A}e^{-\frac{i}{\hbar}Ht}$ Heisenberg operator
- $|\phi\rangle_H = |\phi(t=0)\rangle$ Heisenberg state, time independent
- From its definition, the Heisenberg operator obeys the equation of motion

  $$i\hbar\tfrac{d}{dt}\widehat{A}_H(t) = -He^{\frac{i}{\hbar}Ht}\widehat{A}e^{-\frac{i}{\hbar}Ht} + e^{\frac{i}{\hbar}Ht}\widehat{A}e^{-\frac{i}{\hbar}Ht}H + i\hbar e^{\frac{i}{\hbar}Ht}\tfrac{\partial\widehat{A}}{\partial t}e^{-\frac{i}{\hbar}Ht}$$

  The derivative $\frac{\partial\widehat{A}}{\partial t}$ occurs only if $\widehat{A}$ has explicit time dependence in Schrödinger picture, i.e. t-dependent potential.

  $$\boxed{i\hbar\tfrac{d}{dt}\widehat{A}_H(t) = [\widehat{A}_H(t), H] + i\hbar\tfrac{\partial\widehat{A}_H(t)}{\partial t}} \tag{3.152}$$

  In particular:

  $$\frac{d}{dt}H_H = \frac{\partial}{\partial t} \overset{\text{in general}}{=} 0 \tag{3.153}$$

  Same t-dependence of H in Schrödinger and Heisenberg picture.

Interaction picture

$$H = H_0 + H_{\text{int}} \qquad \text{(solution of } H_0 \text{ known)} \tag{3.154}$$

We propagate the Schrödinger state $|\phi(t)\rangle$ *back in time* to $t = 0$ according to the non-interacting Hamiltonian.

- Interaction state:
  $|\phi(t)\rangle_I = e^{+\frac{i}{\hbar}H_0 t}|\phi(t)\rangle$
- $|\phi(t)\rangle_I$ obeys the equation of motion

$$i\hbar\frac{d}{dt}|\phi(t)\rangle_I = -H_0\cancel{|\phi\rangle_I} + e^{\frac{i}{\hbar}H_0 t}(\cancel{H_0} + H_{\text{int}})|\phi(t)\rangle \tag{3.155}$$

$$\boxed{i\hbar\tfrac{d}{dt}|\phi(t)\rangle_I = e^{\frac{i}{\hbar}H_0 t}H_{\text{int}}e^{-\frac{i}{\hbar}H_0 t}|\phi_I\rangle} \tag{3.156}$$

- Expectation value of any operator $\widehat{A}$:
  $\langle\widehat{A}\rangle = \langle\phi(t)|\widehat{A}|\phi(t)\rangle = {}_I\langle\phi(t)|\underbrace{e^{\frac{i}{\hbar}H_0 t}\widehat{A}e^{-\frac{i}{\hbar}H_0 t}}_{\widehat{A}_I}|\phi(t)\rangle$
- $\widehat{A}_I(t) = e^{\frac{i}{\hbar}H_0 t}\widehat{A}e^{-\frac{i}{\hbar}H_0 t}$

Interaction picture:

1. Operators have time dependence like Heisenberg operators with respect to the non-interacting system H_0, i.e. their time dependence is assumed to be known.
   In particular: $H_{\text{int,I}}(t) = e^{\frac{i}{\hbar}H_0 t}H_{\text{int}}e^{-\frac{i}{\hbar}H_0 t}$
2. The states obey a Schrödinger equation wrt. the interaction Hamiltonian (in interaction picture) $H_{\text{int, I}}(t)$ only (assumed: no explicit t-dependence of H_{int}):
   $i\hbar\frac{d}{dt}|\phi\rangle_I = H_{\text{int,I}}(t)|\phi_I\rangle$

The advantage of the interaction picture is that effects of H_0 and H_{int} are seperated, and that, hence, the motion of the operators is known. These pictures are readily applied to the operators of 2nd quantization, where the *known* motion of $\psi_I(\vec{x}, t)$ will be extensively exploited for many-body perturbation theory.

3.4.2 The Green's function (definition)

We define the retarded (R) and advanced (A) Green's function as the expectation values (using the *Heisenberg picture* for the operators and the states):

$$G^R_{\sigma\sigma'}(x,x') = -i\theta(t-t')\langle[\psi_\sigma(x),\psi^+_{\sigma'}(x')]_\mp\rangle \tag{3.157}$$

$$G^A_{\sigma\sigma'}(x,x') = +i\theta(t-t')\langle[\psi_\sigma,\psi^+_{\sigma'}(x')]_\mp\rangle \tag{3.158}$$

where the commutator $[\ldots,\ldots]_-$ is for bosons and the anticommutator $[\ldots,\ldots]_+$ is for fermions. From now on, we will only consider fermions: $[\ldots,\ldots]_+ \equiv \{\ldots,\ldots\}$

- The expectation value $\langle\ldots\rangle \equiv {}_H\langle\psi_0|\ldots|\psi_0\rangle_H$ is understood to be taken wrt. the Heisenberg ground state. Since all the time dependence is in the operators, we can use the short-hand notation $\langle\ldots\rangle$.
- σ,σ' denote the spin projection $\sigma_z = \pm 1$ or any other, additional quantum number of a particle.

Note:

In the Heisenberg picture, the field operators $\psi,\psi^\dagger$ do not, in general, obey canonical permutation relations because of the factors $e^{\pm\frac{i}{\hbar}Ht}, e^{\pm\frac{i}{\hbar}Ht'}$. Canonical relations hold only for $t=t'$.

For the purpose perturbation theory, we also define the *time-ordered Green's function*:

$$G_{\sigma\sigma'}(x,x') = -i\langle T\psi_\sigma(x)\psi^\dagger_{\sigma'}(x')\rangle \tag{3.159}$$

with

$$T\psi_\sigma(x)\psi^\dagger_{\sigma'}(x') := \begin{cases} \psi_\sigma(x)\psi^\dagger_{\sigma'}(x'), & t>t' \\ \pm\psi^\dagger_{\sigma'}(x')\psi_\sigma(x), & t<t' \end{cases} \tag{3.160}$$

$+$ is for bosons and - for fermions. The case $t=t'$ requires special treatment, see below.

Importance of $G(x,x')$:

From G the ground state expectation value of any single-particle operator $F^{(1)}$ can be calculated:

$$F^{(1)} = \int d^3x\, \psi^\dagger(x) f^{(1)}(\vec{x}) \psi(x) \tag{3.161}$$

(Heisenberg picture: $\psi(x) = e^{\frac{i}{\hbar}Ht}\psi(\vec{x})e^{-\frac{i}{\hbar}Ht}$ etc.)

$$\begin{aligned} \langle F^{(1)} \rangle_{\sigma\sigma'} &= \int d^3x \langle \psi^\dagger_\sigma(x) f^{(1)}(\vec{x}) \psi_{\sigma'}(x) \rangle \\ &= \int d^3x [f^{(1)}(\vec{x})] \langle \psi^\dagger_{\sigma'}(x) \psi_\sigma(x) \rangle \end{aligned}$$

$[f^{(1)}(\vec{x})]$ is the diagonal matrix element of $f^{(1)}(\vec{x})$ in $\vec{x}$ representation.

$$\boxed{\langle F^{(1)} \rangle_{\sigma\sigma'} = \pm i \int d^3x \lim_{\substack{\vec{x}' \to \vec{x} \\ t' \to t+0}} [f^{(1)}(\vec{x})] G(x,x')} \tag{3.162}$$

Examples:

Particle density: $f^{(1)}(\vec{x}) \equiv 1$

$$\boxed{n_\sigma(x) = \pm i \lim_{\substack{\vec{x}' \to \vec{x} \\ t' \to t+0}} G(x,x')} \tag{3.163}$$

Particle current density:

$$\begin{aligned} \vec{j} &= f^{(1)} = \frac{\hbar}{2mi}(\vec{\nabla}_{\vec{x}} - \vec{\nabla}_{\vec{x}'}) \\ &\quad \vec{\nabla}_{\vec{x}} \text{ acting to the right, } \vec{\nabla}_{\vec{x}'} \text{ acting to the left} \\ \int d^3x \langle \vec{j} \rangle_{\sigma\sigma'} &= \frac{\hbar}{2mi}\delta_{\sigma\sigma'} \int d^3x \langle \psi^\dagger_\sigma(x') \vec{\nabla}_{\vec{x}} \psi(x) - \psi^\dagger_\sigma(x') \vec{\nabla}_{\vec{x}'} \psi(x') \rangle \\ &= \pm \frac{\hbar}{2m} \int d^3x \lim_{\substack{\vec{x}' \to \vec{x} \\ t' \to t+0}} (\vec{\nabla}_{\vec{x}} - \vec{\nabla}_{\vec{x}'}) G_{\sigma\sigma}(x,x') \delta_{\sigma\sigma'} \end{aligned}$$

$$\boxed{\langle j_\sigma \rangle = \pm \tfrac{\hbar}{2m} \lim_{\substack{\vec{x}' \to \vec{x} \\ t' \to t+0}} (\vec{\nabla}_{\vec{x}} - \vec{\nabla}_{\vec{x}'}) G_{\sigma\sigma}(x,x')} \tag{3.164}$$

3.4.3 The free Green's function: equations of motion

We first derive the equations of motion for the free Green's function in momentum space. This will establish the connection between the (free) Green's function defined for many-particle systems and the Green's function defined as a resolvent operator of a differential equation.

"Free" Hamilton operator (=single-particle operator):

$$H_0 = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} c^{(+)}_{\vec{k},\sigma} c_{\vec{k},\sigma} \tag{3.165}$$

Remark:

$\vec{k}$ is understood to be the momentum index here, but could be any quantum number in which the single-particle system is diagonal, e.g. l, m for an electron in a H-atom ($\rightarrow$ e-e interaction as perturbation).

Fermions:

Many-body ground state: Fermi sea

$$|0\rangle = |n_{\vec{k}_1\uparrow}, n_{\vec{k}_1\downarrow}, n_{\vec{k}_2\uparrow}, n_{\vec{k}_2\downarrow}, \ldots\rangle \tag{3.166}$$

with $n_{\vec{k},\sigma} = \begin{cases} 1, & |\vec{k}| \leq k_f \\ 0, & |\vec{k}| > k_F \end{cases}$ k_F =Fermi momentum

Short-hand notation:

$$|0\rangle = |n_{\vec{k}\leq k_F,\sigma}, n_{\vec{k}>k_F,\sigma} = 0\rangle \tag{3.167}$$

(**Note:** Efficiency of writing many-body state in occupation number representation.)

Equations of motion for the creation/ destruction operators:

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}c_{\vec{k},\sigma} &= [c_{\vec{k},\sigma}, H_0] \\
\text{fermions:}\quad [c_{\vec{k},\sigma}, H_0] &= \sum_{\vec{k}',\sigma'} \varepsilon_{\vec{k}'}\left(c_{\vec{k},\sigma}c^{(+)}_{\vec{k},\sigma'}c_{\vec{k}',\sigma'} - c^{(+)}_{\vec{k}',\sigma'}c_{\vec{k}',\sigma'}c_{\vec{k}',\sigma'}\right) \\
&= \sum_{\vec{k}',\sigma'} \varepsilon_{\vec{k}'}\Big(\pm c^{(+)}_{\vec{k},\sigma'}\underbrace{c_{\vec{k},\sigma}c_{\vec{k}',\sigma'}}_{\pm c_{\vec{k}'\sigma'}c_{\vec{k},\sigma}} + \delta_{\vec{k}\vec{k}'}\delta_{\sigma\sigma'}c_{\vec{k}',\sigma'} - c^{(+)}_{\vec{k}',\sigma'}c_{\vec{k}',\sigma'}c_{\vec{k},\sigma}\Big) \\
c_{\vec{k},\sigma}(t) &= e^{-\frac{i}{\hbar}\varepsilon_{\vec{k}}t} \\
c^{(+)}_{\vec{k},\sigma}(t) &= e^{+\frac{i}{\hbar}\varepsilon_{\vec{k}}t} \\
i\hbar\frac{\partial}{\partial t}c_{\vec{k},\sigma} &= \varepsilon_{\vec{k}}c_{\vec{k},\sigma} \\
-i\hbar\frac{\partial}{\partial t}c^{(+)}_{\vec{k},\sigma} &= \varepsilon^{(+)}_{\vec{k},\sigma} \qquad (\hbar = 1 \quad \text{below})
\end{aligned}
$$

Equations of motion for $G^{R/A}, G$:

$$
\begin{aligned}
i\frac{\partial}{\partial t}G^R_{\vec{k}\sigma}(t,t') &= i\frac{\partial}{\partial t}\left\{-i\theta(t-t')\left\langle\left(c_{\vec{k}\sigma}(t)c^\dagger_{\vec{k}\sigma}(t') \mp c^\dagger_{\vec{k}\sigma}(t')c_{\vec{k}\sigma}(t)\right)\right\rangle\right\} \\
&= \delta(t-t') + \varepsilon_{\vec{k}}G^R_{\vec{k}\sigma}(t,t') \\
i\frac{\partial}{\partial t}G^A_{\vec{k}\sigma}(t,t') &= i\frac{\partial}{\partial t}\left\{+i\theta(t'-t)\left\langle\left(c_{\vec{k}\sigma}(t)c^\dagger_{\vec{k}\sigma}(t') \mp c^\dagger_{\vec{k}\sigma}(t')c_{\vec{k}\sigma}(t)\right)\right\rangle\right\} \\
&= \delta(t-t') + \varepsilon_{\vec{k}}G^A_{\vec{k}\sigma}(t,t') \\
i\frac{\partial}{\partial t}G_{\vec{k}\sigma}(t,t') &= i\frac{\partial}{\partial t}\left\{(-i)\theta(t-t')\left\langle c_{\vec{k}\sigma}(t)c^\dagger_{\vec{k}\sigma}(t')\right\rangle \pm (-i)\theta(t'-t)\left\langle c^\dagger_{\vec{k}\sigma}(t')c_{\vec{k}\sigma}(t)\right\rangle\right\} \\
&= \left\{\delta(t-t')\left\langle c_{\vec{k}\sigma}(t)c^\dagger_{\vec{k}\sigma}(t')\right\rangle \mp \delta(t-t')\left\langle c^\dagger_{\vec{k}\sigma}(t')c_{\vec{k}\sigma}(t)\right\rangle\right\} + \varepsilon_{\vec{k}}G_{\vec{k}\sigma}(t,t') \\
&= \delta(t-t') + \varepsilon_{\vec{k}}G_{\vec{k}\sigma}(t-t')
\end{aligned}
$$

$$
\boxed{\left[i\tfrac{\partial}{\partial t} - \varepsilon_{\vec{k}}\right]G^{R/A}_{\vec{k}\sigma}(t-t') = \delta(t-t')} \tag{3.168}
$$

- Retarded, advanced, and t-ordered Green's functions have all the same equation of motion.
- The solutions for R,A, t-ordered functions are determined by the different boundary conditions for $t \to \pm\infty$.

- For the free system (H_0 is single-particle operator) the equation of motion, and hence the Green's function, coincide with the those familiar as the resolvent functions of a single-particle differential equation (or from electrodynamics). For many-particle systems our definition of G will give a generalization with decisive advantages.

Free Green's functions in frequency space:

In Fourier transforming wrt. time we have to observe the different boundary conditions for G^R, G^A, G:

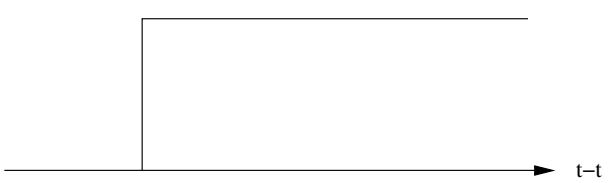


Figure 3.4:

$$\left[i\frac{\partial}{\partial t} - \varepsilon_{\vec{k}}\right] \underbrace{G^R_{\vec{k}\sigma}(t-t')}_{\sim\theta(t-t')} = \delta(t-t') \tag{3.169}$$

Now we multiply this equation by $\int_{-\infty}^{+\infty} dt\, e^{+i(\omega+i\eta)t}$. The infinitesimal factor $\eta > 0$ makes the integral converge for $t \to \infty$. The partial integration over the first factor on the left hand side $(\partial/\partial t)$ leads to ω.

- $$\begin{aligned}(\omega - \varepsilon_{\ k} + i\eta)G^R_{\vec{k}\sigma}(\omega) &= 1\\ \left[i\frac{\partial}{\partial t} - \varepsilon_{\vec{k}}\right] \underbrace{G^A_{\vec{k}\sigma}(t-t')}_{\sim\theta(t'-t)} &= \delta(t-t')\end{aligned}$$

  Again we multiply this equation by $\int_{-\infty}^{+\infty} dt\, e^{+i(\omega-i\eta)t}$ and for $\eta > 0$ this integral also converges for $t \to -\infty$.

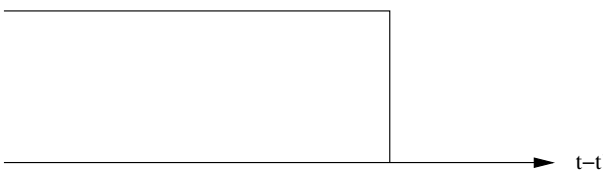


Figure 3.5:

- $[\omega - \varepsilon_{\vec{k}} - i\eta] G^R_{\vec{k}\sigma}(\omega) = 1$

- t-ordered Green's function:
  $\left[i\frac{\partial}{\partial t} - \varepsilon_{\vec{k}}\right] G_{\vec{k}\sigma}(t-t') = \delta(t-t')$

$$\left| \begin{cases} \int dt\, e^{+i(\omega+i\eta)t} & , |\vec{k}| > k_F \quad \left(\text{contribution: } c_{\vec{k}\sigma} c^\dagger_{\vec{k}\sigma}\right) \\ \int dt\, e^{+i(\omega-i\eta)t} & , |\vec{k}| \leq k_F \quad \left(\text{contribution: } c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma}\right) \end{cases} \right.$$

$$\begin{aligned} \left(i\frac{\partial}{\partial t} - \varepsilon_{\vec{k}} + i\eta\right) G_{\vec{k}\sigma}(\omega) &= 1, \qquad |\vec{k}| > k_F \\ \left(i\frac{\partial}{\partial t} - \varepsilon_{\vec{k}} - i\eta\right) G_{\vec{k}\sigma}(\omega) &= 1, \qquad |\vec{k}| \leq k_F \end{aligned}$$

$$\boxed{\begin{aligned} G^{R/A}_{\vec{k}\sigma}(\omega) &= \frac{1}{\omega - \varepsilon_{\vec{k}} \pm i\eta} \\ G_{\vec{k}\sigma}(\omega) &= \frac{\theta(|\vec{k}| - k_F)}{\omega - \varepsilon_{\vec{k}} + i\eta} + \frac{\theta(k_F - |\vec{k}|)}{\omega - \varepsilon_{\vec{k}} - i\eta} \\ &= \frac{1}{\omega - \varepsilon_{\vec{k}} + i\,\mathrm{sgn}(|\vec{k}| - k_F)\eta} \end{aligned}}$$

3.4.4 General form of the interacting Green's function: spectral representation and analytic properties

We now derive and analyze the general form of the Green's function in frequency space.
The ground states of a system of fermions (=Fermi sea) and of bosons (=bose condensate) with fixed, large particle number are fundamentally different, which implies that also the calculations are different. We will restrict ourselves to the case of fermions with spin 1/2 (electrons) from now on.

Fermi sea:
We consider an electron system in a large but finite volume $V = L^3$.

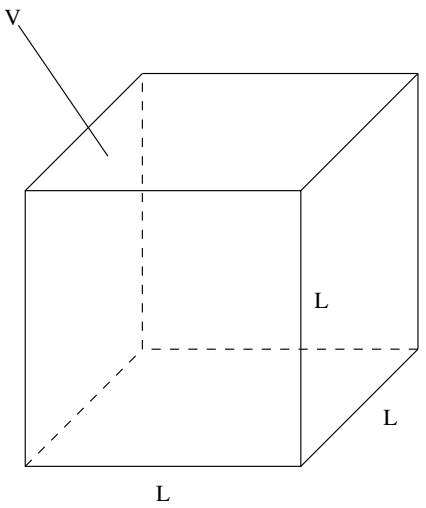


Figure 3.6:

The momentum eigenvalues of the free system are the n quantized:

$$\vec{p} = \hbar \frac{2\pi}{L} \left(n_x \widehat{e}_x + n_y \widehat{e}_y + n_z \widehat{e}_z \right), \qquad n_{x,y,z} = 0, \pm 1, \pm 2, \ldots \tag{3.170}$$

Each momentum eigenstate occupies a volume $\frac{(2\pi\hbar)^3}{V}$ in momentum space.
In the non-interacting ground state, these momentum eigenstates are doubly occupied up to a maximum energy, the Fermi energy E_F, defined such that the total number of *occupied* single-particle states $|\vec{p}, \sigma\rangle$ is equal to the total number of particles N. This antisymmetrized N-particle state is called *Fermi sea*.

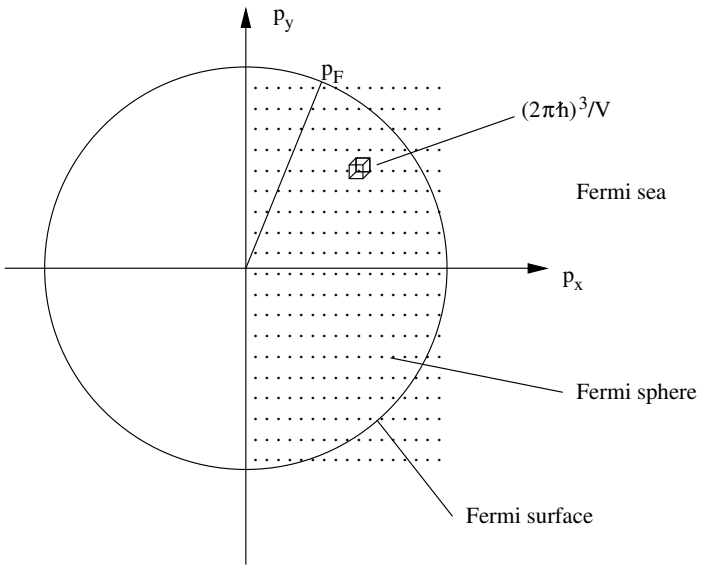


Figure 3.7:

$$|\phi_0\rangle = |n_{p\leq p_F} = 1, n_{p>p_F} = 0\rangle \tag{3.171}$$

The modulus of the maximum momentum of an occupied single-particle state is called Fermi momentum:

$$E_F = \frac{p_F^2}{2m} \tag{3.172}$$

Since the $\vec{p}$ are quantized, all momentum sums can be considered discrete wherever necessary to avoid singular integrals. The limit $V \to \infty$ can be taken at the end of the calculation.

General time dependence and spectral representation of G:

We consider a general, interacting many-body Hamiltonian $H = H_0 + V$:
To make the time dependence explicit, we wrote the Heisenberg operators as

$$\psi(\vec{r}, t) = e^{iHt}\psi(\vec{r})e^{-iHt} \tag{3.173}$$

$$\psi^\dagger(\vec{r}, t) = e^{iHt}\psi^\dagger(\vec{r})e^{-iHt} \tag{3.174}$$

where $\psi(\vec{r}), \psi^\dagger(\vec{r})$ are the field operators in the Schrödinger picture.

We then have (spin index suppressed):

$\underline{t > t'}$:

$$G(\vec{r} - \vec{r}', t - t') = -i \sum_m \left\langle \phi_0 \left| e^{iHt}\psi(\vec{r})e^{-iHt} \right| \phi_m \right\rangle \times \left\langle \phi_m \left| e^{iHt'}\psi^\dagger(\vec{r})e^{-iHt'} \right| \phi_0 \right\rangle \tag{3.175}$$

$$= -i \sum_m \langle \phi_0 | \psi(\vec{r}) | \phi_m \rangle \left\langle \phi_m \left| \psi^\dagger(\vec{r}') \right| \phi_0 \right\rangle \times e^{-i(E_m - E_0)(t' - t)} \tag{3.176}$$

$|\phi_m\rangle \langle\phi_m| = \mathbb{1}$ is the free (N+1)-particle basis (eigenstates of H).

$\underline{t < t'}$:

$$G(\vec{r} - \vec{r}', t - t') = +i \sum_{m'} \left\langle \phi_0 \left| \psi^\dagger(\vec{r}') \right| \phi_{m'} \right\rangle \langle \phi_{m'} | \psi(\vec{r}) | \phi_0 \rangle \, e^{-i(E_m - E_0)(t' - t)}, \tag{3.177}$$

where we have inserted a complete basis of H eigenstates of the (N+1)-particle system $\sum_m |\phi_m\rangle \langle\phi_m|$ and of the (N-1)-particle system $\sum_{m'} |\phi_{m'}\rangle \langle\phi_{m'}|$ respectively.
m, m' runs over all possible states of the many-body system.

$$m: \quad (N+1) - \text{particle system} \tag{3.178}$$

$$m': \quad N - \text{particle system} \tag{3.179}$$

Position dependence of the matrix elements:
The operators and matrix elements in G have the following position dependence:

$$\psi_\sigma(\vec{r}) = e^{-i\vec{p}\vec{r}}\psi(0)e^{i\vec{p}\vec{r}} \tag{3.180}$$

since $\exp(-i\vec{p}\vec{r})$ is the spatial translation operator, and

$$\langle\phi_0 |\psi(\vec{r})| \phi_m\rangle = \langle\phi_0 |\psi(0)| \phi_m\rangle \, e^{+i(\vec{p}_m - \vec{p}_0)\vec{r}} \tag{3.181}$$

with $\vec{p}_0 = 0$ (total momentum of the exact N-particle ground state for a translationally invariant system), $\vec{p}_m$ (total momentum of the (N+1)-particle eigenstate $|\phi_m\rangle$ of H for a translationally invariant system) etc.
Hence, the Green's function has the $\vec{r}$ and t dependence:

$$G(\vec{r} - \vec{r}', t - t') = \begin{cases} -i \sum_m |\langle\phi_0 |\psi(0)| \phi_m\rangle|^2 \, e^{i\vec{p}_m(\vec{r}-\vec{r}')} e^{-i(E_m - E_0)(t-t')} \\ \\ +i \sum_{m'} |\langle\phi_{m'} |\psi(0)| \phi_0\rangle|^2 \, e^{-i\vec{p}_{m'}(\vec{r}-\vec{r}')} e^{i(E_{m'} - E_0)(t-t')} \end{cases} \tag{3.182}$$

The upper equations is valid if $t > t'$ and the lower one if $t < t'$.

Fourier transformation:

$$\int d^3(\vec{r} - \vec{r}') \, e^{-i\vec{p}(\vec{r}-\vec{r}')} \tag{3.183}$$

$$\int d(t - t') \, e^{+i\omega(t-t')} \tag{3.184}$$

For convergence of the t-integral:

$$\omega \rightarrow \omega + i\eta, \qquad (t - t') > 0 \tag{3.185}$$

$$\omega \rightarrow \omega - i\eta, \qquad (t - t') < 0 \tag{3.186}$$

The Fourier transform of $G(\vec{r}-\vec{r}',t-t')$ with respect to $\vec{r}-\vec{r}',t-t'$ is:

$$G_{\vec{p}}(\omega) = (-i)\sum_m |\langle\phi_0|\psi(0)|\phi_m\rangle|^2 (2\pi)^3\delta^{(3)}(\vec{p}-\vec{p}_m) \tag{3.187}$$
$$\times\frac{1}{(-i)}\frac{1}{\omega-(E_m-E_0)+i\eta}$$
$$+i\sum_{m'} |\langle\phi_{m'}|\psi(0)|\phi_0\rangle|^2 (2\pi)^3\delta^{(3)}(\vec{p}+\vec{p}_m) \tag{3.188}$$
$$\times\frac{1}{i}\frac{1}{\omega-(E_{m'}-E_0)-i\eta}$$

It is convenient to write the energy differences $E_m-E_0, E_{m'}-E_0$ in terms of the excitation energies of the N-particle system.
E_0 is the ground state energy of the N-particle system. $E_m, E_{m'}, E_0$ are the total energies of an (excited) (N+1)-, (N-1)-particle state, respectively.

We define the Fermi energy of the *interacting* system generalizing the non-interacting case , as

$$E_F = E_0(N+1)-E_0(N) \approx \frac{dE_0(N)}{dN} = \mu \tag{3.189}$$

i.e., as the change of the *ground* state energy E_0, as *one* particle is added to the system. E_F is also called "chemical potential" μ (at $T=0$).

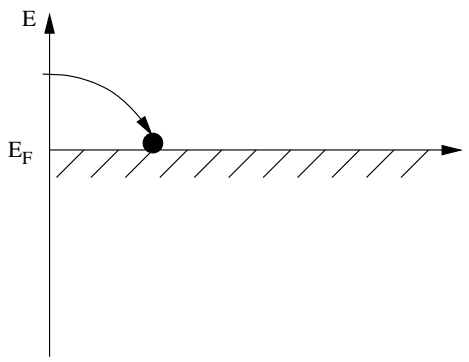


Figure 3.8:

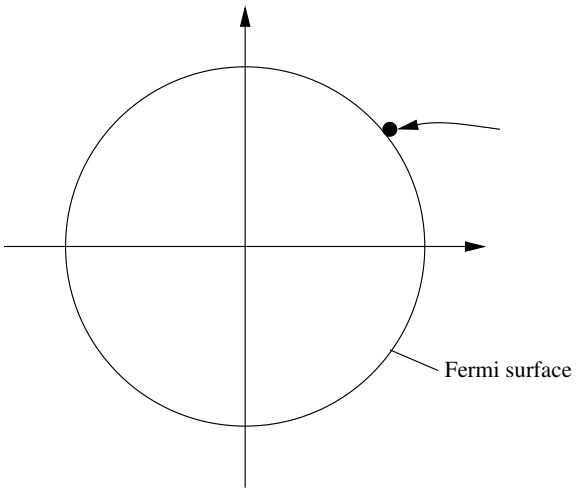


Figure 3.9:

The energy differences $E_m(N+1)-E_0(N)$ and $E_{m'}(N-1)-E_0(N)$ have the character of a single-particle excitation energy, since one particle is added/substracted. It is convenient to measure these differences relative to E_F:

$$E_m(N+1) - E_0(N) = \varepsilon_m + E_F, \qquad \varepsilon_m = E_m(N+1) - E_0(N+1), \quad (3.190)$$

where $\varepsilon_m > 0$ is by definition, the *excitation* energy of the (N+1)-particle system in state m.
For $N \gg 1$ one has

$$E_F = E_0(N+1) - E_0(N) = E_0(N) - E_0(N-1) + \mathcal{O}\left(\frac{1}{N}\right) \quad (3.191)$$

and

$$E_{m'}(N-1) - E_0(N) = \varepsilon_{m'} - E_F, \qquad \varepsilon_{m'} = E_{m'}(N-1) - E_0(N-1) \quad (3.192)$$

with $\varepsilon_{m'} > 0$ the excitation energy of the (N-1)-particle system in state m'.
For $N \gg 1$, the (N+1) and the (N-1)-particle system have the same excitation energies:

$$\varepsilon_{m'} \approx \varepsilon_m, \qquad E_F \approx E'_F \quad (3.193)$$

(**Remark:** even/odd effects in mesoscopic systems with interaction.)

The Green's function then takes the form:

$$G_{\vec{p}}(\omega) = \sum_m |\langle\phi_0 |\psi(0)| \phi_m\rangle|^2 (2\pi)^3 \delta^{(3)}(\vec{p}-\vec{p}_m) \frac{1}{\omega - \varepsilon_m - E_F + i\eta} \quad (3.194)$$

$$+ \sum_{m'} |\langle\phi_{m'} |\psi(0)| \phi_0\rangle|^2 (2\pi)^3 \delta^{(3)}(\vec{p}-\vec{p}_{m'}) \quad (3.195)$$

$$\times \frac{1}{\omega + \varepsilon_{m'} - E_F - i\eta},$$

where $\varepsilon_m > 0, \varepsilon_{m'} > 0$ by definition.

It is convenient to write the sums over the eigenstates $\sum_m, \sum_{m'}$ as a sum over all eigenstates with energie in the interval $[E, E+dE]$ and integrate over $E \geq 0$:

$$\sum_m (\ldots) = \int dE \sum_{\substack{m \\ E \leq \varepsilon_m < E+dE}} (\ldots) \quad (3.196)$$

With the definitions

$$A(\vec{p}, E)dE = (2\pi)^3 \sum_{\substack{m \\ E \leq \varepsilon_m < E+dE}} |\langle\phi_0 |\psi(0)| \phi_m\rangle|^2 \delta^{(3)}(\vec{p}-\vec{p}_m) \quad (3.197)$$

$$B(\vec{p}, E)dE = (2\pi)^3 \sum_{\substack{m' \\ E \leq \varepsilon_{m'} < E+dE}} |\langle\phi_{m'} |\psi(0)| \phi_0\rangle|^2 \delta^{(3)}(\vec{p}-\vec{p}_{m'}) \quad (3.198)$$

we have

$$\boxed{G_{\vec{p}}(\omega) = \int_0^\infty dE \left[\frac{\widetilde{A}(\vec{p},E)}{\omega - E - E_F + i\eta} + \frac{\widetilde{B}(\vec{p},E)}{\omega + E - E_F - i\eta}\right]} \quad (3.199)$$

Lehmann representation

$$\mathrm{Re}\, G_{\vec{p}}(\omega) = \mathcal{P} \int_0^\infty dE \left[\frac{\widetilde{A}(\vec{p}, E)}{\omega - E - E_F} + \frac{\widetilde{B}(\vec{p}, E)}{\omega + E - E_F}\right] \quad (3.200)$$

$$\mathrm{Im}\, G_{\vec{p}}(\omega) = \begin{cases} -\Pi \widetilde{A}(\vec{p}, \omega - E_F), & \omega > E_F \\ +\Pi \widetilde{B}(\vec{p}, -\omega + E_F), & \omega < E_F \end{cases} \quad (3.201)$$

$$\widetilde{A}(\vec{p},\omega - E_F) = \text{probability density for crating a particle with momentum } \vec{p}\text{, energy } \omega \textit{ above } E_F \text{ from the ground state.} \quad (3.202)$$

$$\widetilde{B}(\vec{p},-\omega + E_F) = \text{probability density for destroying a particle with momentum } \vec{p}\text{, energy } \omega \textit{ below } E_F \text{ from the ground state.} \quad (3.203)$$

$$\rightarrow \left|\left| \begin{array}{l} A(\vec{p},\omega) := \widetilde{A}(\vec{p},\omega - E_F) + \widetilde{B}(\vec{p},-\omega + E_F) \\ \text{spectral function} \end{array} \right.$$

(3.110), (3.111)⇒

$$\mathrm{Re}\, G_{\vec{p}}(\omega) = \mathcal{P}\int \frac{d\omega'}{\pi} \frac{\mathrm{Im}\, G_{\vec{p}}(\omega)\mathrm{sgn}\,(\omega' - E_F)}{\omega' - \omega} \quad (3.204)$$

Kramers-Kroenig violated → $G_{\vec{p}}(\omega)$ not analytic in upper or lower half plane.

$$\boxed{A(\vec{p},\omega) = \begin{cases} \widetilde{A}(\vec{p},\omega - E_F), & \omega > E_F \\ \widetilde{B}(\vec{p},-(\omega - E_F)), & \omega < E_F \end{cases}} \quad (3.205)$$

Spectral function with $A \geq 0$ everywhere.

Using (3.110) and (3.111) we obtain:

$$\mathrm{Re}\, G_{\vec{p}}(\omega) = \mathcal{P}\int_{-\infty}^{+\infty} \frac{d\omega'}{\pi} \frac{\mathrm{Im}\, G_{\vec{p}}(\omega)\mathrm{sgn}\,(\omega' - E_F)}{\omega' - \omega} \quad (3.206)$$

Kramers-Kroening relation is violated, i.e. the time-ordered Green's function is neither analytic in the upper nor in the lower complex half plane.
For the retarded and advanced Green's functions we obtain in a similar way:

$$\boxed{\begin{aligned} G^{R/A}_{\vec{p}}(\omega) &= \int_0^\infty dE \left[\frac{\widetilde{A}(\vec{p},E)}{\omega - E - E_F \pm i\eta} + \frac{\widetilde{B}(\vec{p},E)}{\omega + E - E_F \pm i\eta} \right] \\ &= \int_{-\infty}^{+\infty} dE \frac{A(\vec{p},E)}{\omega - E - E_F \pm i\eta} \end{aligned}} \quad (3.207)$$

Spectral representation

It follows that

$$\mathrm{Im}\, G^{R/A}_{\vec{p}}(\omega) = \mp\pi A(\vec{p},\omega - E_F) \quad (3.208)$$

and $G^{R/A}_{\vec{p}}(\omega)$ are analytic in the upper/lower complex half plane. This is - by construction - in accord to the causality/anticausality of $G^{R/A}$.

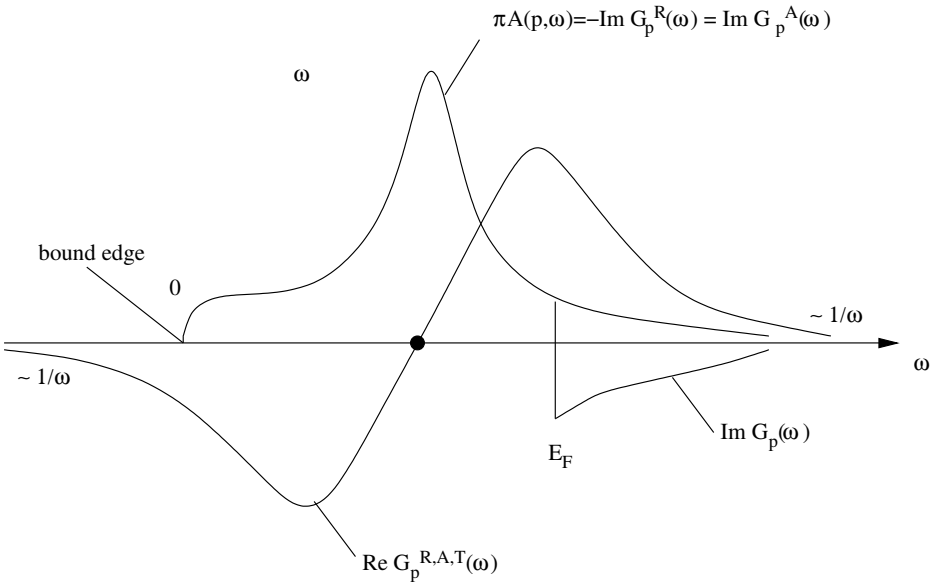


Figure 3.10:

Relevant variable: energy wrt. $E_F : \widetilde{\omega} = \omega - E_F \to \omega$

$$G^A_{\vec{p}} = G^R_{\vec{p}}(\omega)^* \tag{3.209}$$

Relevance of $G^{R/A}$ and of G:

$G^{R/A}$ have the proper analytic and, therefore, causal behavior. However, as we shall see, $G^{R/A}$ are not suitable for constructing perturbation theory (PT).
The time-ordered Green's function allows to contruct PT in a systematical way and, in addition, contains the information about the Fermi energy because of its sign change in $\mathrm{Im}\, G_{\vec{p}}(\omega)$.

Strategy for calculating physical quantities:

1. Calculate $G_{\vec{p}}(\omega)$ using, e.g., PT.

2. Take $|\mathrm{Im}\, G_{\vec{p}}(\omega)| = \pi A(\vec{p},\omega) = \mp \mathrm{Im}\, G^{R/A}_{\vec{p}}(\omega)$.

3. Calculate the full $G^{R/A}$ using Kramers-Kroenig

3.4.5 The physical relevance of the poles of $G^{R/A}_{\vec{p}}(z)$ and of $\mathbf{Im}\, G^{R/A}_{\vec{p}}(\omega)$

$$\begin{aligned} \operatorname{Im} G^{R/A}_{\vec{p}}(\omega) &= \pi A(\vec{p},\omega) \qquad (3.210)\\ &= \text{spectral density} \\ &= \text{density of excitations of the system with energy } \omega \\ &\quad \text{above/below } E_F \text{ and momentum } \vec{p} \\ -\sum_{\vec{p}} \operatorname{Im} G^{R}_{\vec{p}}(\omega) &= N(\omega) \qquad (3.211)\\ &= \text{density of states at energy } \omega \end{aligned}$$

The poles of $G^{R/A}_{\vec{p}}(\omega)$:
The analyticity of $G^{R/A}_{\vec{p}}(z)$ can be expressed by defining another function $\Sigma^{R/A}_{\vec{p}}(z)$ as

$$G^{R/A}_{\vec{p}}(z) = \frac{1}{z + E_F - \varepsilon_{\vec{p}} - \Sigma^{R/A}_{\vec{p}}(z)} \qquad (3.212)$$

with $\varepsilon_{\vec{p}}$ =single-particle eigenenergies of the free system. $\Sigma^{R/A}_{\vec{p}}(z)$ is analytic in the upper/lower half plane and $\operatorname{Im}^{R/A}_{\vec{p}}(\omega) \gtrless^{R}_{A} 0$ on the real axis.

$$\boxed{\Sigma^{R/A}_{\vec{p}} \text{ is called selfenergy}} \qquad (3.213)$$

$G^{R/A}_{\vec{p}}(z)$ has a pole at z_0:

$$z_0 = \varepsilon_{\vec{p}} - E_F + \Sigma^{R/A}_{\vec{p}}(z_0) \qquad (3.214)$$

(which is a nonlinear equation for z_0 via $\Sigma^{R/A}_{\vec{p}}(z_0)$)

Usually this equation has exactly one solution. The physical reason for this will become clear below.
By construction, for the non-interacting system $\Sigma^{R/A}_{\vec{p}}(z) = 0$.
If the interactions are not too strong, then

$$z_0(\vec{p}) \approx \varepsilon_{\vec{p}} - E_F + \Sigma^{R/A}_{\vec{p}}(\varepsilon_{\vec{p}} - E_F). \qquad (3.215)$$

The physical meaning of z_0 becomes evident by Fourier transforming to time space:

$$G^{R/A}_{\vec{p}}(z) = \frac{1}{z + E_F - \varepsilon_{\vec{p}} - \Sigma^{R/A}_{\vec{p}}(z)} \tag{3.216}$$

$$\stackrel{(*)}{=} \frac{\left(1 - \frac{\partial\Sigma}{\partial z}\big|_{z_0}\right)^{-1}}{z - z_0} \tag{3.217}$$

$$(*) \qquad \Sigma_{\vec{p}}(z) \cong \Sigma_{\vec{p}}(z_0) + \left.\frac{\partial\Sigma}{\partial z}\right|_{z_0}(z - z_0) + \ldots \tag{3.218}$$

$$\text{with} \quad z_0 \approx \left(\varepsilon_{\vec{p}} + \operatorname{Re}\Sigma^{R/A}_{\vec{p}}(\varepsilon_{\vec{p}} - E_F) - E_F\right) + i\operatorname{Im}\Sigma^{R/A}_{\vec{p}}(\varepsilon_{\vec{p}}) \tag{3.219}$$

$$G^R_{\vec{p}}(t) = -i\theta(t)\left\langle\left[c_{\vec{p}}(t), c^\dagger_{\vec{p}}(0)\right]_+\right\rangle \tag{3.220}$$

$$= \int\frac{d\omega}{2\pi}e^{-i\omega t}\frac{\left(1 - \frac{\partial\Sigma}{\partial z}\big|_{z_0}\right)^{-1}}{z - z_0} \tag{3.221}$$

$$= \theta(t)\left(1 - \left.\frac{\partial\Sigma}{\partial z}\right|_{z_0}\right)^{-1} e^{-iz_0} \tag{3.222}$$

Physical interpretation of the Green's function and its parameters:

The retarded Green's function

$$G^R_{\vec{p}\sigma}(t) = -i\theta(t)\left\langle\phi_0\left|\left[c_{\vec{p}\sigma}(t), c^\dagger_{\vec{p}\sigma}(0)\right]_+\right|\phi_0\right\rangle \tag{3.223}$$

$$= \theta(t)\left(1 - \left.\frac{\partial\Sigma}{\partial z}\right|_{z=z_0}\right)^{-1}\begin{cases}\exp(-i(\varepsilon_{\vec{p}} + \operatorname{Re}\Sigma^R_{\vec{p}}(\varepsilon_{\vec{p}} - E_F) - E_F)t)\\ \exp(-(-\operatorname{Im}\Sigma^R_{\vec{p}}(\varepsilon_{\vec{p}} - E_F))t)\end{cases}$$

is

- the *amplitude* for creating a particle with momentum$\vec{p}$ and spin σ at time $t' = 0$ in the many-body ground state $|\phi_0\rangle$ and destroying it at a later time $t > 0$;
  plus
- the *amplitude* for destroying a particle with momentum $\vec{p}$ and spin σ at time $t > 0$ and creating it again at an earlier time $t' = 0$.

Thus, $G^R_{\vec{p}\sigma}(t)$ describes the propagation of a particle $(\vec{p}, \sigma)$ from $t' = 0$ to $t > 0$ (in the ground state) and the propagation of a hole (in the Fermi sea, or antiparticle) with $(-\vec{p}, -\sigma)$ backward in time from $t > 0$ to $t' = 0$.

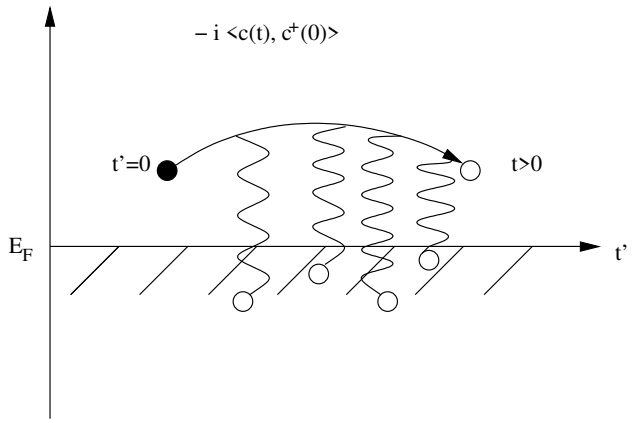


Figure 3.11:

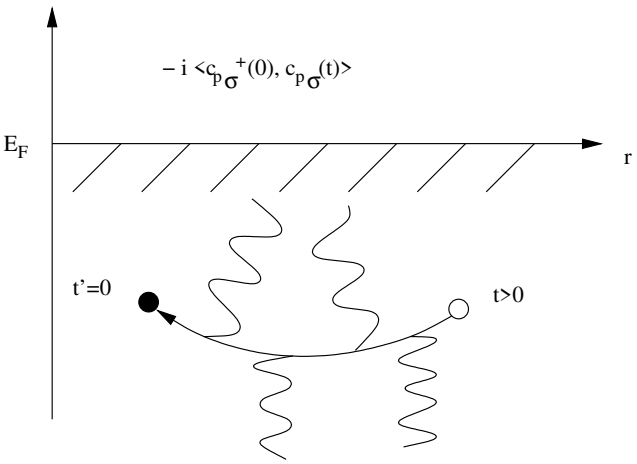


Figure 3.12:

Because of this interpretation, the Green's function is also called (retarded, advanced, time-ordered) *propagator*.

Quasiparticles:
Since for an interacting system the many-body state $c^\dagger_{\vec{p}\sigma}(0)|\phi_0\rangle$ is not an eigenstate of the Hamiltonian, it decays in time, as also seen from the time-dependence

of $G^R_{\vec{p}\sigma}(t)$. The corresponding single-particle excitation of the ground state does, therefore, not correspond to a real particle (which would have infinite life time) and is, hence, called *quasiparticle*. In analogy, the state $c_{\vec{p}\sigma}(t)|\phi_0\rangle$ corresponds to a *quasihole*.
From the time dependence of $G^R_{\vec{p}\sigma}(t)$ we can identify the parameters:

- *Quasiparticle energy* (measured relative to E_F)

$$\widetilde{\varepsilon}_{\vec{p}\sigma} = \varepsilon_{\vec{p}} + \mathrm{Re}\,\Sigma_{\vec{p}\sigma}(\varepsilon_{\vec{p}} - E_F) - E_F \tag{3.224}$$

- *Quasiparticle decay rate*

$$\frac{1}{\tau} = -2\,\mathrm{Im}\,\Sigma_{\vec{p}\sigma}(\varepsilon_{\vec{p}} - E_F) \tag{3.225}$$

  (The factor 2 comes from the fact that G^R is an amplitude and $\frac{1}{\tau}$ is defined for the probability $|G^R|$.)

- *Quasiparticle weight*

$$\left(1 - \left.\frac{\partial\Sigma}{\partial z}\right|_{z=z_0}\right)^{-1} \approx \left(1 - \left.\frac{\partial \mathrm{Re}\,\Sigma}{\partial\omega}\right|_{\omega=\widetilde{\varepsilon}_{\vec{p}}}\right)^{-1} \tag{3.226}$$

  For particle propagation $\left\langle c_{\vec{p}\sigma}(t)c^\dagger_{\vec{p}\sigma}(0)\right\rangle$: $\quad \widetilde{\varepsilon}_{\vec{p}\sigma} > 0$ (3.227)

  For hole propagation $\quad \left\langle c^\dagger_{\vec{p}\sigma}(0)c_{\vec{p}\sigma}(t)\right\rangle$: $\quad \widetilde{\varepsilon}_{\vec{p}\sigma} < 0$ (3.228)

In a relativistic theory a hole (in the Fermi sea) corresponds to an antiparticle (in the Dirac sea) and the propagation backward in time of holes/antiparticles is automatically built into the retarded Green's function.
From the quasiparticle interpretation of $c^\dagger_{\vec{p}\sigma}|\phi_0\rangle$ it is clear that for a "well-behaved" system $G^R_{\vec{p}\sigma}(z)$ should have exactly one pole in the lower half plane for each $(\vec{p},\sigma)$. Exceptions from this rule are possible if the particle-particle interaction is sufficiently singular.

3.4.6 Perturbation theory for G: Wick's theorem, Feynman diagrams, linked cluster theorem

Time dependent perturbation theory for many-body states

In the interaction picture we had in section 3.4.1:

$$
\begin{aligned}
H &= H_0 + V \qquad \text{many-body Hamiltonian} && (3.229)\\
H_0 &= \sum_{\vec{p}\sigma} \varepsilon_{\vec{p}} c^\dagger_{\vec{p}\sigma} c_{\vec{p}\sigma} \qquad \text{single-particle operator} && (3.230)\\
V &= \frac{1}{2}\int \frac{d^3p}{(2\pi)^3}\int \frac{d^3p'}{(2\pi)^3}\int \frac{d^3q}{(2\pi)^3} V(q) c^\dagger_{\vec{p}+\vec{q},\sigma} c^\dagger_{\vec{p}'-\vec{q},\sigma'} c_{\vec{p}'\sigma'} c_{\vec{p}\sigma} && (3.231)\\
&= \frac{1}{2}\int d^3x \int d^3x'\, \psi^\dagger_\sigma(x)\psi^\dagger_{\sigma'}(x') V(x-x')\psi_{\sigma'}(x')\psi_\sigma(x) && (3.232)\\
&\quad \text{two-particle interaction} && (3.233)\\
i\frac{d}{dt}|\phi\rangle_I &= V_I(t)|\phi\rangle_I \qquad \text{state} && (3.234)\\
i\frac{d}{dt}A_I(t) &= [A_I(t), H_0] && (3.235)\\
A_I(t) &= e^{iH_0t} A(0) e^{-iH_0t} \qquad \text{operator, known} && (3.236)
\end{aligned}
$$

Since $[V_I(t), V_I(t')] \neq 0$, formal solution for $|\phi\rangle$:

$$
|\phi(t)\rangle_I = \langle\phi(t_0)\rangle_I - i\int_{t_0}^{t} V_I(t')\,|\phi(t')\rangle\, dt' \tag{3.237}
$$

We now assume that the interaction is switched on adiabatically from $t \to -\infty$ and switched off adiabatically for $t \to +\infty$:

$$
V_I(t) \underset{t\to\pm\infty}{\longrightarrow} 0 \tag{3.238}
$$

Adiabatically means that this t-dependence is slower than any of the intrinsic time scales of the system, i.e. can be neglected for solving the system. For $t \to \pm\infty$ $|\phi(\pm\infty)\rangle_I$ is then known and is an eigenstate of the free system H_0 (e.g. free Fermi sea).
Thus, we have by iteration:

$$
\begin{aligned}
|\phi(t)\rangle_I &= \underbrace{|\phi(-\infty)\rangle_I}_{=|\phi\rangle_{H_0}} - i\int_{-\infty}^{t} dt'\, V_I(t')|\phi(t')\rangle_I && (3.239)\\
&= |\phi(-\infty)\rangle - i\int_{-\infty}^{t} dt'\, V_I(t')|\phi(-\infty)\rangle && (3.240)\\
&\quad +(-i)^2\int_{-\infty}^{t} dt' \int_{-\infty}^{t'} dt''\, V_I(t')V_I(t'')|\phi(-\infty)\rangle \qquad \text{(subscript } I \text{ dropped)}\\
&\overset{(*)}{=} \widehat{T}\left\{\exp\left(-i\int_{-\infty}^{t} dt'\, V_I(t')\right)\right\}|\phi(-\infty)\rangle && (3.241)
\end{aligned}
$$

$$\boxed{S(t_2,t_1)=\widehat{T}\left\{\exp\left(-i\int_{t_1}^{t_2}dtV_I(t')\right)\right\}} \tag{3.242}$$

Time evolution operator in interacting picture. Generally $V(x,x')$ can depend on two times.

$(*)$ Rewriting successive time-integrals as a time-ordered product:

$$\widehat{T}\int_{-\infty}^{t}dt'\int_{-\infty}^{t}dt''\,V_I(t')V_I(t'') \tag{3.243}$$

$$=\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}dt''\,V_I(t')V_I(t'')\underset{\substack{\downarrow\\(**)}}{+}\int_{-\infty}^{t}dt'\int_{t'}^{t}dt''\,V_I(t'')V_I(t') \tag{3.244}$$

$$=\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}dt''\,V_I(t')V_I(t'')+\underbrace{\int_{-\infty}^{t}dt''\int_{t''}^{t}dt'\,V_I(t')V_I(t'')}_{t'\leftrightarrow t} \tag{3.245}$$

$$=2\int_{-\infty}^{t}dt'\int_{-\infty}^{t'}dt''\,V_I(t')V_I(t'') \tag{3.246}$$

$(**)$ V contains even number of operators so that the "+" is valid for bosons *and* fermions.

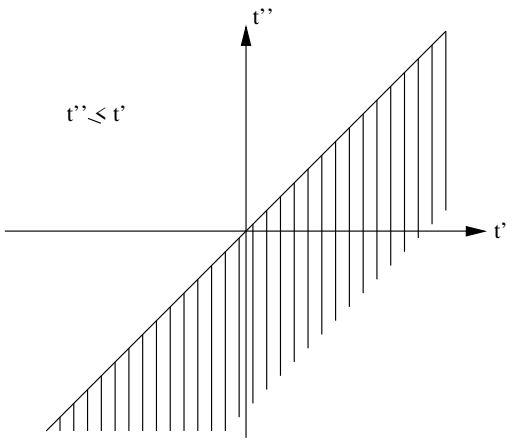


Figure 3.13:

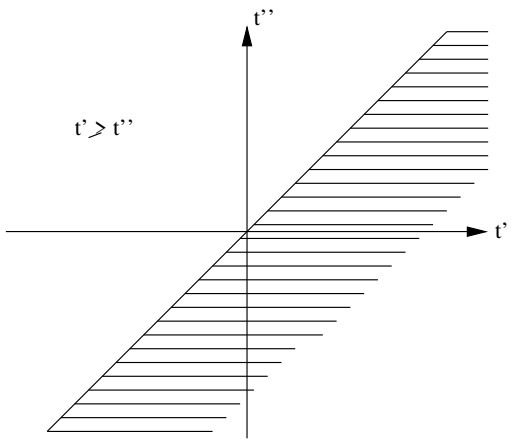


Figure 3.14:

Same integration area and same integrand for both integrals.

For an $k!$-fold time-ordered product one obtains $k!$ equal successive integrals according to the $k!$ orderings of the $V_I(t_j)'$s:

$$\widehat{T}\int_{-\infty}^{t} dt_1 \int_{-\infty}^{t} dt_2 \ldots \int_{-\infty}^{t} dt_k\, V_I(t_1)\ldots V_I(t_k) = \tag{3.247}$$
$$k!\int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} \ldots \int_{-\infty}^{t_{k-1}} dt_k\, V_I(t_1)\ldots V_I(t_k)$$

This proves the equality $(*)$.

$S(t_2,t_1)$ hast the multiplication property, by definition:

$$\boxed{\begin{array}{ll} S(t_2,t_3)S(t_3,t_1) = S(t_2,t_1) & \\ S(t,t) = 1 & \\ [S(t_2,t_3)]^{-1} = S(t_3,t_2) = S^{\dagger}(t_2,t_3) & \text{unitary} \end{array}} \tag{3.248}$$

To calculate the Green's function, we need to evaluate expectation values of the form

$$_H\langle\phi_0|TA_H(t_1)B_H(t_2)C_H(t_3)\ldots|\phi_0\rangle_H \tag{3.249}$$

in the Heisenberg picture. It is useful to write this in the interaction picture, where the t-dependence of the operators is known. S establishes the connection between the Heisenberg and the interaction picture:

$$|\phi(t)\rangle_I = S(t,-\infty)|\phi\rangle_H \tag{3.250}$$

From the expectation value

$$
\begin{aligned}
{}_H\langle\phi|A_H(t)|\phi\rangle_H &= {}_H\langle\phi(t)|A_I(t)|\phi(t)\rangle_I && (3.251)\\
&= \langle\phi_H|[S(t,-\infty)]^{-1}A_I(t)S(t,-\infty)|\phi_H\rangle && (3.252)
\end{aligned}
$$

it follows

$$
A_H(t) = [S(t,-\infty)]^{-1}A_I(t)S(t,-\infty). \tag{3.253}
$$

Connection between Heisenberg and interaction picture operators.

Thus we have

$$
\begin{aligned}
& {}_H\langle\phi_0|T\{A_H(t_1)B_H(t_2)\ldots\}|\phi_0\rangle_H && (3.254)\\
= \quad & {}_H\langle\phi_0|T\{\underbrace{S^{-1}(t_1,-\infty)}_{(1)}A(t_1)\underbrace{S(t_1,-\infty)\underbrace{S^{-1}(t_2,-\infty)}_{S(-\infty,t_2)}}_{S(t_1,t_2)}B(t_2) && (3.255)\\
& \times S(t_2,-\infty)\ldots\}|\phi_0\rangle_H\\
= \quad & {}_H\langle\phi_0|T\{S^{-1}(\infty,-\infty)S(\infty,t_1)A(t_1)S(t_1,t_2)B(t_2) && (3.256)\\
& \times S(t_2,-\infty)\ldots\}|\phi_0\rangle_H\\
= \quad & {}_H\langle\phi_0|S^{-1}(\infty,-\infty)\widehat{T}\{A(t_1)B(t_2)\ldots S(\infty,-\infty)\}|\phi_0\rangle_H, && (3.257)
\end{aligned}
$$

where the time ordering operator $\widehat{T}$ puts the appropriate factors of $S(\infty,-\infty)$ in between the $A, B, \ldots$.

$$
\begin{aligned}
(1) \qquad S^{-1}(t_1,-\infty) &= S(-\infty,t_1) = S(-\infty,\infty)S(\infty,t_1) && (3.258)\\
&= S^{-1}(\infty,-\infty)S(\infty,t_1) && (3.259)
\end{aligned}
$$

$$
{}_H\langle\phi_0|S^{-1}(\infty,-\infty) = [S(\infty,-\infty)|\phi_0\rangle_H]^\dagger \tag{3.260}
$$

The state $S(\infty,-\infty)|\phi_0\rangle_H$ is the free ground state at $t=-\infty$ evolved to $t=+\infty$. Since the interaction is adiabatically switched on and off, this must be again the ground state, i.e. it can differ from $|\phi_0\rangle_H$ only ba a phase factor,

$$
S(\infty,-\infty)|\phi_0\rangle_H = e^{i\alpha}|\phi_0\rangle_H, \tag{3.261}
$$

where

$$
e^{i\alpha} = \quad {}_H\langle\phi_0|S(\infty,-\infty)|\phi_0\rangle_H. \tag{3.262}
$$

Therefore

$$ {}_H\langle\phi_0|\widehat{T}\{A_H(t_1)B_H(t_2)\ldots\}|\phi_0\rangle_H = \frac{{}_H\langle\phi_0|\widehat{T}\{A(t_1)B(t_2)\ldots S(\infty,-\infty)\}|\phi_0\rangle_H}{{}_H\langle\phi_0|S(\infty,-\infty)|\phi_0\rangle_H}, \tag{3.263} $$

where $|\phi_0\rangle_H$ is the (Heisenberg) ground state of the free system, and $A(t_1), B(t_2), \ldots$ are operators in the interaction picture, whose t-dependence is known.
In particular, the t-ordered G function is:

$$ \boxed{G(x,x') = -i\frac{{}_H\langle\phi_0|\widehat{T}\{\psi(\vec{r},t)\psi^\dagger(\vec{r}',t')S(\infty,-\infty)\}|\phi_0\rangle_H}{{}_H\langle\phi_0|S(\infty,-\infty)|\phi_0\rangle_H}} \tag{3.264} $$

- It is clear that the t-ordering is essential for obtaining this formula.
- The phase factor in the denominator will be important.

A perturbation series is generated in a natural way by expanding S in powers of the interaction V. This generates expectation values of products of more and more field operators $\psi, \psi^\dagger$. These high-order expectation values can be factorized into products of free single-particle Green's functions by means of the *Wick theorem*.

Wick's theorem

Let $\psi(\vec{r},t) = \exp(+iH_0t)\,\psi(\vec{r})\exp(-iH_0t)$ be field operators in the interaction picture (or free Heisenberg operators), which have canonical equal-time (anti-) commutation relations,

$$ \left[\psi(\vec{r},t), \psi^\dagger(\vec{r}',t)\right] = \delta^{(3)}(\vec{r}-\vec{r}') \tag{3.265} $$

(general: $\mathcal{C}$-number)

The *free* N-particle Green's function can be written as

$$
\begin{aligned}
& G^{(N),(0)}(x_1,\ldots,X_N;x'_1,\ldots,x'_N) && (3.266)\\
\equiv\ & (-i)^N \quad {}_H\langle\phi_0|T\left\{\psi(x_1)\ldots\psi(x_N)\psi^\dagger(x_1)\ldots\psi^\dagger(x_N)\right\}|\phi_0\rangle_H && (3.267)\\
=\ & (-i)^N \sum_{\substack{\text{permutations}\\ P(x'_1\ldots x'_N)}} (\pm 1)^{\widetilde{P}} G^{(0)}(x_1,x'_{P(1)})G^{(0)}(x_2,x'_{P(2)})\ldots && (3.268)\\
& \times G^{(0)}(x_N,x'_{P(N)})
\end{aligned}
$$

"+" for bosons and "-" for fermions. $\widetilde{P}$ is the number of commutations to bring the N pairs of operators next to each other in the order $\psi(x_1)\psi^\dagger(x'_{P(1)})$.

Example:

$$
G^{(z),(0)}(x_1,x_2;x'_1,x'_2) = \left[G^{(0)}(x_1,x'_1)G^{(0)}(x_2,x'_2) - G^{(0)}(x_1,x'_2)G^{(0)}(x_2,x'_1)\right] \tag{3.269}
$$

Proof: Complete induction

From the equation of motion

$$
\left[i\frac{\partial}{\partial t} - H_0\right] G^{(0)}(x,x') = \delta(t-t')\delta^{(3)}(\vec{r}-\vec{r}') \tag{3.270}
$$

the free 1-particle Green's function is the inverse operator:

$$
G^{(0)}(x,x') = \left[i\frac{\partial}{\partial t} - H_0\right]^{-1} \tag{3.271}
$$

$$
\begin{aligned}
& \left[i\frac{\partial}{\partial t_1} - H_0(x_1)\right](-i)^N \quad {}_H\langle\phi_0|T\{\psi(x_1)\ldots\psi(x_N)\psi^\dagger(x_1)\ldots && (3.272)\\
& \times\psi^\dagger(x'_j)\ldots\psi^\dagger(x_N)\}|\phi_0\rangle_H\\
=\ & \left[i\frac{\partial}{\partial t_1} - H_0(x_1)\right](-i)^N \sum_{j=1}^{N}(\pm 1)^{P_j} \quad {}_H\langle\phi_0|T\{T\{\psi(x_1)\psi^\dagger(x'_j)\} && (3.273)\\
& \times\psi(x_2)\ldots\psi(x_N)\psi^\dagger(x_1)\ldots\underbrace{\cancel{\psi^\dagger(x_j)}}_{\text{missing}}\ldots\psi^\dagger(x_N)\}|\phi_0\rangle_H\\
=\ & (-i)^N \sum_{j=1}^{N}(-1)^{P_j}\delta^{(4)}(x_1-x'_j) \quad {}_H\langle\phi_0|T\{\psi(x_2)\ldots\psi(x_N)\psi^\dagger(x'_1) && (3.274)\\
& \times\ldots\cancel{\psi^\dagger(x'_j)}\ldots\psi^\dagger(x_N)\}|\phi_0\rangle_H
\end{aligned}
$$

P_j is the number of commutations to bring $\psi(x_1), \psi^\dagger(x'_j)$ together.
Acting with inverse operator $\left[i\frac{\partial}{\partial t_1} - H_0(x_1)\right]^{-1}$ on both sides:

$$\begin{aligned} G^{(N),(0)}(x_1,\ldots,x_N,x'_1,\ldots,x'_N) &= (-1)^N \sum_{j=1}^{N} (-1)^{P_j} G^{(0)}(x_1,x'_j) \\ &\quad \times G^{(N-1),(0)}(x_2,\ldots,x_N,x'_1,\ldots,\not{x}'_j,\ldots,x'_N) \end{aligned} \tag{3.275}$$

The Wick theorem follows by repeated action of $\left[i\frac{\partial}{\partial t_i} - H_0(x_i)\right]^{-1}, i = 1,\ldots,N-1$ on $G^{(N),(0)}$.

Note: The essential ingredients for the Wick theorem to be valid are:

- The field operators obey canonical equal-time commutation relations.
- Their t-dependence is according to the free Hamiltonian H_0 (i.e. operators must be in interacting picture).
- The free Hamiltonian H_0 must be a single-particle operators, because otherwise the equation of motion of $G^{(0)}$ would not have the simple form necessary for the proof of the Wick theorem.

Perturbation series:

The exact interacting Green's function can be expanded in powers of the interaction $V_I(t)$:

$$G(x,x') = -i\frac{\langle \widehat{T}\{\psi(x)\psi^\dagger(x')\exp\left(-i\int_{-\infty}^{+\infty}dt_1\int_{-\infty}^{+\infty}dt_2\,V_I(t_1,t_2)\right)\}\rangle}{\langle \widehat{T}\exp\left(-i\int_{-\infty}^{+\infty}dt_1\int_{-\infty}^{+\infty}dt_2\,V_I(t_1,t_2)\right)\rangle} \tag{3.276}$$

with

$$\int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{+\infty} dt_2\, V_I(t_1,t_2) = \frac{1}{2}\int d^4x_1\, \widetilde{V}(x_1-x_2)\psi^\dagger_{\sigma_1}(x_1)\psi^\dagger_{\sigma_2}(x_2) \times\psi_{\sigma_2}(x_2)\psi_{\sigma_1}(x_1) \quad (3.277)$$

$$x = (\vec{r},t,\sigma) \quad \text{etc.} \quad (3.278)$$

$$\psi(x_1) \equiv \psi_1 \quad \text{etc.} \quad (3.279)$$

$$\text{often:} \quad \widetilde{V}(x_1-x_2) = \delta(t_1-t_2)\widetilde{\widetilde{V}}(\vec{r}_1-\vec{r}_2) \quad (3.280)$$

$$\begin{aligned} G(x,x') = {} & -i\frac{1}{\langle S(\infty,-\infty)\rangle}\cdot\Big[\Big\langle \widehat{T}\left\{\psi(x)\psi^\dagger(x')\right\}\Big\rangle \\ & +(-i)\int d^4x_1\int d^4x_2\,\frac{1}{2}V(x_1-x_2) \\ & \times\Big\langle \widehat{T}\Big\{\psi(x)\psi^\dagger(x')\psi^\dagger\psi^\dagger_2\psi_2\psi_1\Big\}\Big\rangle \\ & +\frac{(-i)^2}{2!}\int d^4x_1\ldots\int d^4x_4\,\frac{1}{2}V(x_1-x_2)\frac{1}{2}V(x_3-x_4) \\ & \times\Big\langle \widehat{T}\Big\{\psi(x)\psi^\dagger(x')\psi^\dagger_1\psi^\dagger_2\psi_2\psi_1\psi^\dagger_3\psi^\dagger_4\psi_4\psi_3\Big\}\Big\rangle+\ldots\Big] \end{aligned} \quad (3.281)$$

Using Wick's theorem, each order can be factorized into *free, single-particle* Green's functions G^0:

$$\begin{aligned} G(x,x') = {} & \frac{1}{\langle S(\infty,-\infty)\rangle}\cdot\Big[G^0(x,x') \\ & +(-i)i^3\int d^4x_1\int d^4x_2\,V(x_1-x_2)G^0(x,x_1)G^0(x_1,x') \\ & \times G^0(x_2,x_3) \\ & +(-i)i^3\int d^4x_1\int d^4x_2\,V(x_1-x_2)G^0(x,x_1)G^0(x_1,x_2) \\ & \times G^0(x_2,x)+\ldots\Big] \end{aligned} \quad (3.282)$$

In the k-th order there appear k' equal terms, because a permutation of any two coordinate pairs $(x_1,x_2),(x_3,x_4)$ in the last expression leads to the same term. This cancels exactly the $\frac{1}{k!}$ of the Taylor expansion in each order.

Feynman diagrams:

The mathematical expressions in each order have an extremely useful diagramatic representation:

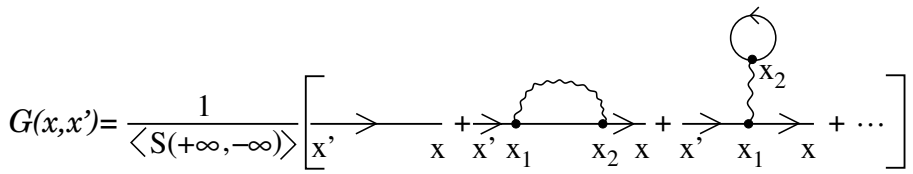


Figure 3.15: Green's function $G(x, x')$ in Feynman diagrams

The prescriptions how to translate a diagram into a mathematical expression are called *Feynman rules* and can be read off from the preceding derivation.

Feynman rules:

(1.) Each solid line with end points x_i, x_j and with a direction marked by the arrow corresponds to a (free) Green's function G^0:

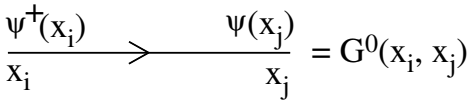


Figure 3.16: Green's function G^0 in Feynman diagram

The foot of the arrow represents a creation operator $\psi^\dagger$, the head of the arrow represents a desctruction operator ψ.

(2.) A wavy line corresponds to the interaction potential

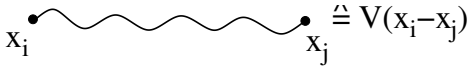


Figure 3.17: Interaction potential in Feynman diagram

(3.) Internal space-time and spin coordinates (*not* at an end point of a diagram)$x_i = (\vec{r}_i, t_i, \sigma_i)$ are integrated (or summed) over:

$$\frac{xi}{x_i} = \int dt_i \int d^3 r_i \sum_{\sigma_i} \qquad \text{"vertex"} \tag{3.283}$$

(4.) The prefactor of a diagram:

i	for each Green's function in the diagram
$(-i)^k$	for a diagram of k-th order in V from the Taylor expansion of $\widehat{T} \exp\left(-i \int dt\, V\right)$
(-1)	for each closed loop of connected fermion Green's function lines

(5.) To obtain all contributions to G at a given order $\mathcal{O}(V)$ draw *all topologically different* Feynman diagrams.

The phase factor $\langle S(+\infty,-\infty)\rangle$ in G can be expanded in a similar way. Since it has no external coordinates and all internal coordinates are integrated over, $\langle S(+\infty,-\infty)\rangle$ contains only closed diagrams:

$$\left\langle \widehat{T}\exp\left(-i\int_{-\infty}^{+\infty}dt_1\int dt_2\,V_I(t_1,t_2)\right)\right\rangle \tag{3.284}$$

$$= 1+(-i)\int d^4x_1\int d^4x_2\,V(x_1-x_2)\left\langle \widehat{t}\left\{\psi_1^\dagger\psi_2^\dagger\psi_2\psi_1\right\}\right\rangle \tag{3.285}$$

$$+\frac{(-i)^2}{2!}\int d^4x_1\ldots\int d^4x_4\,v(x_1-x_2)V(x_3-x_4)$$

$$\times\left\langle \widehat{T}\left\{\psi_1^\dagger\psi_2^\dagger\psi_2\psi_1\psi_3^\dagger\psi_4^\dagger\psi_4\psi_3\right\}\right\rangle+\ldots$$

$$= 1+(-i)i^2\int d^4x_1\int d^4x_2\,V(x_1-x_2)G^0(x_1,x_2)G^0(x_2,x_1) \tag{3.286}$$

$$-(-i)i^2\int d^4x_1\int d^4x_2\,V(x_1-x_2)G^0(x_1,x_1)G^0(x_2,x_2)$$

$$+\ldots$$

The last equation above can be expressed in Feynman diagrams so that we get:

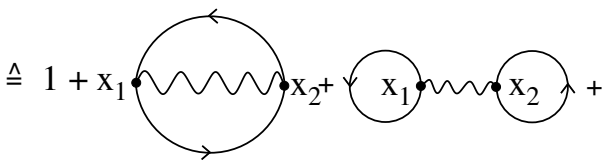
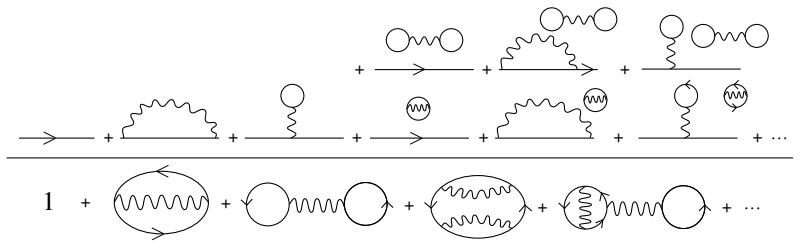
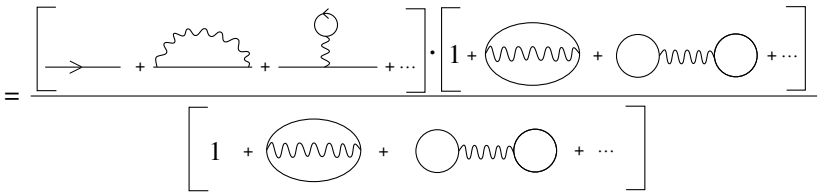


Figure 3.18:

The linked cluster theorem:

The full Green's function, including the phase factor, can be written as:

$G(x,x') =$  (3.198)

$=$  (3.199)

$$= \frac{[\Sigma(\text{all connected diagrams})]\cdot[1+\Sigma(\text{all closed diagrams})]}{[1+\Sigma(\text{all closed diagrams})]} \tag{3.200}$$

$$= \Sigma \text{ all connected diagrams} \tag{3.201}$$

Note the usefulness of diagrams to derive this result.

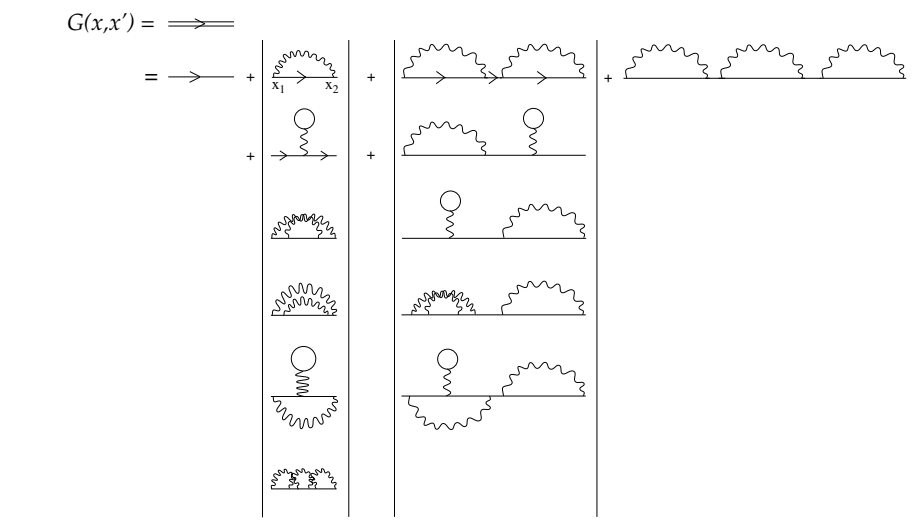
Linked cluster theorem

Only connected diagrams contribute to $G(x, x')$, and the phase factor is cancelled.

$\left[\text{Feynman diagrams in momentum space: } k, \omega \text{ conservation at each vertex}\right]$

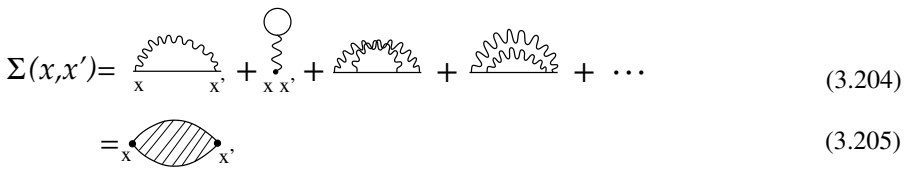
3.4.7 The Dyson equation and the selfenergy

Assuming that the perturbation series for G converges (!), the infinite series can be re-ordered:

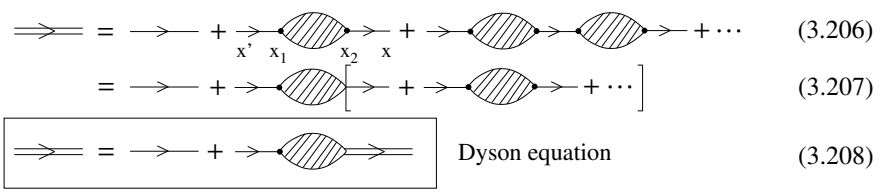


Irreducible diagram:
Diagram, which *cannot* be decomposed into two disconnected parts by cutting one G-line.

Definition:
Selfenergy $\Sigma := \sum$ of all irreducible diagrams including the prefactor from Feynman rules without external lines



Hence:



or in terms of formulas:

$$G(x,x') = G^0(x,x') + \int d^4x_1 \int d^4x_2\, G^0(x,x_2)\Sigma(x_2,x_1)G^0(x_1,x) + \ldots \quad (3.287)$$

$$\boxed{G(x,x') = G^0(x,x') + \int d^4x_1 \int d^4x_2 G^0(x,x_2)\Sigma(x_2,x_1)G(x_1,x)} \quad (3.288)$$

Dyson equation for interacting particles

$$G^0(x,x') = G^0(x-x') \quad (3.289)$$

$$\Sigma(x,x') = \Sigma(x-x') \quad (3.290)$$

$$G(x,x') = G(x-x') \qquad \text{translational invariance} \quad (3.291)$$

In a translational invariant system:

$$G_{\vec{p}} = G^{(0)}_{\vec{p}}(\omega) + G^{(0)}_{\vec{p}}(\omega)\Sigma_{\vec{p}}(\omega)G_{\vec{p}}(\omega) \qquad \text{Dyson equation} \quad (3.292)$$

$$G_{\vec{p}}(\omega) = \frac{1}{\omega - \varepsilon_{\vec{p}} - E_F - \Sigma_{\vec{p}}(\omega)} \quad (3.293)$$