Quantum Field Theory
and Keldysh Green’s Function
in Quantum Transport

An application to the Aharonov-Bohm effect in a double quantum dot

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Abstract

The following report gives an overview to quantum field theory of non-equilibrium states based on the formalism of the Keldysh Green’s function. Quantum field is utilized in various parts of physical theory, for example in relativistic quantum theory as well as in condensed matter theory. Here we want to concentrate on the quantum statistical treatment of non-equilibrium states, namely transport phenomena. In order to describe appropriate systems of non-equilibrium theoretically we can use the formally and structurally equivalent formalism as for equilibrium statistical mechanics, as we will see.

Therefore the basics of quantum mechanics and second quantization will be introduced at first. Then we will turn to quantum dynamics and define the Green’s functions. Moreover, the contour formalism will be introduced. To study the perturbation theory of the contour-ordered Green’s function we will discuss the Wick theorem. Here we will give a perspective to Feynman diagrammatics and the Dyson equation. Finally we will deal with a closed Aharonov-Bohm interferometer containing two non-interacting single-level quantum dots as an example for the theory introduced before and discuss the transmission through this device.
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1 Introduction

Quantum field theory serves as a quantum mechanical description of processes, which allow transitions between states of different numbers of particles. Quantum field theory therefore is quantum mechanics of an arbitrary number of particles [Ra07].

This kind of theory is applied in relativistic quantum theory as well as in condensed matter theory. The latter one considers non-relativistic many-body systems. The application of quantum field theory in condensed matter theory can be attributed to the smart description it provides in respect to the quantum statistics of the particles, namely bosons and fermions. Moreover the treatment of non-equilibrium states and thus transport phenomena is possible by means of non-equilibrium field theory [Ra07].

This review concentrates on the description of non-equilibrium theory based on the Keldysh technique, which dates back to Schwinger 1961 [Sc61] and Keldysh 1964 [Ke64]. Introducing this technique the computation is similar to the one of standard quantum field theory for systems in equilibrium [RS86].

The following summary of the Projektpraktikum carried out in AG Belzig at the university of Konstanz gives an overview of the work done during this period of time. This includes an introduction to the techniques of quantum field theory that are important for condensed matter physics and the study of a specific example.

The structure of this report is the following: In chapter 2 the basic principles of quantum mechanics of one particle as well as of $N$ particles will be recalled. Moreover, we will expand the considerations on multi-particle systems of fermions and the appropriate fermionic quantum fields, before the operators on the multi-particle state space will be introduced.

In chapter 3 we will turn to quantum dynamics and define the Green’s functions. Furthermore, we will regard the contour formalism. Here we will adapt to the formulation introduced by Keldysh. In order to apply perturbation theory we will discuss Wick’s theorem. In this context we will give a perspective to Feynman diagrammatics and the Dyson equation. In addition, a first example on the Keldysh Green’s function will be presented.

In chapter 4 we apply the real-time Green’s function method of the transport theory on an explicit example. We will deal with the electron transport through a closed Aharonov-Bohm interferometer containing two non-interacting single-level quantum dots. After discussing the Hamiltonian of the system we will present the derivation of the Green’s functions, which is used to calculate the total transmission and the linear conductance of the device. Finally, we will discuss the results focusing on special regimes.

With chapter 5 the report will be rounded off by an outlook and a summary.
2 Quantum mechanics and second quantization

In quantum mechanics the state of a physical system is completely characterized by a vector $|\psi\rangle$ in a Hilbert space $\mathcal{H}$. In the following sections, which are mainly adapted to [Ra07], we will deal with these states for systems with many particles.

2.1 Single-particle systems

For a single-particle system the wave-function $\psi(x)$ of a state $|\psi\rangle$ is given by its projection onto a position state $|x\rangle$,

$$\psi(x) = \langle x | \psi \rangle,$$

where $|x\rangle$ denotes the eigenstate of position. The wave function can be interpreted as the probability amplitude for the particle being located at the position $x$ in question.

Another important representation of the states is the one in terms of the eigenstates of momentum, denoted by $|p\rangle$. The states of both representations form a complete set of basis vectors for the Hilbert space.

Measurable quantities or so-called observables, are in quantum mechanics expressed by hermitian operators on $\mathcal{H}$. Examples are the operator of space $\hat{x}$ or the operator of momentum $\hat{p}$, as well as the Hamilton operator $\hat{H}$ (in short Hamiltonian).

The Hamiltonian $\hat{H} = H(\hat{p}, \hat{x})$ determines the dynamics of a system. Considering a single particle (mass $m$) in the non-relativistic case in a potential $V(x, t)$ the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}, t). \quad (2.1)$$

The dynamics of a state vector $|\psi(t)\rangle$, which describes at each instant of time the system completely, is given by the time dependent Schrödinger equation

$$i \frac{d|\psi(t)\rangle}{dt} = \hat{H} |\psi(t)\rangle. \quad (2.2)$$

Due to linearity of the Schrödinger equation the unitary time-evolution operator $\hat{U}(t, t')$ can be introduced, which connects state vectors at the time $t$ and $t'$,

$$|\psi(t)\rangle = \hat{U}(t, t') |\psi(t')\rangle. \quad (2.3)$$

Using $\hat{U}(t, t')$ as an ansatz for the Schrödinger equation (2.2) we have

$$\hat{U}(t, t') = \sum_{n=0}^{\infty} \frac{1}{i^n} \int_{t'}^{t} dt_1 \int_{t'}^{t_1} dt_2 \ldots \int_{t'}^{t_{n-1}} dt_n \hat{H}(t_1)\hat{H}(t_2)\ldots\hat{H}(t_n)$$

$$= T \exp \left( -i \int_{t'}^{t} d\bar{t} \hat{H}(\bar{t}) \right). \quad (2.4)$$

1 In order to be able to distinguish between variables and operators we explicitly label the latter ones with a hat within this chapter. Later we will relinquish on this notation when operators on the multi-particle space are considered.

2 Units are chosen to put $\hbar = 1$. 
The time-ordering operator \( T \) thereby is defined by the last equality. Regarding a time-independent Hamiltonian, that means \( \partial_t \hat{H} = 0 \), the time-evolution operator is
\[
\hat{U}(t, t') = e^{-i\hat{H}(t-t')}.
\] (2.5)

In general the equations (2.2) and (2.3) are associated to initial conditions for the states. The solution \( \psi_{x',t'}(x, t) \) of the Schrödinger equation with a particular initial state \( \psi(x', t') \), where the particle is definitely at position \( x' \) at time \( t' \), can be expressed in terms of the Green’s function \( G(x, t; x', t') \):
\[
\psi_{x',t'}(x, t) = \langle x, t | x', t' \rangle = \langle x | \hat{U}(t, t') | x' \rangle \equiv G(x, t; x', t') .
\]

Hence, the Green’s function is a solution of the Schrödinger equation and the general result for the wave function with an arbitrary initial state \( \psi(x', t') \) reads
\[
\psi(x, t) = \int dx' G(x, t; x', t') \psi(x', t') .
\]

The Green’s function can also be referred to as a propagator of the wave function, which completely specifies the quantum dynamics of the particle.

### 2.2 N-particle systems

Until now only single-particle systems have been considered. In this section we will discuss the quantum mechanics of a \( N \)-particle system.

The \( N \)-particle state space \( \mathcal{H}^{(N)} = \mathcal{H}_1 \otimes \mathcal{H}_1 \otimes \ldots \otimes \mathcal{H}_N \) is generated by the tensor product of the single-particle Hilbert spaces \( \mathcal{H}_i \) \((i = 1, \ldots N)\). For distinguishable particles the tensor product states, which are for instance in terms of the momentum
\[
|p_1\rangle \otimes |p_2\rangle \otimes \ldots \otimes |p_N\rangle \equiv |p_1, p_2, \ldots, p_N\rangle ,
\]
are an orthonormal basis of this space \( \mathcal{H}^{(N)} \). These states are eigenstates of the single-particle momentum operator \( \hat{p}_i \) and hence eigenstates of the total momentum operator \( \hat{P}_N = \sum_i \hat{p}_i \). In general, an arbitrary orthonormal set of complete single-particle states can be used as a basis.

For an assembly of identical and therefore not distinguishable particles, for examples electrons, an interchange of two particles is not measurable. Hence, states, which only differ by two interchanged particles, are described by the same vector. Any \( N \)-particle state \( |p_1, p_2, \ldots, p_N\rangle \) of identical particles is either symmetric or antisymmetric with respect to interchange of pairs of particles, for instance
\[
|p_1, p_2, \ldots, p_N\rangle = \pm |p_2, p_1, \ldots, p_N\rangle ,
\]
where the upper (lower) sign corresponds to bosons (fermions). Thus the definition of states, which are either symmetric or antisymmetric with respect to interchange of pairs of identical particles, allows to describe these assemblies of identical particles. These
states can be obtained by the linear symmetrization operator $\hat{S}$ for bosons and the linear antisymmetrization operator $\hat{A}$ for fermions:

$$\hat{S}|p_1, p_2, \ldots, p_N\rangle = \frac{1}{N!} \sum_{P} \hat{A}|p_{P_1}, p_{P_2}, \ldots, p_{P_N}\rangle$$

$$\hat{A}|p_1, p_2, \ldots, p_N\rangle = \frac{1}{N!} \sum_{P} \text{sign}(P)|p_{P_1}, p_{P_2}, \ldots, p_{P_N}\rangle.$$  \hspace{1cm} (2.6)

Here the summations are over all permutations $P$ of the particles and $\text{sign}(P)$ equals +1 for an even number of transpositions needed to build the permutation $P$ or −1 for an odd number, respectively.

Then the Pauli’s exclusion principle for fermions follows directly. Assuming that there are two identical single-particle states, after the antisymmetrization each term emerges two times but with different sign in the antisymmetrized states, so that it equals to the zero vector. Hence, two fermions can not occupy the same state.

Since the (anti-)symmetrization operator $\hat{S}$ ($\hat{A}$) is a projection operator, which projects any state onto either of the two orthogonal subspaces of symmetric or antisymmetric states, the state space for a physical system of $N$ identical particles is accordingly the symmetric subspace $B^{(N)}$ for bosons or the antisymmetric subspace $F^{(N)}$ for fermions. These spaces are obtained by projection of the states of $\mathcal{H}^{(N)}$ using the appropriate (depending on the statistics of the particles) (anti-)symmetrization operator.

In the following parts we will focus on the fermions, but the implementation for bosons is nearly identical to the one for the fermions, when we regard that the antisymmetrization has to be replaced by symmetrization. In the antisymmetric $N$-particle states space $F^{(N)}$, a basis of orthogonal and normalized antisymmetric states is defined by

$$|p_1 \wedge p_2 \wedge \ldots \wedge p_N\rangle = \sqrt{N!} \hat{A}|p_1, p_2, \ldots, p_N\rangle$$

$$= \frac{1}{\sqrt{N!}} \sum_{P} \text{sign}(P)|p_{P_1}, p_{P_2}, \ldots, p_{P_N}\rangle ,$$

where the pre-factor $\sqrt{N!}$ is due to the normalization of the states. The scalar product of theses states (regarding $\hat{A}^\dagger \hat{A} = \hat{A}^2 = \hat{A}$ and equation (2.6))

$$\langle p_1 \wedge \ldots \wedge p_N | p'_1 \wedge \ldots \wedge p'_N\rangle = \sum_{P} \text{sign}(P) \langle p_1 | p'_{P_1}\rangle \ldots \langle p_N | p'_{P_N}\rangle$$

$$= \det((\langle p_i | p'_j\rangle)) ,$$

equals $\text{sign}(P)$ if the primed set of momenta is a permutation of the unprimed set and is zero otherwise. According to the last equality it also can be expressed by the Slater determinant, which is the determinant of the $N \times N$ matrix with entries $\langle p_i | p'_j\rangle$.

### 2.3 Multi-particle systems and quantum fields

Up to now we have considered one Hilbert space $\mathcal{H}^{(N)}$ for a defined number $N$ of particles. Moreover, the antisymmetrized subspace $F^{(N)}$ for $N$ identical particles was defined.
In order to regard an arbitrary number of particles, we introduce the so-called Fock space \( \mathcal{F} \), given by the direct sum of the state spaces

\[
\mathcal{F} = \mathcal{F}^{(0)} \oplus \mathcal{F}^{(1)} \oplus \mathcal{F}^{(2)} \oplus \ldots = \bigoplus_{N=0}^{\infty} \mathcal{F}^{(N)} .
\]

Here the space \( \mathcal{F}^{(0)} \) is the space of states without any particles, which only consists of one the state, the vacuum state \( |0\rangle \).

Standard single-particle operators, like the momentum \( \hat{\mathbf{p}} \), or the two-particle interaction \( \hat{V}(\hat{x}_i, \hat{x}_j) \) conserve the number of particles and therefore only operate on one \( N \)-particle state space \( \mathcal{F}_N \). Nevertheless, it is useful to define operators, which connect various sectors of the Fock space, for instance \( \mathcal{F}^{(N)} \) and \( \mathcal{F}^{(N')} \) with \( N \neq N' \).

This kind of operators are, for instance, the creation operators \( (a_p^\dagger) \) and the annihilation operators \( (a_p, \) here corresponding to a momentum value \( p \)). Such creation operators for fermions transform an antisymmetrized \( N \)-particle state into the antisymmetrized \( (N+1) \)-particle state, where an additional fermion has momentum \( p \). The annihilation operators for fermions whereas transform an antisymmetrized \( N \)-particle state into the antisymmetrized \( (N-1) \)-particle state, where the particle in state \( p \) is annihilated or, if none of the fermions occupies the momentum state \( p \), produces the zero vector:

\[
a_p^\dagger |p_1 \wedge p_2 \wedge \ldots \wedge p_N\rangle = |p \wedge p_1 \wedge p_2 \wedge \ldots \wedge p_N\rangle
\]

\[
a_p |p_1 \wedge p_2 \wedge \ldots \wedge p_N\rangle = \sum_{n=1}^{N} (-1)^{n-1} \langle p | p_n \rangle \langle p_1 \wedge \ldots \langle \text{no } p_n \ldots \wedge p_N \rangle . \quad (2.7)
\]

The (anti-)commutation rules for the creation and annihilation operators for fermions are

\[
\{a_p, a^\dagger_{p'}\} = 0, \quad \{a_p, a_{p'}\} = 0, \quad \{a_p, a^\dagger_{p'}\} = \langle p | p' \rangle . \quad (2.8)
\]

Here it directly results \((a_p^\dagger)^2 = 0\) as well as \(a_p^2 = 0\), thus Pauli’s exclusion principle can be seen once again.

The number operator \( \hat{n}_p \) for state \( p \) is defined by \( \hat{n}_p = a_p^\dagger a_p \) and counts the number of particles in the eigenstate with momentum \( p \). Its eigenvalues can be either 0 or 1, depending on the state is occupied or not.

An arbitrary state vector can be expressed in terms of creation operators and the vacuum state by

\[
|p_1 \wedge p_2 \wedge \ldots \wedge p_N\rangle = a_{p_1}^\dagger a_{p_2}^\dagger \ldots a_{p_N}^\dagger |0\rangle .
\]

The creation and annihilation operators can be defined in a more general way for any other complete set of single-particle states labelled by the an arbitrary index instead of \( p \). For instance, we can apply Fourier transformation and introduce the creation and annihilation operator \( a_p^\dagger \equiv \psi^\dagger(\mathbf{x}) \) and \( a_p \equiv \psi(\mathbf{x}) \) of the space states (field operators):

\[
\psi^\dagger(\mathbf{x}) = \int \frac{dp}{(2\pi)^{3/2}} e^{-ip \cdot x} a_p^\dagger \quad \quad a_p^\dagger = \int \frac{dx}{(2\pi)^{3/2}} e^{ip \cdot x} \psi^\dagger(\mathbf{x})
\]

\[
\psi(\mathbf{x}) = \int \frac{dp}{(2\pi)^{3/2}} e^{ip \cdot x} a_p \quad \quad a_p = \int \frac{dx}{(2\pi)^{3/2}} e^{-ip \cdot x} \psi(\mathbf{x}). \quad (2.9)
\]
The field operators fulfill the anti-commutation relations of equation (2.8), too.

Up to now we have seen that the description of an assembly of fermions in terms of the antisymmetry of the state vectors requires a substantial amount of indices-writing and therefore is quite messy. This becomes even more apparent when we consider quantum mechanical systems that are in a superposition of states with an arbitrary number of particles. The definition of the creation and annihilation operators or equivalently the quantum fields simplifies the characterization of the quantum statistics of such an assembly a lot. Any state in the multi-particle state space could be simply expressed by operating with the creation field on the vacuum state. Thus the all states of a many-body system are expressed in terms of these two operators and for a description of the assembly we just have to regard the simple anti-commutation relations (2.8).

2.4 Non-interacting electron gas

In this context we want to consider as a striking example a three dimensional system of \( N \) non-interacting spin one-half (denoted by \( \sigma \) ) fermions or in other words an ideal Fermi gas. The ground state \( |\Phi_0\rangle \), the so-called Fermi sea, is obtained from the vacuum state according to

\[
|\Phi_0\rangle = \prod_{p,|p| \leq p_F} \prod_{\sigma = \uparrow, \downarrow} a_{p,\sigma}^\dagger |0\rangle .
\]

Then we can compute one-particle Green’s function (density matrix) for this system:

\[
G_{\sigma}(x' - x') \equiv \langle \Phi_0 | \psi_{\sigma}(x) \psi_{\sigma}(x') | \Phi_0 \rangle = \frac{1}{(2\pi)^3} \int dp \int dp' \ e^{-ipx} e^{ip'x'} \langle \Phi_0 | a_{p,\sigma}^\dagger a_{p',\sigma} | \Phi_0 \rangle \\
= \frac{1}{(2\pi)^3} \int dp \ e^{-ip(x' - x')} \ \theta(p_F - |p|) ,
\]

having used equation (2.9) and the fact that all fermions occupy each single states within the Fermi sphere in the momentum space. In three dimensional spherical coordinates we obtain (defining \( x = |x - x'| \)):

\[
G_{\sigma}(x - x') = \frac{2\pi}{(2\pi)^3} \int_0^{k_F} dp \ p^2 \int_{-1}^{1} d(cos \theta) \ e^{-ip|x - x'| \cos \theta} = \frac{1}{2\pi} \int_0^{k_F} dp \ p \sin (px) \\
= \frac{1}{2\pi^2 x^3} (\sin (k_F x) - k_F x \cos (k_F x)) \\
= \frac{3n}{2} \frac{\sin (k_F |x - x'|) - k_F |x - x'| \cos (k_F |x - x'|)}{(k_F |x - x'|)^3} ,
\]

(2.11)
with the Fermi momentum $k_F^3 = 3\pi^2 n$, where $n$ gives the density of the fermions in the real space:

$$n = \frac{N}{V} = \frac{1}{V} \int d^3p \frac{2V}{(2\pi)^3} = \frac{2}{(2\pi)^3} \int_0^{k_F} dp \ 4\pi p^2 = \frac{k_F^3}{3\pi^2}. $$

Thus the one-particle correlation function is the probability amplitude for a particle being absent at position $x$, if at position $x'$ a particle is removed from the Fermi sea\(^3\). Or equivalently it specifies the overlap between the state, where a particle at position $x'$ has been removed from the ground state, and the state, where a particle at position $x$ has been removed from the ground state.

Due to the Pauli principle we can even observe that non-interacting fermions with the same spin are correlated. The pair correlation function $g_{\sigma\sigma'}(x - x')$ is related to the one-particle Green’s function according to:

$$g_{\sigma\sigma'}(x - x') \equiv \left< \Phi_0 \mid \psi_\sigma(x) \psi_\sigma^\dagger(x') \psi_{\sigma'}(x') \psi_{\sigma'}(x) \right| \Phi_0 \right>$$

$$= \frac{1}{(2\pi)^6} \int dp \ dp' \ dq \ dq' \ e^{-i(p-p') \cdot (x-x')} \left< \Phi_0 \mid a_p^\dagger \ a_{q'}^\dagger \ a_{q'} \ a_{p'} \right| \Phi_0 \right>, $$

once again having used equation (2.9).

Considering at first $\sigma \neq \sigma'$. In this case $q = q'$ and $p = p'$ has to be crucial for having $g_{\sigma\sigma'}(x - x')$ unequal to zero. Then we obtain $g_{\sigma\sigma'}(x - x') = (n/2)^2$.

For $\sigma = \sigma'$ there are two possibilities for $g_{\sigma\sigma'}(x - x')$ being finite, namely $q = q'$ and $p = p'$ or $q = q'$ and $p = q'$, respectively. In accordance with Pauli’s principle, $q \neq p$ has to be disregarded, since $(a_p^\dagger)^2 = 0$. Taking these facts into account the pair correlation function results in

$$g_{\sigma\sigma}(x - x') = \frac{1}{(2\pi)^6} \int dp \ dq \ \left(1 - e^{-i(p-q) \cdot (x-x')} \right) n_{p,\sigma} n_{q,\sigma}$$

$$= \left(\frac{n}{2}\right)^2 - G_\sigma(x - x').$$

Thus the pair correlation function, which can be interpreted as the probability that a particle with spin $\sigma'$ occupies position $x'$, if a particle with spin $\sigma$ at position $x$ has been removed, reads

$$g_{\sigma\sigma'}(x - x') = \begin{cases} \left(\frac{n}{2}\right)^2 & \text{for } \sigma \neq \sigma' \\ \left(\frac{n}{2}\right)^2 - G_\sigma(x - x')^2 & \text{for } \sigma = \sigma' \end{cases} \quad (2.12)$$

In figure 1 the one-particle correlation function (equation (2.11)) as well as the pair correlation function (equation (2.12)) for $\sigma = \sigma'$ for non-interacting fermions is depicted. In particular the anti-bunching of the ideal Fermi gas is visible, since due to Pauli’s exclusion principle in maximum only one particle can be at position $x$ with spin $\sigma$. If this particle is removed, there is no particle with spin $\sigma$ at position $x$ that means $g_{\sigma,\sigma}(0) = 0$.

---

\(^3\)One can also say that the one-particle correlations function is the probability amplitude for having a hole at position $x'$, if at position $x$ a hole was created in the Fermi sea.
Fig. 1: The one-particle Green's function (a) and the pair correlations function (b) for non-interacting spin one-half fermions. As following from equation (2.10) the one-particle Green's function is the three dimensional Fourier transform of the density in momentum space (see inset in (a)). The pair correlation function (b) oscillates with the wave number \( k_F \). Moreover, the anti-bunching of the non-interacting fermions is visible and can be attributed to the Pauli’s exclusion principle.

2.5 Operators on the Fock space

In this section we will introduce the elevation of a known \( N \)-particle operator (for instance a Hamiltonian) to its form on the multi-particle states space. As already mentioned physical quantities are expressed by operators in quantum mechanics. In his spectral representation an operator \( \hat{A} \) is given by

\[
\hat{A} = \sum_a a |a\rangle \langle a| ,
\]

with the eigenvalues \( a \) and the corresponding eigenstates \( |a\rangle \) of the operator. In the following we will generalize this operator in the multi-particle space, so that the restriction of the yielded operator to any \( N \)-particle subspace reduces it to the operator in question for the system consisting of \( N \) identical particles.

Let us consider a general one-particle operator, \( \hat{f}^{(1)} \), which constructs a corresponding operator on the \( N \)-particle system (index \( i \) denotes the particle) according to

\[
\hat{F}_N^{(1)} = \sum_{i=1}^N \hat{f}_i^{(1)} .
\]

Taking for example \( \hat{f}^{(1)} = |\mu_2\rangle \langle \mu_1| \), the \( N \)-particle space operator \( \hat{F}_N^{(\mu_1|\mu_2)} \) operates on an arbitrary \( N \)-particle state owing to

\[
\hat{F}_N^{(1)} |\lambda_1 \land \lambda_2 \land \ldots \land \lambda_N\rangle = |\mu_1| \lambda_1\rangle |\mu_2 \land \lambda_2 \land \ldots \land \lambda_N\rangle
+ |\mu_1| \lambda_2\rangle |\lambda_1 \land \mu_2 \land \lambda_3 \ldots \land \lambda_N\rangle + \ldots
+ |\mu_1| \lambda_N\rangle |\lambda_1 \land \lambda_2 \land \ldots \land \lambda_{N-1} \land \mu_2\rangle .
\]
Taking the antisymmetrization for the exchange of two fermions into account, it results

\[ \hat{F}^{(1)}_N |\lambda_1 \wedge \ldots \wedge \lambda_N\rangle = \sum_{n=1}^N \langle \mu_1 | \lambda_n \rangle (-1)^{n-1} |\mu_2 \wedge \lambda_1 \wedge \ldots (\text{no } \lambda_n) \ldots \wedge \lambda_N\rangle . \]

Comparing with equation (2.7), the obtained state is equivalent to the one when operating with the operator \( a_{\mu_2}^\dagger a_{\mu_1} \) on the state, thus the one-particle operator \( |\mu_2\rangle \langle \mu_1| \) corresponds to the operator \( F^{(1)} \) in the multi-particle space,

\[ F^{(1)} = a_{\mu_2}^\dagger a_{\mu_1} . \]

Speaking more generally in an arbitrary basis \( |\lambda\rangle \) an arbitrary one-particle operator has the form

\[ \hat{f}^{(1)} = \sum_{\lambda,\lambda'} |\lambda\rangle \langle \lambda' | \hat{f}^{(1)} |\lambda'\rangle . \]

The corresponding operator \( \hat{F}^{(1)}_N \) on the \( N \)-particle system is due to linearity given by

\[ F^{(1)} = \sum_{\lambda,\lambda'} \langle \lambda | \hat{f}^{(1)} |\lambda'\rangle a_{\lambda}^\dagger a_{\lambda'} . \quad (2.13) \]

As an example for application of equation (2.13) the total momentum operator \( P \) in the multi-particle space is regarded both in momentum and in position representation of the field:

\[ P = \int dp \ p a_{p}^\dagger a_{p} = \int dx \ \psi^\dagger(x) (-i\hbar \nabla_x) \psi(x) . \]

Furthermore, the Hamiltonian (2.1) of a non-relativistic particle shall be considered. Owing to equation (2.13) the corresponding Hamiltonian on the multi-particle space is

\[ H = \int dx \ \psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x,t) \right) \psi(x) . \]

For free non-relativistic particles thus the kinetic energy operator has the form

\[ H = \int dx \ \psi^\dagger(x) \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi(x) = \sum_p \varepsilon_p a_{p}^\dagger a_{p} , \]

given in the position and momentum representation, respectively.

Up to now we have only considered operators without interaction between the particles. Let us consider identical fermions interacting through an instantaneous two-body potential \( V^{(2)}(x_i, x_j) \). The interaction operator in the two-particle state space representation is then given by (factor 1/2 due to double counting of the integrals)

\[ \hat{V}^{(2)} = \frac{1}{2} \int dx_1 \int dx_2 \ |x_1 \wedge x_2\rangle V^{(2)}(x_1, x_2) \langle x_1 \wedge x_2| . \]
In an analogous way as for the one-particle operator above, it is possible to show that the two-body interaction operator on an $N$-particle basis states,

$$V^{(2)}_N |x_1 \wedge x_2 \wedge \ldots \wedge x_N\rangle = \frac{1}{2} \sum_{i \neq j} V^{(2)}(x_i, x_j) |x_1 \wedge x_2 \wedge \ldots \wedge x_N\rangle,$$

is in the Fock space represented by the operator

$$V = \frac{1}{2} \int dx \int dx' \psi^\dagger(x) V^{(2)}(x, x') \psi(x'') \psi(x).$$

This operator is as well as the one-particle operators above so-called normal-ordered, since all annihilation operators appear to the right of any creation operator. As a consequence we can directly see that the vacuum state has zero energy and momentum.

Now we can write down the Hamiltonian for non-relativistic identical particles, which interact through an instantaneous two-body interaction, in the Fock space:

$$H = \int dx \psi^\dagger(x) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}\right) \psi(x) + \frac{1}{2} \int dx \int dx' \psi^\dagger(x) V^{(2)}(x, x') \psi(x'') \psi(x).$$

### 2.6 Statistical operator

If we expand our considerations from an isolated system to a generic open system, the state vector $|\Psi\rangle$ will be in a mixture of states and thus we have to regard the density matrix or the statistical operator

$$\rho \equiv \sum_k p_k |\psi_k\rangle \langle \psi_k|,$$

where $p_k$ is the probability with which the quantum state $|\psi_k\rangle$ occurs in the multi-particle state. Using the statistical operator the average value of a physical quantity $A$ can be expressed by the trace in the multi-particle state via

$$\langle A \rangle = \text{Tr}(\rho A) = \sum_k p_k \langle \psi_k | A | \psi_k \rangle.$$

Assuming a physical system described by a time-independent Hamiltonian $H = H_0 + H^i$, where $H_0$ represents the free particles and the interaction between the particles is described by $H^i$, the statistical operator in thermodynamic equilibrium at a temperature $T$ is

$$\rho_T(H) = \frac{1}{Z} e^{-\frac{H}{k_B T}}$$

with $Z = \text{Tr} e^{-\frac{H}{k_B T}}$.

Here we use the canonical ensemble. Shifting from the canonical to the grand canonical ensemble, we measure the particle energies relative to their chemical potential $\mu$, so that we have to replace $H \rightarrow H - \sum_s \mu_s N_s$ [RS86].
3 Quantum dynamics and Green’s functions

In order to describe the quantum dynamics of a system described by a Hamiltonian $H(t)$ we can use different ways expressed by the so-called pictures.

3.1 Quantum mechanical pictures

In the Schrödinger picture the state vectors $|\psi(t)\rangle$ or equivalently the statistical operator $\rho(t)$ are considered to be time-dependent, whereas the observables are time-independent (compare to equations (2.2) to (2.4)) [Ra07]. Nevertheless, it is convenient to transfer the dynamics to the physical quantities $A$, which is done in the Heisenberg picture (here with respect to $H(t)$). The transformation is unitary and given by

$$|\psi_H(t)\rangle \equiv U^\dagger(t,t_0)|\psi(t)\rangle \quad \text{and} \quad A_H(t) \equiv U^\dagger(t,t_0) A U(t,t_0) ,$$

(3.1)

where $U(t,t_0)$ is the time-evolution operator (see equation (2.4))

$$U(t,t_0) = T e^{-\frac{i}{\hbar} \int_{t_0}^{t} dt \, H(t)} ,$$

(3.2)

and $t_0$ is an arbitrary reference time, where the two pictures coincides [Ra07].

The generic, total Hamiltonian $H(t) = H + H'(t)$ we want to consider here can be split into a time-independent, equilibrium Hamiltonian $H = H_0 + H'$, where $H_0$ once again represents the free particles and $H'$ the interaction between them (isolated system, see section 2.6), and a contribution $H'(t)$, which is related to a disturbance the system is exposed to (perturbation) [RS86].

In an analogous manner as the transformation from the Schrödinger to the Heisenberg picture we can define the interaction picture (with respect to $H$). The transformation is given by the same unitary operator $U$ as in the case of the Heisenberg picture (equation 3.2), if we replace the total Hamiltonian $H(t)$ by the one of the isolated system $H$ (leading to equation (2.5), since $H$ is time-independent) [Ra07].

3.2 Green’s functions

Experiments on quantum dynamics in general have only access to special measurable quantities, for example density and current. Therefore it is convenient in the quantum dynamics theory to introduce correlations functions or so-called Green’s functions, which constitute a connection between these and the calculable quantities of theory [Ra07].

Using the abbreviation $(t_1, x_1) \equiv 1$, we first define the $G$-lesser and $G$-greater Green’s

---

4In the following the Hamiltonian $H(t)$ describes the regarded system as well as an external disturbance. In order to distinguish it from the Hamiltonian $H$ representing the system itself (see section 2.6), we chose this notation, which should not be mixed up with the Hilbert space.

5The $G$-lesser Green’s function is the amplitude to miss a particle at position $x_{1'}$ at the time $t_{1'}$, if at time $t_1$ a particle was removed at position $x_1$.

6The $G$-greater Green’s function is the amplitude for the process of an added a particle at position $x_1$ at time $t_1$, if at time $t_{1'}$ a particle was added at position $x_{1'}$. 


function by
\[
G^<(1,1') = \mp i \left\langle \psi_H^\dagger(1')\psi_H(1) \right\rangle,
\]
\[
G^>(1,1') = -i \left\langle \psi_H(1)\psi_H^\dagger(1') \right\rangle,
\]
where the upper sign is for the Bose and the lower sign for the Fermi field in the Heisenberg picture, respectively. For the calculation of a perturbative expansion, we shall later encounter the time-ordered as well as the anti-time-ordered Green’s function:
\[
G(1,1') = -i \left\langle T(\psi_H(1)\psi_H^\dagger(1')) \right\rangle = \begin{cases} 
G^<(1,1') & \text{for } t_{1'} > t_1 \\
G^>(1,1') & \text{for } t_1 > t_{1'}
\end{cases}
\]
\[
\tilde{G}(1,1') = -i \left\langle \tilde{T}(\psi_H(1)\psi_H^\dagger(1')) \right\rangle,
\]
where the time-ordering operator $T$ orders the product of operators according to their time arguments into a time-descending sequence and $\tilde{T}$ orders anti-time that means oppositely to that of $T$ [Ra07].

Other combinations of field correlations are given by the retarded, the advanced and the Keldysh or kinetic Green’s function:
\[
G_R(1,1') = -i \theta(t_1 - t_{1'}) \left\langle \left[ \psi_H(1),\psi_H^\dagger(1') \right]_\mp \right\rangle = \theta(t_1 - t_{1'}) (G^>(1,1') - G^<(1,1'))
\]
\[
G_A(1,1') = i \theta(t_{1'} - t_1) \left\langle \left[ \psi_H(1),\psi_H^\dagger(1') \right]_\mp \right\rangle = -\theta(t_{1'} - t_1) (G^>(1,1') - G^<(1,1'))
\]
\[
G_K(1,1') = -i \left\langle \left[ \psi_H(1),\psi_H^\dagger(1') \right]_\mp \right\rangle = G^>(1,1') + G^<(1,1').
\]

Analogously to the time-ordered Green’s function (3.4) we can define the so-called contour-ordered Green’s function by replacing the time ordering operator $T$ by the contour ordering operator $T_c$ of the contour $c$. Here the contour $c$ is a contour along the real-time axis starting and ending at $t_0$ and passing through $t_1$ and $t_{1'}$ once (see figure 2). In a same manner than the time-ordering, the contour-ordering operator orders the operators owing to the position on the contour of their time arguments, so that the time-ordering relations ($>,$ $<$) have to be replaced by contour-ordering relations ($>_c,$ $<_c$). Figure 2 depicts the case $t_1 > _c t_{1'}$ [RS86, Ra07].

**Fig. 2:** The closed time path contour $c$, which starts from $t_0$, proceeds along the real-time axis to pass $t_{1'}$ and $t_1$ and then returns back to $t_0$. 
3.3 Interaction picture on the Keldysh contour

Quantum dynamics of a many-body system are determined by the time development of the field operators in the Heisenberg picture, since measurable physical quantities of a system are expressed by strings of Heisenberg operators. Thus the dynamics of a system is described by the correlations functions of the field operators - the Green’s functions.

Due to the crucial role of the time-ordering in the evolution operator (see equation (2.4)), we will concentrate in the following perturbation considerations on the time-ordered Green’s function.

The standard transformation of an observable $O_H(t)$ in the Heisenberg picture to the corresponding observable $O_H(t)$ in the interaction picture is (compare to equation (3.1)):

$$O_H(t) = U(t, t_0) O_H(t) U(t, t_0)$$

with $U(t, t_0) = T \exp \left[ -i \int_{t_0}^{t} dt' H_H(t') \right]$, (3.6)

where $H'_{H}(t)$ represents $H'(t)$ in the interaction picture with respect to $H$. In terms of the contour $c_t$ we can rewrite the transformation to $c_t$:

$$O_H(t) = T_{c_t} \left( \exp \left[ -i \int_{c_t} d\tau H'_H(\tau) \right] O_H(t) \right).$$

Here $\tau$ denotes the contour variable from the contour $c_t$, which starts and ends at $t_0$ and passes through $t$ by proceeding along the real-time axis (see figure 3). As above, the contour ordering symbol $T_{c_t}$ orders products of operators according to the position of their contour argument on the closed contour [RS86, Ra07].

![Fig. 3: The contour $c_t$ proceeding from $t_0$ along the real time axis to $t$ and then back to $t_0$.](image)

With the latter equation (3.7) the contour-ordered Green’s function $G(1, 1')$ can be studied. Therefore we start by the definition of the $G(1, 1')$ (replace $T$ by $T_{c_t}$ in equation (3.4)) and have a separate look at $G^< (1, 1')$ and $G^> (1, 1')$ (once again for contour ordered times). Since the considerations are analogously we shall only investigate $G^> (1, 1')$ and thus $t_1 >_c t_{1'}$. Applying equation (3.7) we yield:

$$G^> (1, 1') = -i \left\langle \psi_H(1) \psi_H^\dagger (1') \right\rangle$$

$$= -i \left\langle T_{c_{t1}} e^{-i \int_{c_{t1}} d\tau H'_H(\tau)} \psi_H(1) \right\rangle \left\langle T_{c_{t1'}} e^{-i \int_{c_{t1'}} d\tau H'_H(\tau)} \psi_H^\dagger (1') \right\rangle$$

$$= -i \left\langle T_{c_{t1} + c_{t1'}} \left( e^{-i \int_{c_{t1} + c_{t1'}} d\tau H'_H(\tau)} \psi_H(1) \psi_H^\dagger (1') \right) \right\rangle.$$
We combined the both contours \( c_1 \) (\( c_{t'} \)), which start and end at \( t_0 \) and pass through \( t_1 \) (\( t' \)), together to the combined contour \( c_1 + c_{t'} \), which starts at \( t_0 \), passes through \( \min\{t_1, t'\} \), returns to \( t_0 \), stretches to \( \max\{t_1, t'\} \) and then ends at \( t_0 \) (see figure 4). This can be done, since the closed part of the path in between (marked green in the figure) has not any involvement of the field operators, so that this contributions equals to the unit operator [RS86, Ra07].

**Fig. 4:** The combined contour \( c_1 + c_{t'} \) stretching from \( t_0 \) to \( \min\{t_1, t'\} \) and back to \( t_0 \) and then forward to \( \max\{t_1, t'\} \) before returning back to \( t_0 \). The green marked part is closed contour, which has no involvement of a field operator, thus giving the unit operator.

Combining the result for \( G^{<}(1, 1') \) and the one for \( G^{>}(1, 1') \) we finally yield

\[
G(1, 1') = -i \left\langle T_c \left( \psi_H(1) \psi_H^\dagger(1') \right) \right\rangle = -i \left\langle T_c \left( e^{-i \int_0^1 d\tau H'_{H_0}(\tau) \psi_H(1) \psi_H^\dagger(1')} \right) \right\rangle.
\]

In general, the only method to describe the dynamics of a system in non-equilibrium is given by perturbation theory. Hence, the aim is to achieve a perturbative study of the contour-ordered Green’s function. For that reason the Hamiltonian is divided into two parts, one part representing a well-understood problem and one non-trivial part, whose effect shall be studied order by order [Ra07].

The system we want to look at is described by the Hamiltonian \( H = H_0 + H^i \) (see above), where \( H_0 \) needs to be quadratic in fields in order to allow a perturbative expansion of the contour-ordered Green’s function. Transforming to the interaction picture with respect to \( H_0 \) we yield from equation (3.7):

\[
O_{H}(t) = T_{c_i} \left( \exp \left[ -i \int_{c_i} d\tau \left( H_{H_0}^{i}(\tau) + H^i_{H_0}(\tau) \right) \right] O_{H_0}(t) \right).
\]

Analogous considerations as above for the contour-ordered Green’s function allow us to get the contour-ordered Green’s function in the interaction picture

\[
G(1, 1') = -i \frac{\text{Tr} \left( e^{-\beta H} T_c \left( e^{-i \int_0^1 d\tau \left( H_{H_0}^{i}(\tau) + H^i_{H_0}(\tau) \right) \psi_{H_0}(1) \psi_{H_0}^\dagger(1')} \right) \right)}{\text{Tr} e^{-\beta H}},
\]

where the average is expressed in terms of the trace over the statistical operator and normalized with the partition function (see section 2.6). Now we can replace

\[
e^{-\beta H} = e^{-\beta H_0} e^{i H_0 (-i \beta)} T_{c_a} e^{-i \int_0^1 d\tau H^i(\tau)} = e^{-\beta H_0} T_{c_a} e^{-i \int_0^1 d\tau H^i_{H_0} (\tau)}
\]

with \( H^i_{H_0}(t) \) being the operator \( H^i \) in the interaction picture with respect to \( H_0 \). Moreover, we used Dyson’s formula\(^8\) and regarded the assumption that \( H \) is time-independent. The

\(^8\)Dyson’s formula connects the unitary transformations matrices of the interaction picture with respect to \( H (\Phi_H(t, t_0)) \) and the one with respect to \( H_0 (\Phi_{H_0}(t, t_0)) \) to the transformation matrix \( V(t, t_0) \) of the transformation from the interaction picture with respect to \( H \) to the one with respect to \( H_0 \). The formula reads \( V(t, t_0) = U_{H_0}(t, t_0) U_H(t, t_0) \) or explicitly \( T e^{-i \int_0^1 d\tau H_{H_0}(\tau)} = e^{i H_0 (t-t_0)} T e^{-i \int_0^1 d\tau H(t)} \).
contour $c_a$ stretches down into the lower complex time plane from $t_0$ to $t_0 - i\beta$. Plugging the latter equation into the expression for the contour-ordered Green’s function (3.8) and defining the total contour $c_t$, which contains beside $c$ the appendix contour $c_a$ (see figure 5), we yield [RS86, Ra07]:

$$G(1, 1') = -i \frac{\text{Tr} \left( e^{-\beta H_0} T_{c_t} \left( e^{-i \int_{c_t} d\tau H_{00}(\tau)} e^{-i \int_{c} d\tau H'_{00}(\tau)} \psi_{H_0}(1) \psi_{H_0}^+(1') \right) \right)}{\text{Tr} \left( e^{-\beta H_0} T_{c_t} \left( e^{-i \int_{c_t} d\tau H_{00}(\tau)} e^{-i \int_{c} d\tau H'_{00}(\tau)} \psi_{H_0}(1) \psi_{H_0}^+(1') \right) \right)}.$$  (3.9)

**Fig. 5:** The total contour $c_t$ containing both the contour $c$ and the appendix contour $c_a$. It proceeds from $t_0$ to max{$t_1, t_1'$}, then back to $t_0$ and has in addition to the contour $c$ the appendix, which stretches further down into the lower complex time plane from $t_0$ to $t_0 - i\beta$.

On the expression (3.9) we can apply Wick’s theorem just as in equilibrium theory in order to obtain the perturbative expansion of the contour-ordered Green’s function. Speaking formally the only difference between the equilibrium and the non-equilibrium theory is given by the fact that the integration over the inverse temperature (for finite temperature) or rather the real axis (for zero temperature) has to be replaced by the integration over a contour. Hence, mapping onto the associated Feynman diagrams of the contour-ordered Green’s function is precisely the same as in equilibrium theory [RS86].

Before we discuss Wick’s theorem and the Keldysh formalism, some remarks are in order. Note, that on the appendix contour part only interactions are alive, whereas the external perturbation vanishes on this part of the contour. Since we do not consider initial correlations that means we are not interested in physics on short time scales of the order of the collision time scale due to the interactions, we can assume $t_0 \rightarrow -\infty$. Moreover, the Green’s function falls off sufficiently rapidly, thus the contribution from the imaginary part of the contour $c_i$ vanishes. In other words we can say that a propagator with one of its arguments on the imaginary time appendix is damped on the time scale of the scattering time of the system. Therefore the initial time $t_0$, where the system is perturbed by the external field, exceeds the microscopic scattering times of the systems by far and thus can be effectively approximated by $t_0 \rightarrow -\infty$ [RS86, Ra07].

Thus the contours $c_i$ and $c$ are now identical and both start and end at $-\infty$. Extending them beyond the largest time, we can define the Schwinger’s closed time path [Sc61], the Schwinger-Keldysh or rather the real-time contour $c_k$, which starts at time $t = -\infty$ and proceeds to time $t = \infty$ and then returns back again to time $t = -\infty$ (see figure 6). Using this contour the contour-ordered or closed time path Green’s function finally reads

$$G(1, 1') = -i \text{Tr} \left( \rho_0 T_{c_k} \left( e^{-i \int_{c_k} d\tau (H_{00}(\tau) + H'_{00}(\tau))} \psi_{H_0}(1) \psi_{H_0}^+(1') \right) \right),$$  (3.10)
with the statistical operator $\rho_0$ for the equilibrium state of the non-interacting system at the temperature $T$

$$
\rho_0 = \frac{e^{-H_0/k_B T}}{\text{Tr} \ e^{-H_0/k_B T}}.
$$

Fig. 6: The Schwinger-Keldysh or real-time contour $c_k$ consists of two parts: $c_1$ extending from $-\infty$ to $\infty$ and $c_2$ extending from $\infty$ to $-\infty$.

### 3.4 Keldysh formulation

The contour-ordered Green’s function $G_{c_k}$ on the Keldysh contour (equation (3.10)) can be mapped onto the Keldysh space, where it is represented by a matrix:

$$
G_{c_k}(1, 1') \mapsto \hat{G} \equiv \begin{bmatrix}
\hat{G}_{11} & \hat{G}_{12} \\
\hat{G}_{21} & \hat{G}_{22}
\end{bmatrix} \equiv \begin{bmatrix}
\hat{G}^{++} & \hat{G}^{+-} \\
\hat{G}^{-+} & \hat{G}^{--}
\end{bmatrix}.
$$

(3.11)

For $t_1$ and $t_1'$ residing on the branch $c_i$ and $c_j$ the component $\hat{G}_{ij}$ is defined as $G_{c_k}(1, 1')$. Analogously the “+” (“-”) sign denotes the upper (lower) branch of the contour. Explicitly these components are given by

$$
\begin{align*}
\hat{G}_{11}(1, 1') &\equiv \hat{G}^{++}(1, 1') = -i \langle T (\psi_H(1) \psi_H(1')) \rangle \\
\hat{G}_{12}(1, 1') &\equiv \hat{G}^{+-}(1, 1') = G^< (1, 1') \\
\hat{G}_{21}(1, 1') &\equiv \hat{G}^{-+}(1, 1') = G^> (1, 1') \\
\hat{G}_{22}(1, 1') &\equiv \hat{G}^{--}(1, 1') = -i \langle \tilde{T} (\psi_H(1) \psi_H(1')) \rangle.
\end{align*}
$$

(3.12)

Performing a “rotation” in Keldysh space [Ke64], it is possible to map this representation of $\hat{G}$ onto

$$
\hat{G} \mapsto \begin{bmatrix}
0 & G^A \\
G^R & G^K
\end{bmatrix},
$$

with the already defined retarded, advanced and Keldysh Green’s functions $G^R$, $G^A$ and $G^K$, respectively (see equation (3.5)). Compared to the representation above this one has the advantage that the components of $\hat{G}$ are not linearly dependent any more, thus redundancy is removed [RS86].
As an example for a perturbative expansion of the contour-ordered Green’s function, let us calculate the lowest order terms for the case of a coupling of particles to an external classical field \( V(\mathbf{x},t) \). Owing to equation (3.10) the contour-ordered Green’s function is

\[
G(1, 1') = -i \text{ Tr} \left( \rho_0 T_c \left( e^{-i \int_c \! d\tau \int d\mathbf{x} \, V(\mathbf{x},\tau) \psi_{H_0}(\mathbf{x},\tau) \psi_{H_0}^\dagger(1) \psi_{H_0}^\dagger(1')} \right) \right) . \tag{3.13}
\]

Doing an expansion of the exponential, we yield for the zeroth-order term just the free contour Green’s function and for the first-order term an expression with an average over strings of field operators [Ra07]:

\[
G^{(0)}(1, 1') = -i \text{ Tr} \left( \rho_0 T_c \left( \psi_{H_0}(1) \psi_{H_0}^\dagger(1') \right) \right) \\
G^{(1)}(1, 1') = (-i)^2 \int d\mathbf{x}_2 \int_c d\tau_2 \, V(2) \text{ Tr} \left( \rho_0 T_c \left( \psi_{H_0}^\dagger(2) \psi_{H_0}(2) \psi_{H_0}(1) \psi_{H_0}^\dagger(1') \right) \right) . \tag{3.14}
\]

### 3.5 Wick’s theorem

If we apply the perturbative expansion on the exponential in the generic expression for the contour-order Green’s function (3.10), we get products of interaction Hamiltonians appearing under contour ordering. In the interaction picture these are in general strings of field operators weighted by the statistical operator of the free part of the Hamiltonian, which is quadratic in these fields. In order to decompose such strings into products involving the free contour Green’s function we use Wick’s theorem [Ra07].

Wick’s theorem allows to decompose a quadratically weighted trace of a contour-ordered string of field operators into a sum over all possible pairwise products:

\[
\langle T_c (c(\tau_n) c(\tau_{n-1}) \ldots c(\tau_2) c(\tau_1)) \rangle = \sum_{a.p.p.} \prod_{q,q'} \langle T_c (c_q(\tau) c_{q'}(\tau')) \rangle , \tag{3.15}
\]

where \( c \) denote either a creation or annihilation operator and the sum is over all possible pairs (a.p.p.) of the \( n \) operators, not distinguishing ordering within pairs. In this regard we relinquish to show the proof of Wick’s theorem, since it goes beyond the constraint right here. A detailed proof can be found in chapter 4.3.3 of [Ra07].

Instead we want to have a look at some examples. If the regarded string on the left side of equation (3.15) contains an odd number of operators, the expression equals to zero, due to the fact that the expectation value is with respect to the thermal equilibrium state. An odd number of operators indeed leads to a matrix element between states with different numbers of particles, which is zero due to orthogonality of the states. Taking as an instance for an even number of operators a string with four operators into account, we yield by using Wick’s theorem

\[
\langle T_{c_1} (a(\tau_1) a^\dagger(\tau_2) a(\tau_3) a^\dagger(\tau_4)) \rangle = \langle T_{c_1} (a(\tau_1) a^\dagger(\tau_2)) \rangle \langle T_{c_1} (a(\tau_3) a^\dagger(\tau_4)) \rangle + \langle T_{c_1} (a(\tau_1) a^\dagger(\tau_4)) \rangle \langle T_{c_1} (a(\tau_3) a^\dagger(\tau_2)) \rangle ,
\]
where terms that do not pair creation and annihilation operators are deleted, due to the same reason as explained for an odd number of operators [Ra07].

Since Wick’s theorem establishes a connection between strings of field operators and the free thermal equilibrium contour-ordered Green’s functions, which are precisely given by the right side of the equation (3.15), the perturbative expansion of the contour-order Green’s function can be expressed in terms of the free thermal equilibrium contour-ordered Green’s function. Indeed, these expressions yielded from perturbation theory are in the most cases unwieldy. That is why it is convenient to employ the method introduced by Feynman, which represents the perturbative expressions by diagrams [Ra07].

### 3.6 Aside: Feynman diagrammatics

In this regard we will only discuss the non-equilibrium Feynman diagrammatics for the special case considered already before, namely for the coupling of an assembly of identical particles to an external classical field $V(x,t)$. The contour-ordered Green’s function for this purpose is given by equation (3.13). The first-order term of the perturbative expansion (3.14) can be rewritten by applying Wick’s theorem to

$$G^{(1)}(1,1') = \int dx_2 \int d\tau_2 \, G^{(0)}(1,2) \, V(x_2) \, G^{(0)}(2,1') \, ,$$

and equivalent expressions can be yielded for higher order terms. The perturbative expansion of the contour-ordered Green’s function in diagrammatics are depicted in figure 7, where the zeroth-order term and the first-order term of the Green’s function are given by the first and second diagram in the infinite series, respectively [Ra07, RS86].

$\textbf{Fig. 7:}$ Perturbative expansion of the contour-ordered Green’s function $G(1,1')$ (equation (3.13)). The zeroth-order and first-order terms (compare to equation (3.14)) are represented by the first and second diagram in the infinite series, respectively.

The infinite expansion of exponential in the considered contour-ordered Green’s function for a particle coupled to a scalar potential (see figure 7) can be captured in the Dyson equation

$$G(1,1') = G_0(1,1') + \int dx_2 \int d\tau_2 \, G_0(1,2) \, V(x_2, \tau_2) \, G(2,1') \, ,$$

with $G_0(1,1') \equiv G^{(0)}(1,1')$ being the free thermal equilibrium contour-ordered Green’s function [Ra07, RS86].

$^9$Notice, that $n$-th order expressions in perturbation theory lead to $n$ identical contributions. These factor cancels out each time with the factor of the exponential expansion.
The corresponding Hamiltonian is given by

\[ H_0 = \sum_n \varepsilon_n \, c_n^\dagger \, c_n = \sum_n H_n , \]

with \( H_n = \varepsilon_n \, c_n^\dagger \, c_n \) as the single level Hamiltonian and \( c_n^\dagger \) (\( c_n \)) being the creation (annihilation) operator for fermions. In the Green’s functions the field operators occur time-dependent and thus in the interaction picture, which means \( c_n(t) = e^{iH_0 t} \, c_n \, e^{-iH_0 t} \) (compare to equation (3.1)). Differentiate \( c_n(t) \) with respect to \( t \) results in:

\[
\frac{dc_n(t)}{dt} = i \, e^{iH_0 t} \left[ H_0, c_n \right] \, e^{-iH_0 t} = -i \, \varepsilon_n \, c_n(t) ,
\]

where we have used the fact that

\[
\left[ H_0, c_n \right] = \sum_m \varepsilon_m \left( c_m^\dagger \, c_m \, c_n - c_n \, c_m^\dagger \, c_m \right) = \sum_m \varepsilon_m \left( -\delta_{nm} c_m \right) = -\varepsilon_n \, c_n .
\]

3.7 Example on Keldysh Green’s function

As a first example we want to calculate the contour-ordered Green’s function in Keldysh space (see equations (3.11) and (3.12)) for a system with discrete fermion energy levels \( \varepsilon_n \). The equation of motion (3.16) for \( c_n(t) \) we yield:

\[
\frac{dc_n(t)}{dt} = c_n \, e^{-i\varepsilon_n t} ,
\]

If we plug this equation in the definition of the Green’s function, its components read

\[
G_{nm}^{++}(1,1') = i \, \langle c_n(1) \, c_m^\dagger(1') \rangle = i \, e^{i\varepsilon_n t'} \, e^{-i\varepsilon_m t_1} \, \langle c_n^\dagger \, c_m \rangle = i \, e^{i\varepsilon_n (t'-t_1)} \, f(\varepsilon_n) \, \delta_{nm}
\]

\[
G_{nm}^{--}(1,1') = -i \, \langle c_n(1) \, c_m^\dagger(1') \rangle = -i \, e^{-i\varepsilon_n (t_1-t')} \left( 1 - f(\varepsilon_n) \right) \, \delta_{nm} .
\]

Here \( \langle c_n^\dagger \, c_m \rangle = f(\varepsilon_n) \, \delta_{nm} \) describes the thermal equilibrium occupation of the levels given by the Fermi distribution and we have used \( [c_n, c_m^\dagger] = \delta_{nm} \). Referred to equation (3.12) \( G_{nm}^{++} \) and \( G_{nm}^{--} \) can be expressed in terms of these two Green’s function

\[
G_{nm}^{++}(1,1') = -i \, \langle T(c_n(1) \, c_m^\dagger(1')) \rangle = G_{nm}^{--}(1,1') \, \theta(t_1 - t') + G_{nm}^{--}(1,1') \, \theta(t_1 - t')
\]

\[
G_{nm}^{--}(1,1') = -i \, \langle T(c_n(1) \, c_m^\dagger(1')) \rangle = G_{nm}^{++}(1,1') \, \theta(t_1 - t') + G_{nm}^{++}(1,1') \, \theta(t_1 - t') .
\]

Same could be done for the retarded, advanced and Keldysh Green’s function (compare to equation (3.5)). For the retarded Green’s function we explicitly yield

\[
G_{nm}^R(1,1') = \theta(t_1 - t') \left( G_{nm}^{++}(1,1') - G_{nm}^{--}(1,1') \right) = -i \, e^{i\varepsilon_n (t_1 - t')} \, \theta(t_1 - t') \, \delta_{nm} .
\]

For our calculations in the next chapter we need to perform a Fourier transformation from time to frequency space of the retarded Green’s function. To have a first feeling about the Fourier transformation we want to perform such already here for this example. Therefore we simplify the problem by considering only the Hamiltonian of one level \( H_n \).
and set $t_1 = 0$. Doing this we can just neglect the indices $n$ and we get for the retarded Green’s function

$$G^R(t) = -i \theta(t) e^{-i\epsilon t}.$$  

If we perform the direct Fourier transformation of $G^R(t)$ we see that we have to add a small purely complex variable $i\eta$ with $\eta \to 0^+$ to the frequency in order to solve the integral. This variable causes a necessary decrease of the function to be integrated and we get

$$G^R(\omega) = -i \int_{-\infty}^{\infty} dt \theta(t) e^{-i\epsilon t} e^{i(\omega+i\eta)t} = -i \int_0^{\infty} dt e^{-\eta t} e^{-i(\epsilon-i\omega)t}$$

$$= \frac{1}{(\omega + i\eta) - \epsilon} = \frac{1}{\omega - \epsilon} - i\pi \delta(\omega - \epsilon),$$  

(3.17)

having used the representation of the delta distribution for $\eta \to 0$ in the last equality. The first term in the last expression is the so-called principal part.

We should obtain the same result, if we perform the Fourier transformation on the equation of motion for the Green’s function. The equation of motion is

$$i \frac{d}{dt} G^R(t) = \delta(t) + \epsilon G^R(t).$$

To get the Green’s function in frequency domain, we perform a Fourier transformation of the equation of motion. If we apply the standard rule for time derivations and replace $i \frac{d}{dt} G^R(t) \to \omega G^R(\omega)$, the result we get after solving for $G^R(\omega)$ is:

$$\omega G^R(\omega) = 1 + \epsilon G^R(\omega) \quad \Rightarrow \quad G^R(\omega) = \frac{1}{\omega - \epsilon}.$$  

(3.18)

Comparing the both results (3.17) and (3.18) we recognize that in the latter one the small variable $\eta$ is missing in the denominator, which is crucial for the back transformation, where the Residue theorem has to be regarded. Therefore we see that we have to be careful by performing the Fourier transformation on the equation of motion in order to obtain the Green’s functions in frequency domain.
4 Electron transport through closed Aharonov-Bohm interferometer

As a more striking example for the introduced theory we want to study the electron transport through a closed Aharonov-Bohm interferometer adapted to [KK02].

4.1 Model

We consider a closed Aharonov-Bohm interferometer containing two non-interacting single-level quantum dots like depicted in figure 8. The two quantum dots are coupled to leads and the magnetic flux in the closed loop can be varied.

The Hamiltonian of the whole system is given by the standard Hamiltonians for such a problem (see for example also [CC71, YW14, LA14]):

\[
H = H_{\text{leads}} + H_{\text{dots}} + H_{\text{tunnelling}}
\]

\[
= \sum_{kr} \varepsilon_{kr} a_{kr}^\dagger a_{kr} + \sum_{i=1,2} \varepsilon_i c_i^\dagger c_i + \sum_{kri} \left( t_{ri} a_{kr}^\dagger c_i + t_{ri}^* c_i^\dagger a_{kr} \right),
\]

where \(a_{kr}^\dagger\) and \(a_{kr}\) are the creation and annihilation operators for electrons with quantum number \(k\) in the left and right lead \((r = L, R)\) respectively. The Fermi operators for the dot states with the energies \(\varepsilon_i\) (measured from the Fermi energy), which can be varied by applied gate voltages, are \(c_i^\dagger\) and \(c_i\) \((i = 1, 2)\). We assume that the tunnel matrix elements \(t_{ri}\) are energy-independent and moreover that the coupling strength \(|t_{ri}| = t\) is symmetric.

\[\text{Fig. 8: Schematic model of the regarded system. A closed Aharonov-Bohm interferometer contains two non-interacting single-level quantum dots, which are indirectly coupled to each other via the leads.}\]

Since there is tunnelling from the leads to the dots, each dot has a finite linewidth \(\Gamma = \Gamma_L + \Gamma_R\), which can be expressed in terms of the density of states \(N_r\) in the lead \(r = L, R\) by \(\Gamma_r = 2\pi t^2 N_r\).

The phase shift induced by the magnetic flux \(\Phi\) is modelled by an Aharonov-Bohm phase and can be incorporated via the tunnel matrix elements, which become in a symmetric gauge \(t_{L1}^* = t_{L2} = t_{R2}^* = t_{R1} = te^{i\varphi/4}\), where \(\varphi \equiv 2\pi \Phi/\Phi_0\) with the flux quantum \(\Phi_0 = h/e\) (see figure 8).
For the further considerations it is convenient to define the average level energy 
$$\bar{\varepsilon} = (\varepsilon_1 + \varepsilon_2)/2$$ and the energy difference between the two levels of the dots 
$$\Delta \varepsilon = \varepsilon_2 - \varepsilon_1$$. Notice that in the regarded model there is no direct interaction between the two quantum dots, neither Coulomb repulsion or tunnel coupling. In fact the levels are coupled indirectly to each other via the coupling to the leads.

Performing an appropriate experiment the accessible quantity is the linear conductance 
$$G_{\text{lin}} = \left( \frac{\partial I}{\partial V} \right)_{V=0}$$, which can be expressed in terms of the transmission $$T(\omega)$$ for an electron with energy $$\omega$$ and the derivative of the Fermi-Dirac distribution by

$$G_{\text{lin}} = -\frac{e^2}{h} \int d\omega \ T(\omega) \ f'(\omega) \ . \tag{4.2}$$

According to [MW92] the transmission $$T(\omega)$$ is given by

$$T(\omega) = \text{Tr} \left( G^A(\omega) \Gamma^R G^R(\omega) \Gamma^L \right) \ , \tag{4.3}$$

with the retarded and advanced dot Green’s functions $$G^R(\omega)$$ and $$G^A(\omega)$$, respectively. The tunnel coupling to the left and right lead is described by $$\Gamma^L$$ and $$\Gamma^R$$. Since the underlying model contains two quantum dots, all these quantities have a $$2 \times 2$$ matrix structure.

### 4.2 Derivation of the Green’s function

In order to derive the retarded and advanced Green’s functions in frequency domain, we start at the definition for the (dot-dot) retarded Green’s function in time domain (compare to equation (3.5) with $$t_\nu = 0$$):

$$G_{ij}^R(t) = -i \theta(t) \left\langle \left\{ c_i(t), c_j^\dagger(0) \right\} \right\rangle \ , \tag{4.4}$$

where the indices $$ij$$ refer to the dots ($$i, j = 1, 2$$). Since we want to employ the equation-of-motion approach in order to obtain the exact equilibrium Green’s function, we first consider the derivation of $$c_i(t) = e^{iHt} c_i e^{-iHt}$$:

$$\frac{dc_i(t)}{dt} = iH e^{iHt} c_i e^{-iHt} + e^{iHt} c_i (-iH) e^{-iHt} = -i e^{iHt} [c_i, H] e^{-iHt} \ .$$

Thus the equation of motion for $$G_{ij}^R(t)$$ is

$$i \frac{d}{dt} G_{ij}^R(t) = \frac{d}{dt} \left( \theta(t) \left\langle \left\{ c_i(t), c_j^\dagger(0) \right\} \right\rangle \right)
= \delta(t) \left\langle \left\{ c_i(0), c_j^\dagger(0) \right\} \right\rangle + \theta(t) \left\langle \left\{ \frac{d}{dt} c_i(t), c_j^\dagger(0) \right\} \right\rangle
= \delta(t) \delta_{ij} - i \theta(t) \left\langle \left\{ e^{iHt} [c_i, H] e^{-iHt}, c_j^\dagger(0) \right\} \right\rangle \ . \tag{4.5}$$
In order to dissolve the commutator we consider the three parts of the Hamiltonian separately. Since we have $[c_i, a_{kr}^\dagger a_{kr}] = 0$, the commutator with the Hamiltonian of the leads equals to zero $[c_i, H_{\text{leads}}] = 0$. The commutator with the dot Hamiltonian is

$$[c_i, H_{\text{dots}}] = \sum_j \varepsilon_j [c_i, c_j^\dagger c_j] = \varepsilon_i c_i,$$

and the commutator with the tunnelling Hamiltonian is

$$[c_i, H_{\text{tunnelling}}] = \sum_{krj} \left( t_{rj} [c_i, a_{kr}^\dagger c_j] + t_{rj}^* [c_i, c_j^\dagger a_{kr}] \right) = \sum_{kr} t_{ri}^* a_{kr}.$$

Using this equations we can rewrite the equation of motion for $G_{ij}^R(t)$ (4.5) to

$$i \frac{d}{dt} G_{ij}^R(t) = \delta(t) \delta_{ij} + \varepsilon_i G_{ij}^R(t) + \sum_{kr} t_{ri}^* G_{krj}^R(t),$$

having introduced the lead-dot retarded Green’s function

$$G_{krj}^R(t) = -i \theta(t) \left\{ \{ a_{kr}(t), c_j^\dagger(0) \} \right\}.$$

Thus we have related the derivative of the dot-dot Green’s function to itself and the new introduced lead-dot Green’s functions. Since the aim is to get a closed equation for the dot-dot Green’s function, the equation of motion for the lead-dot Green’s function is considered:

$$i \frac{d}{dt} G_{krj}^R(t) = -i \theta(t) \left\{ e^{iHt} [a_{kr}, H] e^{-iHt}, c_j^\dagger(0) \right\}.$$

Once again we have a separate look on the commutator for the three parts of the Hamiltonian. The commutator with the Hamiltonian of the dots is zero $[a_{kr}, H_{\text{dots}}] = 0$, since $[a_{kr}, c_i^\dagger c_i] = 0$. For the other two commutators we yield

$$[a_{kr}, H_{\text{leads}}] = \sum_{k'r'} \varepsilon_{k'r'} [a_{kr}, a_{k'r'}^\dagger a_{kr}] = \varepsilon_{kr} a_{kr},$$

$$[a_{kr}, H_{\text{tunnelling}}] = \sum_{k'r'i} \left( t_{r'i} [a_{kr}, a_{k'r'}^\dagger c_i] + t_{r'i}^* [a_{kr}, c_i^\dagger a_{k'r'}] \right) = \sum_i t_{ri} a_{kr}.$$

Plugging these commutators in the equation of motion (4.8) it results:

$$i \frac{d}{dt} G_{krj}^R(t) = \varepsilon_{kr} G_{krj}^R(t) + \sum_i t_{ri} G_{ij}^R(t).$$

If we apply the Fourier transformation from time space to frequency space we have to introduce a small purely complex variable $i\eta$ with $\eta \to 0^+$ in the exponent in order to
have a function that decreases to zero for $t \to \infty$ (compare to example discussed in section 3.7). Considering this we yield from equations (4.6) and (4.9)

\[
(\omega + i\eta) \, G^R_{ij}(\omega) = \delta_{ij} + \varepsilon_i \, G^R_{ij}(\omega) + \sum_{kr} t^*_{ri} \, G^R_{krj}(\omega)
\]

\[
(\omega + i\eta) \, G^R_{krj}(\omega) = \varepsilon_{kr} \, G^R_{krj}(\omega) + \sum_i t_{ri} \, G^R_{ij}(\omega).
\]  

(4.10)

Solving the first equation for $G^R_{ij}(\omega)$ and introducing the free retarded Green’s function $g^R_i(\omega) = (\omega - \varepsilon_i + i\eta)^{-1}$, which excludes the tunnelling between the leads and the dots (compare to example of section 3.7), it results

\[
G^R_{ij}(\omega) = g^R_i(\omega) \, \delta_{ij} + g^R_i(\omega) \sum_{kr} t^*_{ri} \, G^R_{krj}(\omega),
\]

with represents the Dyson equation for the system with respect to the tunnelling Hamiltonian.

Starting with the equations (4.10) and plugging them into each others iteratively we can derive a closed set of equations for the components of the retarded Green’s function.

Representatively we shall do this for $G^R_{11}(\omega)$ and $G^R_{21}(\omega)$ (we will use the abbreviation $G^R_{ij}(\omega) \equiv G_{ij}$). In this case we start with equation (4.10) for $G_{11}$:

\[
(\omega + i\eta) \, G_{11} = 1 + \varepsilon_1 \, G_{11} + \sum_k (t^*_{L1} \, G_{kL1} + t^*_{R1} \, G_{kR1}),
\]

and plug in the equations (4.10) for $G_{kL1}$ and $G_{kR1}$:

\[
(\omega + i\eta) \, G_{11} = 1 + \varepsilon_1 \, G_{11} + \sum_k \left[ t^*_{L1} \left( -\frac{t_{L1} \, G_{11} + t_{L2} \, G_{21}}{\varepsilon_{kL} - \omega - i\eta} \right) + t^*_{R1} \left( -\frac{t_{R1} \, G_{11} + t_{R2} \, G_{21}}{\varepsilon_{kR} - \omega - i\eta} \right) \right],
\]

Since neither $t_{ri}$ nor the Green’s functions in this expression are $k$-dependent, we can define the abbreviation $A_r = \sum_k (\varepsilon_{kr} - \omega - i\eta)^{-1}$. Doing the same calculations for $G_{21}$ we get the equation system:

\[
(\omega + i\eta) \, G_{11} = 1 + G_{11} \left( \varepsilon_1 - t^2 (A_L + A_R) \right) - t^2 \, G_{21} \left( A_L \, e^{i\varphi/2} + A_R \, e^{-i\varphi/2} \right)
\]

\[
(\omega + i\eta) \, G_{21} = G_{21} \left( \varepsilon_2 - t^2 (A_L + A_R) \right) - t^2 \, G_{11} \left( A_L \, e^{-i\varphi/2} + A_R \, e^{i\varphi/2} \right),
\]

which we solve for $G_{11}$ and $G_{21}$. Eventually we obtain the solutions:

\[
G_{11} = \left[ \omega + i\eta - \varepsilon_1 + t^2 (A_L + A_R) - t^4 \cdot \frac{A_L^2 + A_R^2 + A_L A_R (e^{-i\varphi} + e^{i\varphi})}{\omega + i\eta - \varepsilon_2 + t^2 (A_L + A_R)} \right]^{-1}
\]

\[
G_{21} = \left[ t^2 (A_L \, e^{i\varphi/2} + A_R \, e^{-i\varphi/2}) - (\omega + i\eta - \varepsilon_1 + t^2 (A_L + A_R)) (\omega + i\eta - \varepsilon_2 + t^2 (A_L + A_R)) \right]^{-1}.
\]
For the further evaluation we consider

\[
t^2(A_L + A_R) = t^2 \sum_{kr} \frac{1}{\epsilon_{kr} - \omega - i\eta} = t^2 \sum_{kr} \frac{1}{\epsilon_{kr} - \omega} + i\pi t^2 \sum_{kr} \delta(\epsilon_{kr} - \omega)
\]

\[
= t^2 \sum_r \int d\omega' \frac{N_r}{\omega' - \omega} + i\pi t^2 \sum_r N_r = \Delta \varepsilon(\omega) + i\frac{\Gamma}{2} \approx i\frac{\Gamma}{2},
\]

where we have assumed that the energy deviation \(\Delta \varepsilon(\omega)\) (principal part) is small, since we consider only a narrow frequency band in the energy dispersion, and thus we have neglected the first term and used the relation between the density of states and the linewidth \(\Gamma = \Gamma_L + \Gamma_R\) of the dot levels.

With this expression and under the further assumption that the two leads are equal and thus symmetric, which means \(\Gamma_L = \Gamma_R\), we can finally yield

\[
G_{11} = \frac{\omega - \varepsilon_2 + i\frac{\Gamma}{2}}{\frac{1}{4} \Gamma^2 \cos^2 \frac{\varphi}{2} + (\omega - \varepsilon_1 + i\frac{\Gamma}{2}) (\omega - \varepsilon_2 + i\frac{\Gamma}{2})},
\]

\[
G_{21} = \frac{-i\frac{\Gamma}{2} \cos \frac{\varphi}{2}}{\frac{1}{4} \Gamma^2 \cos^2 \frac{\varphi}{2} + (\omega - \varepsilon_1 + i\frac{\Gamma}{2}) (\omega - \varepsilon_2 + i\frac{\Gamma}{2})}.
\]

If we do analogous calculations for \(G_{22}\) and \(G_{12}\) we get for the retarded Green’s function:

\[
G^R(\omega) = \frac{1}{\frac{1}{4} \Gamma^2 \cos^2 \frac{\varphi}{2} + (\omega - \varepsilon_1 + i\frac{\Gamma}{2}) (\omega - \varepsilon_2 + i\frac{\Gamma}{2})} \begin{pmatrix} \omega - \varepsilon_2 + i\frac{\Gamma}{2} & -i\frac{\Gamma}{2} \cos \frac{\varphi}{2} \\ -i\frac{\Gamma}{2} \cos \frac{\varphi}{2} & \omega - \varepsilon_1 + i\frac{\Gamma}{2} \end{pmatrix}^{-1},
\]

(4.11)

and for the advanced Green’s function \(G^A(\omega)\) the complex conjugate.

Now we can apply equation (4.3) in order to obtain the transmission \(T(\omega)\). Therefore we have to regard the tunnel coupling matrices, which are for the symmetric leads considered here, described by

\[
\Gamma^L = \frac{\Gamma}{2} \begin{pmatrix} 1 & e^{i\varphi/2} \\ e^{-i\varphi/2} & 1 \end{pmatrix},
\]

and once again the complex conjugate for \(\Gamma^R\).

Finally, the transmission reads:

\[
T(\omega) = \frac{\Gamma^2 \left[ (\omega - \bar{\varepsilon})^2 \cos^2 \frac{\varphi}{2} + \left( \frac{\Delta \varepsilon}{2} \right)^2 \sin^2 \frac{\varphi}{2} \right]}{\left[ (\omega - \bar{\varepsilon})^2 - (\frac{\Delta \varepsilon}{2})^2 - (\frac{\Gamma}{2})^2 \sin^2 \frac{\varphi}{2} \right]^2 + (\omega - \bar{\varepsilon})^2 \Gamma^2},
\]

(4.12)

and thus the linear conductance can be determined via equation (4.2).
4.3 Discussion of the results

As a last point we want to discuss the obtained transmission through the regarded device for several special regimes. Therefore we variate the magnetic flux $\Phi$ for certain values of the average level energy $\bar{\varepsilon}$ and the energy difference $\Delta \varepsilon$.

First of all we consider the simplest case for $\bar{\varepsilon} = 0$ as well as $\Delta \varepsilon = 0$. Then the energy levels in the two dots are equal to the Fermi energy of the leads. The transmission for the magnetic flux values of $\Phi = 0, \frac{1}{4} \Phi_0, \frac{1}{2} \Phi_0$ with the magnetic flux quantum $\Phi_0 = h/e$ are depicted in figure 9a. The spectra for $\Phi = \frac{3}{4} \Phi_0$ and $\Phi = \Phi_0$ are the same as for $\Phi = \frac{1}{4} \Phi_0$ and $\Phi = 0$, respectively.

Fig. 9: Transmission $T(\omega)$ for various magnetic fluxes applied ($\Phi = 0, \frac{1}{4} \Phi_0, \frac{1}{2} \Phi_0$). (a) Average level energy $\bar{\varepsilon} = 0$ and energy difference $\Delta \varepsilon = 0$. (b) Average level energy $\bar{\varepsilon} = 0$ and energy difference $\Delta \varepsilon = \Gamma$.

With equation (4.12) we can calculate the transmission for this regime:

$$T(\omega) = \frac{\Gamma^2 \omega^2 \cos^2 \frac{\varphi}{2}}{\left[\omega^2 - \left(\frac{\Gamma}{2}\right)^2 \sin^2 \frac{\varphi}{2}\right]^2 + \omega^2 \Gamma^2}.$$  

For $\Phi = 0$ and so $\varphi = 0$ (blue curve) we recognize that the transmission is equivalent to the one of a single dot, but has the double width $\Gamma$ (instead of $\Gamma/2$). For $\omega = 0$ we have complete transmission ($T = 1$), which decreases with increasing detuning of the electron frequency with respect to the energy levels in the dots.

Applying a magnetic flux of $\Phi = \frac{1}{4} \Phi_0$ the transmission decreases in general (red curve). That can be attributed to the cosine function in numerator. Moreover, we recognize the feature of totally suppressed transmission for $\omega = 0$, which appears as a sharp dip in transmission spectrum. Owing to [KK02] this anomaly of suppressed transmission is not captured by a first- or second-order perturbation expansion in $\Gamma$. We affiliate this feature to the fact of destructive interference of electron waves. One electron wave passing only one dot thereby interferes with electron waves that are backscattered at the leads.
multiple times and go multiple round-trips via both dots and thus accumulate different phases, which cancel out in the end.

For $\Phi = \frac{1}{2}\Phi_0$ (green curve) the transmission is suppressed independently of $\omega$ due to destructive interference of the electron waves going through one dot with the electron waves through the other dot.

Increasing the magnetic flux further the transmission has the inverse increasing behaviour, since the flux appears in the transmission in the quadratic cosine and sine function. Moreover, both the numerator and the denominator are periodic in $\Phi_0$, thus we get same results if we add multiples of the magnetic flux quantum to the magnetic flux.

Next we want to consider the regime $\bar{\epsilon} = \Gamma$ and $\Delta \epsilon = 0$. Here both dots are shifted in the same manner away from the Fermi energy of the leads by $\Gamma$. Therefore the transmission spectra are also shifted by $\Gamma$, but are apart from that equal to the one shown in figure 9a.

We obtain more interesting features for the regime $\bar{\epsilon} = 0$ and $\Delta \epsilon = \Gamma$, which is presented in figure 9b for the magnetic flux values of $\Phi = 0, \frac{1}{4}\Phi_0, \frac{1}{2}\Phi_0$. The energy levels in both dots have now a energy difference $\Gamma$ and are symmetric with respect to the Fermi energy of the leads. The spectra for $\Phi = \frac{3}{4}\Phi_0$ and $\Phi = \Phi_0$ are here once again the same as for $\Phi = \frac{1}{4}\Phi_0$ and $\Phi = 0$, respectively.

For $\Phi = 0$ (blue curve) the transmission is suppressed for $\omega = 0$ and has two maxima values next to it. The two maxima values we affiliate to resonant tunnelling through one of the dots. The suppressed transmission is a so-called Fano-resonance, where the electron waves through both dots interfere destructively.

The two maxima move closer together and the linewidth decreases for finite magnetic flux like $\Phi = \frac{1}{4}\Phi_0$ (red curve). Also the transmission is not suppressed any more completely for $\omega = 0$ due to the additional phase shift that electron waves accumulate on the ways through the dots.

For $\Phi = \frac{1}{2}\Phi_0$ (green curve) the suppression of transmission for $\omega = 0$ vanishes completely and we get a broadened maxima of full transmission but with a narrowed linewidth at $\omega = 0$. Here we have resonant tunnelling, since electron waves going through one of the dots interfere constructively.

For more physically motivated explanations of the features presented here, one has to evaluate the Green’s function describing the transmission from the left to right lead, which goes beyond the constraints right here.
5 Summary and outlook

Within the presented report on the Projektpraktikum we have studied the formalism of quantum field theory of non-equilibrium states based on the Keldysh Green's function and presented an application of these technique for a striking example.

Therefore first of all the basic principles of quantum mechanics and second quantization have been recalled. Especially the definition of the creation and annihilation fields on the multi-particle state space have simplified the description a lot, since the whole kinematics of a many-body system as well as the operators representing its physical quantities thus were expressed in terms of just these two objects.

Then we have dealt with quantum dynamics and the study of the correlations functions for the quantum fields or the Green’s functions for non-equilibrium states. Here the perturbation theory on the Green’s function including the closed time path formalism and Wick’s theorem have been discussed and the Keldysh formulation has been introduced. In addition we have related our considerations to further quantum theory, namely the Feynman diagrammatics and the Dyson equation.

Last but not least we have concentrated on transport phenomena and presented a striking application of the theory introduced before. In this regard we have studied the transport through an closed Aharonov-Bohm interferometer containing two non-interacting single level quantum dots. We have derived an exact expression for the transmission through the device by calculating the Green’s functions and finally discussed the results for specific regimes.

Further work for the future is on the one hand the explanation of the features in the transmission spectrum presented in the last chapter by elevating the Green’s function describing the transmission from the left to right lead. Additionally, the considerations done here for two single-level dots can be expanded to a plaquette of single-level dots (compare to [LA14]) or to multiple-level dots.
References


