Kapitel 8

Nonequilibrium Green Functions

Real-time nonequilibrium Green functions (NEGFs)[1] naturally appear in the extension of the ground state Green functions theory and of the Matsubara formalism of (equilibrium) quantum many-body theory [54, 55] to situations out of equilibrium. In this respect, the term "one-particle NEGF", cf. Section 8.2.3, has a complex meaning including the notion "propagator" (retarded Green function) as well as "correlation function". The great success of NEGFs is, in general, due to the fact that fundamentals of ground state and equilibrium theory that include Feynman rules and diagram techniques, can be applied, without major conceptual modifications, also to nonequilibrium situations. This circumstance is sometimes referred to as "analytic continuation".

Nonequilibrium Green functions are one of the most powerful approaches to nonequilibrium quantum statistical mechanics and quantum kinetic equations [Bon98]. Their development was pioneered by *Martin* [56] and *Schwinger* [Sch61] and was expedited by *Kadanoff* and *Baym* [27] in the USA and, in parallel, by *Keldysh* [Kel64] in the USSR, see also Ref. [BJST19]. The main achievements were rendered in the late 1950s and early 1960s and were stimulated by quantum field theory. Since then, NEGFs have become standard tools to derive quantum transport models on various levels of sophistication, e.g., [23, 24, 25, 58, HK09], and have been applied to give quantum corrections and many-body improvements to the Boltzmann equation [59, 60, SKB00]. On the other hand, NEGFs have nowadays[2] reached the potential to nume-

[1] This chapter is based on a number of previous book chapters and reviews. In particular, it is an extension of the presentation given in [BB13] and has been written together with Simon Groth.

[2] Due to the continuously increasing power of computers.

rically treat time-dependent quantum systems *from first principles*[3]. To this end, one solves the basic equations of motion for the one-particle NEGF – the Keldysh-Kadanoff-Baym equations (KBEs) – and obtains statistical and dynamical information about the system even in the presence of strong external driving forces, far from the linear response regime.

8.1 Introduction

Our goal is the description of time-dependent processes in a fully interacting quantum many-body system of identical particles. Using second quantization with creation ($\hat{f}_i^\dagger$) and annihilation ($\hat{f}_i$) operators acting on a many-particle state $|\{n\}\rangle$ in Fock space[4], that are constructed from a complete set of single-particle orbitals, $|i\rangle$, we consider a generic time-dependent many-body hamiltonian,

$$\hat{H}(t) = \sum_{ij} \langle i|h(t)|j\rangle \, \hat{f}_i^\dagger \, \hat{f}_j + \frac{1}{2} \sum_{ij,kl} \langle ij|w|kl\rangle \, \hat{f}_i^\dagger \, \hat{f}_j^\dagger \, \hat{f}_l \, \hat{f}_k \; , \tag{8.1}$$
$$h(t) = t + v(t) \; ,$$

where t (v) is the kinetic (potential) energy of a single particle, w denotes the two-body interaction potential, and $\langle i|h(t)|j\rangle$ and $\langle ij|w|kl\rangle$ are the corresponding single-particle and two-particle matrix elements, cf. Chap. 3. The great advantage of the second quantization formulation is that the commutation (bosons) and anticommutation (fermions) relations[5] ,

$$[\hat{f}_i, \hat{f}_j^\dagger]_\mp = \delta_{ij} \; , \qquad [\hat{f}_i, \hat{f}_j]_\mp = [\hat{f}_i^\dagger, \hat{f}_j^\dagger]_\mp = 0 \; . \tag{8.2}$$

take care of the correct symmetry of the many-body state. Moreover, the creation and annihilation operators often facilitate a simple form of single-particle operators. While the number operator is just $\hat{n}_i = \hat{f}_i^\dagger \, \hat{f}_i$, the one-particle reduced density matrix (1pRDM) operator reads,

$$\hat{n}_{ij} = \hat{f}_i^\dagger \, \hat{f}_j \; . \tag{8.3}$$

This matrix of operators yields, after ensemble averaging, the familiar one-particle density matrix $n_{ij} = \langle \hat{n}_{ij} \rangle$. Below, we will express it in terms of the single-particle Green function, cf. Eq. (8.73).

[3] By this we mean that the equations of motion are formally exact with the accuracy determined by the choice (approximation) of a single function – the self-energy.

[4] $\hat{f}_i^\dagger$ ($\hat{f}_i$) adds (removes) a particle to (from) a spin orbital $|i\rangle$, e.g., Ref. [35] and Ch. 3.

[5] The (anti-)commutator is defined as $[\hat{a}, \hat{b}]_\mp = \hat{a}\hat{b} \mp \hat{b}\hat{a}$ where the minus (plus) refers to bosons (fermions), cf. Sec. 3.4.

In quantum mechanics, there exist different ways ("pictures") to account for time dependencies in a system. Despite their mathematical equivalence, the one or the other may allow for a more advantageous formulation of the problem considered in a particular case [for details, see Ch. 5]. NEGFs make essential use of the Heisenberg picture (H). In contrast to the Schrödinger picture (S), where the system's state vector $|\Psi_{\rm S}^{(N)}\rangle$ evolves in time and operators of observables are stationary[6], the Heisenberg picture allows for the operators to evolve in time while the state vectors remain time-independent. The transformation between S and H is mediated by the unitary time evolution operator[7], that obeys the Schrödinger equation,

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\hat{U}(t,t') = \hat{H}_{\rm S}(t)\,\hat{U}(t,t')\;, \tag{8.4}$$

or equivalently,

$$\mathrm{i}\hbar\frac{\partial}{\partial t'}\hat{U}(t,t') = -\hat{U}(t,t')\,\hat{H}_{\rm S}(t')\;, \tag{8.5}$$

with the initial condition $\hat{U}(t,t)=1$. The solution is[8],

$$\hat{U}(t,t') := \hat{T}\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t'}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\rm S}(\bar{t})} \quad,\ \text{if}\quad t>t'\;, \tag{8.6}$$

$$\hat{U}(t,t') := \hat{\tilde{T}}\mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\int_{t}^{t'}\mathrm{d}\bar{t}\,\hat{H}_{\rm S}(\bar{t})} \quad,\ \text{if}\quad t<t'\;, \tag{8.7}$$

$$\hat{U}(t,t')\,\hat{U}(t',t) = 1\;,$$

satisfying the group property

$$\hat{U}(t,t_1)\hat{U}(t_1,t') = \hat{U}(t,t')\,,\quad \text{where } t\geq t_1\geq t'\;, \tag{8.8}$$

and $\hat{H}_{\rm S}(t)$ is the full Hamiltonian. Further, we introduced the chronological ($\hat{T}$) and anti-chronological ($\hat{\tilde{T}}$) time-ordering operators defined by the following action on a product of arbitrary time-dependent operators:

$$\hat{T}\left\{\hat{A}_1(t_1)\,\ldots\,\hat{A}_n(t_n)\right\} = \sum_{\mathcal{P}}\Theta(t_{\mathcal{P}(1)}-t_{\mathcal{P}(2)})\,\ldots\,\Theta(t_{\mathcal{P}(n-1)}-t_{\mathcal{P}(n)}) \times \hat{A}_{\mathcal{P}(1)}(t_{\mathcal{P}(1)})\,\ldots\,\hat{A}_{\mathcal{P}(n)}(t_{\mathcal{P}(n)})\;, \tag{8.9}$$

$$\hat{\tilde{T}}\left\{\hat{A}_1(t_1)\,\ldots\,\hat{A}_n(t_n)\right\} = \sum_{\mathcal{P}}\Theta(t_{\mathcal{P}(1)}-t_{\mathcal{P}(2)})\,\ldots\,\Theta(t_{\mathcal{P}(n-1)}-t_{\mathcal{P}(n)}) \times \hat{A}_{\mathcal{P}(n)}(t_{\mathcal{P}(n)})\,\ldots\,\hat{A}_{\mathcal{P}(1)}(t_{\mathcal{P}(1)})\;, \tag{8.10}$$

[6] If they do not have an explicit time-dependence like for example a time dependent potential $\hat{v}(t)$.

[7] In matrix representation, the unitarity is expressed by $\hat{U}^\dagger\hat{U}=1$.

[8] The solution (8.6) is obtained by integrating equation Eq. (8.4) from t' to t leading to the integral-equation $\hat{U}(t,t') = 1 - \mathrm{i}\hbar\int_{t'}^{t}\mathrm{d}\hat{H}(\bar{t})\,\hat{U}(\bar{t},t')$, which can be iterated yielding Eq. (8.6). Similarly, the solution (8.7) is derived from Eq. (8.5).

where the sum runs over all permutations $\mathcal{P}$ of the n-tuple $(1, 2, \ldots, n)$, and the step function is defined by

$$\Theta(t - t') = \begin{cases} 1 & \text{if} \quad t > t' \,, \\ 0 & \text{if} \quad t < t' \,. \end{cases} \tag{8.11}$$

Thus, the two time-ordering operators are not defined for equal times of the operators to be ordered[9]!

Next, the Heisenberg operator $\hat{A}_{\mathrm{H}}$ corresponding to the Schrödinger operator $\hat{A}_{\mathrm{S}}$ is defined as

$$\hat{A}_{\mathrm{H}}(t) := \hat{U}(t_0, t)\, \hat{A}_{\mathrm{S}}\, \hat{U}(t, t_0) \,, \tag{8.12}$$

and fulfills the Heisenberg equation:

$$\mathrm{i}\hbar \frac{d}{dt} \hat{A}_{\mathrm{H}}(t) = \mathrm{i}\hbar \frac{\partial}{\partial t} \hat{A}_{\mathrm{H}}(t) = \left[\hat{A}_{\mathrm{H}}(t), \hat{H}_{\mathrm{H}}(t) \right]_- + \mathrm{i}\hbar \left(\frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \right)_{\mathrm{H}} . \tag{8.13}$$

As noted already above, the corresponding state vector[10]

$$|\Psi_{\mathrm{H}}^{(N)}(t)\rangle = \hat{U}(t_0, t)\, |\Psi_{\mathrm{S}}^{(N)}(t)\rangle = \hat{U}(t_0, t)\, \hat{U}(t, t_0)\, |\Psi_{\mathrm{S}}^{(N)}(t_0)\rangle = |\Psi_{\mathrm{S}}^{(N)}(t_0)\rangle \,, \tag{8.14}$$

remains constant (t_0 only gives a reference time) and any not explicitly time-dependent operator that commutes with the Hamiltonian is a constant of motion, as is obvious from Eq. (8.13).

Proof that Eq. (8.12) is a solution of the Heisenberg equation (8.13) (assuming $\frac{\partial \hat{A}_{\mathrm{S}}}{\partial t} \equiv 0$): Using the definition of the evolution operator Eq.

[9] It is not necessary to define the case of equal times, since under the integrals in the expansion of the evolution operator, the value of each integral is not influenced by the value of the integrand at the integral borders.

[10] In a third (intermediate) picture – the interaction (or Dirac) picture (I) –, the state vector $|\Psi_{\mathrm{I}}^{(N)}\rangle$ carries the (trivial) time dependence of some not explicitly time-dependent part $\hat{H}_0$ of the full Hamiltonian $\hat{H}(t)$.

(8.6), we calculate:

$$\begin{aligned}
\mathrm{i}\hbar\frac{d\hat{A}_{\mathrm{H}}}{dt} &= \mathrm{i}\hbar\frac{d}{dt}\hat{\bar{T}}\left\{\mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\}\hat{A}_{\mathrm{S}}\hat{T}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\} \\
&= -\hat{\bar{T}}\left\{\hat{H}_{\mathrm{S}}(t)\mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\}\hat{A}_{\mathrm{S}}\hat{T}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\} \\
&\quad +\hat{\bar{T}}\left\{\mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\}\hat{A}_{\mathrm{S}}\hat{T}\left\{\hat{H}_{\mathrm{S}}(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\} \\
&= -\hat{U}(t_0,t)\hat{H}_{\mathrm{S}}(t)\hat{A}_{\mathrm{S}}\hat{U}(t,t_0)+\hat{U}(t_0,t)\hat{A}_{\mathrm{S}}\hat{H}_{\mathrm{S}}(t)\hat{U}(t,t_0) \\
&= -\hat{U}(t_0,t)\hat{H}_{\mathrm{S}}(t)\hat{U}(t,t_0)\hat{U}(t_0,t)\hat{A}_{\mathrm{S}}\hat{U}(t,t_0) \\
&\quad +\hat{U}(t_0,t)\hat{A}_{\mathrm{S}}\hat{U}(t,t_0)\hat{U}(t_0,t)\hat{H}_{\mathrm{S}}(t)\hat{U}(t,t_0) \\
&= \left[\hat{A}_{\mathrm{H}},\hat{H}_{\mathrm{H}}\right]_{-} . \qquad (8.15)
\end{aligned}$$

In prospect to the next section, this simple proof has been given to point out the importance of the two different time-ordering operators when writing down the explicit form of the evolution operators in the solution of the Heisenberg equation[11].

Combining the Heisenberg picture with the scond quantization, the creation and annihilation operators in Eqs. (8.1) to (8.3) become time-dependent, i.e., we replace $\hat{f}_i \to \hat{f}_{i,\mathrm{H}}(t)$. The (anti-)commutation relations of Eq. (8.2) then remain valid in the equal-time limit only, for different times there is no relation.

Initial state. Many situations require to properly define the initial state at some reference time t_0. In equilibrium, this may be an eigenstate of the system (for a pure quantum state) or a mixture of eigenstates defined through the statistical operator $\hat{\rho}$. For an interacting many-body system, there are basically two different ways to account for stationary (generally correlated) initial states:

i. through an adiabatic switch-on of the interaction [Kel64, Fuj65, Hal75, 62], where the system passes through a sequence of intermediate eigenstates, or

ii. by starting from a (correlated) many-body state formulated in the picture of the grand canonical ensemble (GCE), e.g. [62, 63].

Of course, other approaches exist which *a priori* define (non-)correlated nonequilibrium initial states, see, e.g., [BSH99, SBK03, KSB05] and references therein.

[11] One might ask why we could apply the time-ordering in Eq. (8.15) since we did not define the case of equal times. This problem can be circumvented by casting the integrals in the exponents into Riemann sums. Thereby the Hamiltonians in the exponents will always be evaluated at times smaller than t allowing us to apply the time-ordering operators as defined.

In this chapter, we mainly follow approach ii., because the mathematical methods behind nonequilibrium Green functions are most comprehensively developed along this line. However, strategy i. is not irrelevant, and we will later emphasize its significance when using the generalized Kadanoff-Baym ansatz (GKBA), see Section 8.9.2 and the G1–G2-scheme [SJB20].

8.2 Nonequilibrium Green functions

8.2.1 Keldysh Contour

From now on, we suppose that the quantum many-body system of Eq. (8.1) [system a) in Fig. 8.1] exchanges particles and energy with a reservoir [system b)]. In addition, we assume that both are in equilibrium for times $t \leq t_0$, i.e. the external potential $v(t) = 0$, for times $t \leq t_0$. In equilibrium, the reservoir has the temperature[12] $T = (k_\mathrm{B}\beta)^{-1}$ and chemical potential μ. The system and the reservoir are entangled which is the consequence of the coupling between them, see Fig. 8.1. Therefore, the reduced density matrix of the system must describe an ensemble of states (rather than a pure state), namely the grand canonical ensemble in this specific setup. Carrying out the trace over the reservoir under the assumption of a weak coupling between the reservoir and the system leads to the well-known grand canonical density matrix[13]:

$$\hat{\rho}_\mathrm{GCE} = \frac{1}{Z_0}\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})} , \tag{8.16}$$

$$Z_0 = \mathrm{Tr}\left\{\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}\right\} , \tag{8.17}$$

where $\hat{H}$ must be a time-independent (equilibrium) Hamiltonian and $\hat{N}$ is the number operator. The trace is performed by summing over a complete set of states in the Fock space (commonly in occupation number representation).

With that, we can compute averages of an operator $\hat{A}$, for times $t \leq t_0$ according to[14]

$$\left\langle \hat{A} \right\rangle (t \leq t_0) = \mathrm{Tr}\left\{\hat{\rho}_\mathrm{S}(t \leq t_0)\hat{A}_\mathrm{S}\right\} = \frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{-\beta(\hat{H}_\mathrm{S}(t_0)-\mu\hat{N}_\mathrm{S})}\,\hat{A}_\mathrm{S}\right\} . \tag{8.18}$$

For times $t > t_0$, the system hamiltonian has changed and become time-dependent, so we have to use the time-dependent non-equilibrium density

[12] Note that out of equilibrium there is no such thing as "temperature".

[13] Eq. (8.16) can also be derived by maximizing the entropy of the system which is as well only valid for the equilibrium case.

[14] Again the subscript S in $\hat{A}_\mathrm{S}$ indicates the Schrödinger and $\hat{A}_\mathrm{H}$ the Heisenberg picture.

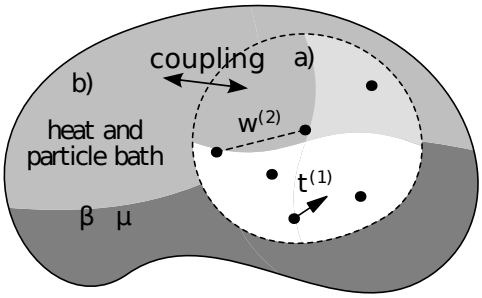

Abbildung 8.1: Grand canonical ensemble (GCE) with inverse temperature $\beta = 1/(k_{\rm B}T)$ and chemical potential μ. Whereas system b) denotes the heat and particle reservoir, system a) is the basic (open) system under investigation. In general, particles (black dots) and energy can be transferred between a) and b). Further, $w^{(2)} = w$ denotes the two-body interaction between identical particles with kinetic energy $t^{(1)} = t$.

matrix for the calculation of the averages. Therefore, we have to return to the **general form of the density operator** and express it **in terms of the equilibrium density matrix** Eq. (8.16) via the evolution operator[15]:

$$\begin{aligned}
\hat{\rho}_{\rm S}(t) &= \sum_r W_r |\Psi_{\rm S}^r(t)\rangle\langle\Psi_{\rm S}^r(t)| && (8.19)\\
&= \sum_r W_r \hat{U}(t,t_0)|\Psi_{\rm S}^r(t_0)\rangle\langle\Psi_{\rm S}^r(t_0)|\hat{U}(t_0,t)\\
&= \hat{U}(t,t_0)\hat{\rho}_{\rm S}(t_0)\hat{U}(t_0,t)\\
&= \hat{U}(t,t_0)\frac{1}{Z_0}{\rm e}^{-\beta\left(\hat{H}_{\rm S}(t_0)-\mu\hat{N}_{\rm S}\right)}\hat{U}(t_0,t)\,, && (8.20)
\end{aligned}$$

with non-negative real probabilities W_r that sum to unity. Note that the evolution operators appear here (3rd and 4th lines) differently than in a standard Heisenberg operator, Eq. (8.12), because $\hat{\rho}$ is not a conventional operator but is constructed from state vectors.

Further, we make use of the formal equality of the canonical density operator and the evolution operator of the time-independent system described by

[15]Note the inverse ordering of the two time evolution operators, as compared to a standard Heisenberg operator, in the final result. This arises due to the peculiar "ket-bra" structure of the two states, in the definition of $\hat{\rho}_{\rm S}$.

$\hat{H}_{\rm S}(t_0)$ in imaginary time, i.e.

$$\begin{aligned} \mathrm{e}^{-\beta\hat{H}_{\rm S}(t_0)} &= \mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\hat{H}_{\rm S}(t_0)[t_0-(t_0-\mathrm{i}\hbar\beta)]} \\ &= \hat{\tilde{T}}_I \mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\hat{H}_{\rm S}(t_0)[t_0-(t_0-\mathrm{i}\hbar\beta)]} \qquad (8.21) \\ &= \hat{\tilde{T}}_I \mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\int_{t_0-\mathrm{i}\hbar\beta}^{t_0}\mathrm{d}\bar{t}\,\hat{H}_{\rm S}(t_0)} \\ &\equiv \hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\;, \qquad (8.22) \end{aligned}$$

where we introduced the anti-chronological time-ordering operator $\hat{\tilde{T}}_I$ for imaginary times $(t_0-\mathrm{i}\hbar\tau)\in[t_0-\mathrm{i}\hbar\beta,t_0], \tau\in\mathbb{R}$ (chronological with respect to τ). Its action is also defined by Eq. (8.10) when replacing t_1 by $t_0-\mathrm{i}\hbar\tau_1$. In fact, we could have added any time-ordering operator in Eq. (8.21), because there is no product of time-dependent operators to be ordered. We chose the anti-chronological order to identify the expression with the evolution operator defined in Eq. (8.7)[16]. Finally, the subscript "0" in $\hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)$ indicates that this evolution operator has to be evaluated using the time-independent Hamiltonian $\hat{H}_{\rm S}(t_0)$.

Combining Eq. (8.20) and (8.22), the time-dependent averages of observables for $t\geq t_0$ become

$$\begin{aligned} \left\langle\hat{A}\right\rangle(t) &= \mathrm{Tr}\left\{\hat{\rho}_{\rm S}(t)\hat{A}_{\rm S}\right\} \\ &= \frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_{\rm S}}\hat{U}(t,t_0)\hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\hat{U}(t_0,t)\hat{A}_{\rm S}\right\} \\ &= \frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_{\rm S}}\hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\hat{U}(t_0,t)\hat{A}_{\rm S}\hat{U}(t,t_0)\right\} \qquad (8.23) \\ &= \frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_{\rm S}}\hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\hat{A}_{\rm H}(t)\right\} \\ &= \mathrm{Tr}\left\{\hat{\rho}_{\rm H}\hat{A}_{\rm H}(t)\right\} =: \left\langle\hat{A}_{\rm H}(t)\right\rangle\;, \qquad (8.24) \end{aligned}$$

where we took advantage of the fact that all Hamiltonians investigated here commute with the number operator[17], i.e.

$$\left[\hat{H}_{\rm S}(t),\hat{N}_{\rm S}\right]=0 \iff \mathrm{e}^{-\beta(\hat{H}_{\rm S}(t)-\mu\hat{N}_{\rm S})}=\mathrm{e}^{-\beta\hat{H}_{\rm S}(t)}\mathrm{e}^{\beta\mu\hat{N}_{\rm S}}\;, \qquad (8.25)$$

and, in Eq. (8.23), we used the cyclic invariance of the trace. The last line in Eq. (8.24) has been given to define what is meant by averaging over a Heisenberg

[16]Note that $t_0-\mathrm{i}\hbar\beta$ is "smaller" than t_0 with respect to the imaginary part.

[17]These are all Hamiltonians with an equal number of creation and annihilation operators.

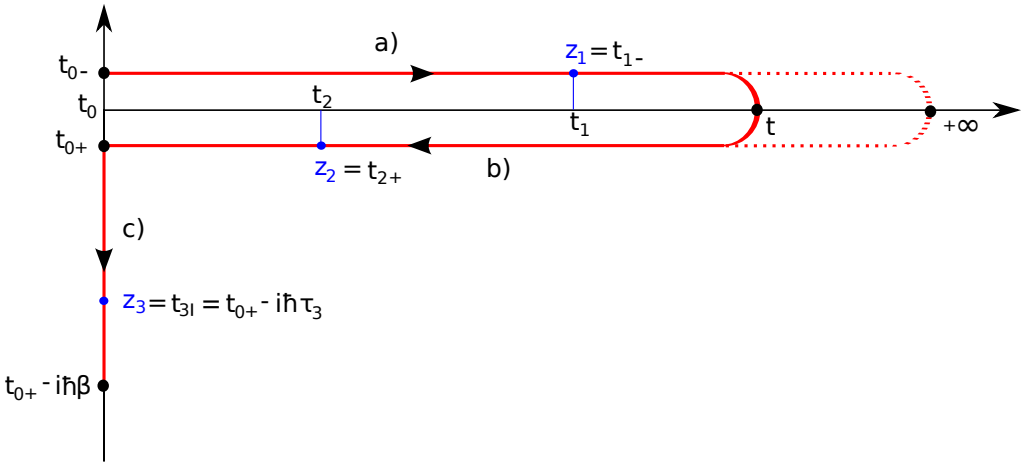

Abbildung 8.2: Keldysh contour $\mathcal{C}$ full (red) line including three different branches: the upper branch a) with chronological time-ordering $\hat{T}$ evolving with $\hat{H}_{\rm S}(\bar{t})$, the lower branch b) with anti-chronological time-ordering $\hat{\tilde{T}}$ evolving with $\hat{H}_{\rm S}(\bar{t})$ and the imaginary branch c) with anti-chronological time-ordering $\hat{\tilde{T}}_I$ with respect to $t_0 - i\hbar\tau$ (chronological with respect to τ) evolving with $\hat{H}_{\rm S}(t_0)$. On $\mathcal{C}$ it is $z_1 < z_2 < z_3$. The dashed line shows the extended contour reaching to plus infinity.

operator[18]. For further investigation of the third line in Eq. (8.23) we write down the evolution operators explicitly:

$$\left\langle \hat{A} \right\rangle (t) = \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_{\rm S}} \hat{\tilde{T}}_I \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t_0 - \mathrm{i}\hbar\beta} \mathrm{d}\bar{t}\, \hat{H}_{\rm S}(t_0)} \right\} \right.$$
$$\left. \times \hat{\tilde{T}} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t}^{t_0} \mathrm{d}\bar{t}\, \hat{H}_{\rm S}(\bar{t})} \right\} \hat{A}_{\rm S} \hat{T} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} \mathrm{d}\bar{t}\, \hat{H}_{\rm S}(\bar{t})} \right\} \right\} . \quad (8.26)$$

When acting on a ket-vector under the trace (meaning we read from right to left), first, the ket-vector is propagated on the real time axis from t_0 to t (chronological time ordering, cf. the integration limits in the right exponential) where the operator $\hat{A}_{\rm S}(t)$ acts. Second, the ket-vector is evolved back from t to t_0 (anti-chronological time-ordering) and third, an additional evolution of the ket-vector occurs along the imaginary axis from t_0 to $t_0 - i\hbar\beta$ (again anti-chronological time-ordering). This forward and backward propagation is a direct consequence of the Heisenberg representation of operators.

[18]By definition $\hat{\rho}_{\rm H} \equiv \hat{\rho}_{\rm S}(t_0)$. Therefore, it is the time independent density operator $\hat{\rho}_{\rm S}(t_0)$ that enters the trace when averaging a Heisenberg operator.

However, for a variety of many-body approaches (e.g. Feynman diagram technique), it is required to work with **time-ordered operator products**. To achieve this, in the present case, one can apply a simple trick which is originally due to Keldysh [Kel64]: we design a "time contour"[19] $\mathcal{C}$ consisting of three branches (see Fig. 8.2), From now on, we will use the letter z to denote a contour time variable lying on one of the three branches or, equivalently, we use the letter t and explicitly specify the corresponding branch with the subscripts[20] $-, +, |$ (cf. Fig. 8.2). With this notation, the contour can be written as the union of the three branches:

$$\mathcal{C} \;=\; [t_{0-}, t] \cup [t, t_{0+}] \cup [t_{0+}, t_{0+} - \mathrm{i}\hbar\beta] \; . \tag{8.27}$$

With this special contour, the action of all operators appears in a "forward" ("chronological") order.

8.2.2 Algebra on the Keldysh contour

In this section we consider in more detail how to understand Heisenberg operators on the Keldysh contour. The following equations define the three possible cases:

$$\begin{aligned}
\hat{A}_{\mathrm{H}}(t_{1-}) &:= \hat{U}(t_0, t_1)\hat{A}_{\mathrm{S}}\hat{U}(t_1, t_0) && (8.28)\\
\hat{A}_{\mathrm{H}}(t_{1+}) &:= \hat{U}(t_0, t_1)\hat{A}_{\mathrm{S}}\hat{U}(t_1, t_0) && (8.29)\\
\hat{A}_{\mathrm{H}}(t_{1|}) &:= \hat{A}_{\mathrm{H}}(t_0 - \mathrm{i}\tau_1) \\
&= \hat{U}_0(t_0, t_0 - \mathrm{i}\tau_1)\hat{A}_{\mathrm{S}}\hat{U}_0(t_0 - \mathrm{i}\tau_1, t_0) \\
&= \mathrm{e}^{+\frac{\tau_1}{\hbar}\hat{H}_{\mathrm{S}}(t_0)}\hat{A}_{\mathrm{S}}\mathrm{e}^{-\frac{\tau_1}{\hbar}\hat{H}_{\mathrm{S}}(t_0)}, \quad \text{with} \quad \tau_1 \in \mathbb{R} \; . && (8.30)
\end{aligned}$$

Therefore, it is irrelevant for the operators whether the contour argument lies on the upper or lower branch for it is always the corresponding real time (see Fig. 8.2) that is used for evaluation of the evolution operator. Moreover, one should note that the imaginary time evolution operator is not unitary, i.e. $\hat{U}_0^\dagger(t_0, t_0 - \mathrm{i}\tau_1) \neq \hat{U}_0(t_0 - \mathrm{i}\tau_1, t_0)$.

Now, we define a generalized time-ordering operator $\hat{T}_{\mathcal{C}}$, which works chronologically (anti-chronologically) on the upper (lower and imaginary) branch of the contour, thereby arranging imaginary times which originate from the vertical branch behind (i.e. "later" than) purely real times. For a contour-ordered

[19] or Keldysh or round-trip contour

[20] The upper branch is indicated with "-" since it is "earlier" on the contour.

product of operators $\hat{A}_{1,\mathrm{H}}(z_1)\ldots\hat{A}_{n,\mathrm{H}}(z_n)$, we have $(z_1,\ldots z_n\in\mathcal{C})$,

$$\hat{T}_{\mathcal{C}}\{\hat{A}_{1,\mathrm{H}}(z_1)\ldots\hat{A}_{n,\mathrm{H}}(z_n)\} := \sum_{\mathcal{P}}\theta_{\mathcal{C}}(z_{\mathcal{P}(1)}-z_{\mathcal{P}(2)})\ldots\theta_{\mathcal{C}}(z_{\mathcal{P}(n-1)}-z_{\mathcal{P}(n)}) \times\hat{A}_{\mathcal{P}(1),\mathrm{H}}(z_{\mathcal{P}(1)})\ldots\hat{A}_{\mathcal{P}(n),\mathrm{H}}(z_{\mathcal{P}(n)})\,, \quad (8.31)$$

with

$$\theta_{\mathcal{C}}(z-z') := \begin{cases}1\,, & \text{if} \quad z>z' \quad \text{on} \quad \mathcal{C}\\ 0\,, & \text{if} \quad z<z' \quad \text{on} \quad \mathcal{C}\,,\end{cases} \quad (8.32)$$

again leaving out the definition for equal contour times. Thus, the contour time-ordering operator simply puts the latest times on the contour to the leftmost place in a contour ordered product. Of course, the definition of the contour Heisenberg operator (Eq. (8.28) should only be used after the contour time-ordering operator has been applied. By defining also the Hamiltonian on the contour[21],

$$\hat{H}_{\mathrm{S}}(\bar{z}) := \begin{cases}H_{\mathrm{S}}(\bar{t})\,, & \text{if} \quad z\in[t_{0-},t]\cup[t,t_{0+}]\,,\\ H_{\mathrm{S}}(t_0)\,, & \text{if} \quad z\in[t_{0+},t_{0+}-\mathrm{i}\hbar\beta]\,,\end{cases} \quad (8.33)$$

we can finally rewrite the time-dependent average of an observable (Eq. (8.26)) and find the following important expression:

$$\left\langle\hat{A}\right\rangle(z) := \frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_{\mathrm{S}}}\hat{T}_{\mathcal{C}}\left\{\mathrm{e}^{\left(-\frac{\mathrm{i}}{\hbar}\int_{\mathcal{C}}\mathrm{d}\bar{z}\,\hat{H}_{\mathrm{S}}(\bar{z})\right)}\hat{A}_{\mathrm{S}}|_z\right\}\right\} \quad (8.34)$$
$$:= \frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_{\mathrm{S}}}\hat{U}_{\mathcal{C}}\,\hat{A}_{\mathrm{S}}|_z\right\}\,,$$

where the notation $\hat{A}_{\mathrm{S}}|_z$ is only used to specify the **contour time** at which the (in general) time-independent Schrödinger operator has to act. We refer to $\hat{U}_{\mathcal{C}}$ as the generalized time evolution operator or **contour time evolution operator**, which is defined by the following equations:

[21] $\bar{t}$ denotes the real time belonging to the contour time $\bar{z}$.

$$\begin{aligned}
\hat{U}_{\mathcal{C}}(t_{0+}-\mathrm{i}\hbar\beta,t_{0-}) &:= \hat{T}_{\mathcal{C}}\,\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{\mathcal{C}}\mathrm{d}\bar{z}\,\hat{H}_{\mathrm{S}}(\bar{z})} && (8.35)\\
&:= \hat{T}_{\mathcal{C}}\exp\Bigg\{-\frac{\mathrm{i}}{\hbar}\Bigg(\int_{t_{0+}}^{t_{0+}-\mathrm{i}\hbar\beta}\mathrm{d}\bar{t}_{|}\,\hat{H}_{\mathrm{S}}(\bar{t}_{|})\\
&\qquad +\int_{t}^{t_{0+}}\mathrm{d}\bar{t}_{+}\,\hat{H}_{\mathrm{S}}(\bar{t}_{+})+\int_{t_{0-}}^{t}\mathrm{d}\bar{t}_{-}\,\hat{H}_{\mathrm{S}}(\bar{t}_{-})\Bigg)\Bigg\} && (8.36)\\
&= \hat{\hat{T}}_{I}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t_0-\mathrm{i}\hbar\beta}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(t_0)}\right\}\hat{\hat{T}}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t}^{t_0}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\}\\
&\qquad\times\hat{T}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_0}^{t}\mathrm{d}\bar{t}\,\hat{H}_{\mathrm{S}}(\bar{t})}\right\} && (8.37)\\
&= \hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\hat{U}(t_0,t)\hat{U}(t,t_0)\\
&= \hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\,. && (8.38)
\end{aligned}$$

Going from Eq. (8.36) to Eq. (8.37), we applied the contour time-ordering operator and used the relation between the contour and the real time Hamiltonian Eq. (8.33). These two steps must be done at once, since the three time-ordering operators in the third line are defined for real times only ($\hat{T}_{\mathcal{C}}$ for contour times only). The last three lines are not correct, if the generalized evolution operator appears together with a Schrödinger operator like in Eq. (8.34). In that case $\hat{A}_{\mathrm{S}}|_z$ has to be inserted at the proper position in between the contour integrals. Nevertheless, we can obviously express the grand partition function in terms of the generalized evolution operator:

$$Z_0 = \mathrm{Tr}\,\{\mathrm{e}^{\beta\mu\hat{N}_{\mathrm{S}}}\hat{U}_{\mathcal{C}}\}. \tag{8.39}$$

For a better understanding of the introduced Keldysh contour and the contour function $\left\langle\hat{A}(z)\right\rangle$ a few remarks should be made:

i) The spacing between the upper and the lower branch in Fig. 8.2 is to be understood as an illustrative help only. In fact both branches lie exactly on top of each other. That is why the time t lies on both branches, i.e. $t = t_- = t_+$, if t is the turning point of the contour on the real axis[22] .

ii) As a result of the group property of the evolution operator, the contour can easily be extended to infinity on the real axis. For that purpose let us

[22]In the second remark, we extend the contour and shift the turning point on the real axis to $+\infty$. Then we should replace "t" by ∞ in the definitions Eq. (8.33) and (8.27) since in that case the relation $\infty = \infty_- = \infty_+$ holds.

consider the contour time-dependent average $\left\langle \hat{A} \right\rangle (z)$ for the case when z lies on the upper branch, i.e. $z = t_{1-} \in [t_{0-}, t]$

$$\begin{aligned}
\left\langle \hat{A} \right\rangle (t_{1-}) &= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_\mathcal{C} \mathrm{d}\bar{z}\, \hat{H}_\mathrm{S}(\bar{z})} \hat{A}_\mathrm{S}|_{t_{1-}} \right\} \right\} && (8.40) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{0+}}^{t_{0+}-\mathrm{i}\hbar\beta} d\bar{t}_|\, \hat{H}_\mathrm{S}(\bar{t}_|)} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t}^{t_{0+}} d\bar{t}_+ \hat{H}_\mathrm{S}(\bar{t}_+)} \right.\right. \\
&\qquad \left.\left. \times \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{1-}}^{t} \mathrm{d}\bar{t}_-\, \hat{H}_\mathrm{S}(\bar{t}_-)} \right\} \hat{A}_\mathrm{S} \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{0-}}^{t_{1-}} \mathrm{d}\bar{t}_-\, \hat{H}_\mathrm{S}(\bar{t}_-)} \right\} \right\} && (8.41) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{0+}}^{t_{0+}-\mathrm{i}\hbar\beta} \mathrm{d}\bar{t}_|\, \hat{H}_\mathrm{S}(\bar{t}_|)} \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{\infty}^{t_{0+}} \mathrm{d}\bar{t}_+\, \hat{H}_\mathrm{S}(\bar{t}_+)} \right.\right. \\
&\qquad \left.\left. \times \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{1-}}^{\infty} \mathrm{d}\bar{t}_-\, \hat{H}_\mathrm{S}(\bar{t}_-)} \right\} \hat{A}_\mathrm{S} \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{0-}}^{t_{1-}} \mathrm{d}\bar{t}_-\, \hat{H}_\mathrm{S}(\bar{t}_-)} \right\} \right\} && (8.42) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0) \times \right. \\
&\qquad \left. \hat{U}(t_0, \infty) \hat{U}(\infty, t_1) \hat{A}_\mathrm{S} \hat{U}(t_1, t_0) \right\} && (8.43) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0) \hat{U}(t_0, t_1) \hat{A}_\mathrm{S} \hat{U}(t_1, t_0) \right\} && (8.44) \\
&= \left\langle \hat{A} \right\rangle (t_1), && (8.45)
\end{aligned}$$

where t_1 is the corresponding real time of t_{1-}. The extension of the contour occurred in Eq. (8.42) by adding the terms

$$\int_\infty^t \mathrm{d}\bar{t}_+\, \hat{H}_\mathrm{S}(\bar{t}_+) + \int_t^\infty \mathrm{d}\bar{t}_-\, \hat{H}_\mathrm{S}(\bar{t}_-)\,, \tag{8.46}$$

in the exponents. These two terms cancel each other under the contour time-ordering operator which is shown in Eq. (8.43) and (8.44). Since we could have done the same calculation for $z = t_{1+} \in [t, t_{0+}]$, we are free to extend the contour up to infinity (see Fig. 8.2 dashed line) and replace "t" by "∞" in the definitions (8.33) and (8.27). Moreover, we found that the following relation between the real and contour time-dependent average of an observable holds:

$$\begin{aligned}
\left\langle \hat{A} \right\rangle (t_{1-}) &= \left\langle \hat{A} \right\rangle (t_1), \quad \forall \quad t_{1-} \in [t_{0-}, \infty]\,, \\
\left\langle \hat{A} \right\rangle (t_{1+}) &= \left\langle \hat{A} \right\rangle (t_1), \quad \forall \quad t_{1-} \in [\infty, t_{0+}]\,. && (8.47)
\end{aligned}$$

This is not surprising when remembering the definition of the Heisenberg operators on the contour, Eq. (8.28). Still, it shows that our introduced contour formalism is consistent, which is always a nice result.

iii) Now, let us investigate the case when z lies on the imaginary branch, i.e. $z = t_{1|} = t_{0+} - \mathrm{i}\tau_1 \in [t_{0+}, t_{0+} - \mathrm{i}\hbar\beta]$. We then have

$$\begin{aligned}
\left\langle \hat{A} \right\rangle (t_{1|}) &= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_\mathcal{C} \mathrm{d}\bar{z}\, \hat{H}_\mathrm{S}(\bar{z}} \hat{A}_\mathrm{S}|_{t_{1|}} \right\} \right\} && (8.48) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{0+}-\mathrm{i}\tau_1}^{t_{0+}-\mathrm{i}\hbar\beta} \mathrm{d}\bar{t}_{|}\, \hat{H}_\mathrm{S}(\bar{t}_{|})} \right\} \hat{A}_\mathrm{S} \right. \\
&\quad \left. \times \hat{T}_\mathcal{C} \left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{t_{0+}}^{t_{0+}-\mathrm{i}\tau_1} \mathrm{d}\bar{t}_{|}\, \hat{H}_\mathrm{S}(\bar{t}_{|})} \right\} \underbrace{\hat{U}(t_0, \infty)\hat{U}(\infty, t_0)}_{\hat{1}} \right\} && (8.49) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{U}(t_0 - \mathrm{i}\hbar\beta, t_0 - \mathrm{i}\tau_1) \right. \\
&\quad \left. \times \hat{A}_\mathrm{S} \hat{U}(t_0 - \mathrm{i}\tau_1, t_0) \right\} && (8.50) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{U}(t_0 - \mathrm{i}\tau_1, t_0) \right. \\
&\quad \left. \times \hat{U}(t_0 - \mathrm{i}\hbar\beta, t_0 - \mathrm{i}\tau_1) \hat{A}_\mathrm{S} \right\} && (8.51) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{U}(t_0 - \mathrm{i}\hbar\beta, t_0 - \mathrm{i}\tau_1) \right. \\
&\quad \left. \times \hat{U}(t_0 - \mathrm{i}\tau_1, t_0) \hat{A}_\mathrm{S} \right\} && (8.52) \\
&= \frac{1}{Z_0} \mathrm{Tr} \left\{ \mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}} \hat{U}(t_0 - \mathrm{i}\hbar\beta, t_0) \hat{A}_\mathrm{S} \right\} && (8.53) \\
&= \mathrm{Tr} \left\{ \hat{\rho}(t_0) \hat{A}_\mathrm{S} \right\} = \left\langle \hat{A} \right\rangle (t_0), \quad \forall \tau_1 \in \left[0, \frac{\hbar}{\beta} \right] . && (8.54)
\end{aligned}$$

First, we used the cyclic invariance of the trace, in Eq. (8.51), and second, the fact that Hamiltonians of different times commute under a time-ordered product of equal type, so we could commute the two evolution operators, Eq. (8.52), to apply the group property. Since $t_{1|}$ was arbitrary, we found the interesting relation:

$$\left\langle \hat{A} \right\rangle (t_{0+} - \mathrm{i}\tau) = \left\langle \hat{A}(t_0) \right\rangle , \quad \forall \quad \tau_1 \in [0, \beta] . \tag{8.55}$$

That means the contour time-dependent average $\left\langle \hat{A} \right\rangle (z)$ will always be the average of the unperturbed system $\left\langle \hat{A} \right\rangle (t_0)$ when z lies on the imaginary branch.

iv) It is crucial not to confuse $\left\langle \hat{A}_H \right\rangle (z)$ with $\left\langle \hat{A}_H \right\rangle (t)$ because mathematically these are completely different functions. The link between them is given by Eqs. (8.55) and (8.47). Furthermore[23], $\left\langle \hat{A}_H \right\rangle (z)$ can be considered the simplest form of a contour-ordered function. In general these are of the form:

$$\left\langle \hat{T}_{\mathcal{C}} \left\{ \hat{A}_{1,\mathrm{H}}(z_1) \hat{A}_{2,\mathrm{H}}(z_2) \dots \hat{A}_{n,\mathrm{H}}(z_n) \right\} \right\rangle , \tag{8.56}$$

i.e. an average of a contour-ordered product of Heisenberg operators[24]. In that case, relation (8.55) holds only for equal times ($z_1 = z_2 = \ldots = z_n$), where z_1 lies on the imaginary branch. If the times are different, the operators will separate the evolution along the imaginary branch into more than just two parts (cf. Eq. (8.49)), so we could not reconstruct the equilibrium density matrix by using the cyclic invariance of the trace. Nevertheless, if a physical observable, described by a single first quantized operator, is generalized to the contour, as done in this chapter, relation (8.55) holds.

v) Naturally, in case of a time-independent Hamiltonian (equilibrium), it is

$$\left\langle \hat{A} \right\rangle (z) = \left\langle \hat{A}_{\mathrm{H}}(z) \right\rangle = \left\langle \hat{A} \right\rangle (t_0), \quad \forall\, z, \tag{8.57}$$

i.e. the expectation value of a time-dependent Heisenberg operator is always time-independent in equilibrium. This is readily seen in Eq. (8.43), if one uses again the cyclic invariance of the trace and the fact that

$$\left[\mathrm{e}^{\beta\mu\hat{N}_{\mathrm{S}}} \hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0), \hat{U}(t_0, t_1) \right]_- = \left[\mathrm{e}^{-\beta(\hat{H}_{\mathrm{S},0} - \mu\hat{N}_{\mathrm{S}})}, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}_{\mathrm{S},0}(t_0 - t_1)} \right]_- = 0 \,. \tag{8.58}$$

vi) The presence of the Keldysh contour assesses a contour algebra which was described in detail by *DuBois* [DuB67] and *Langreth* [64] and which culminates in the application of the Langreth-Wilkins rules [65], see Table 8.1.

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[23] Note that $\left\langle \hat{A}_{\mathrm{S}} \right\rangle (z) = \left\langle \hat{A}_{\mathrm{H}} \right\rangle (z)$. The difference lies only in the averaging, i.e. the Schrödinger operator is averaged with $\hat{\rho}(t)$ whereas the Heisenberg operator is averaged with $\hat{\rho}(t_0)$. That is why we did not write a subscript in $\left\langle \hat{A} \right\rangle (z)$ for they both refer to the same expression when writing the averaging explicitly (cf. Eq. (8.34).

[24] $\left\langle \hat{T}_{\mathcal{C}} \hat{A}_{\mathrm{H}}(z) \right\rangle = \left\langle \hat{A}_{\mathrm{H}}(z) \right\rangle = \left\langle \hat{A} \right\rangle (z)$

8.2.3 One-Particle Nonequilibrium Green Function

In Sec. 8.2.1 we have introduced the contour formalism for the computation of the time-dependent expectation value of an arbitrary operator $\hat{A}$ in first quantization. Now, we will combine the contour formalism with the second quantization, which directly brings us to the *Nonequilibrium Green Functions* (NEGF). Let us write a general operator $\hat{A}$ of one-particle type in second quantization in the Heisenberg picture:

$$\begin{aligned}
\hat{A}_{\mathrm{H}}(t) &= \hat{U}(t_0,t)\hat{A}_{\mathrm{S}}\hat{U}(t,t_0) \\
&= \sum_{j,i} a_{ji}\hat{U}(t_0,t)\hat{f}^{\dagger}_{j,\mathrm{S}}\hat{f}_{i,\mathrm{S}}\hat{U}(t,t_0) \\
&= \sum_{j,i} a_{ji}\hat{U}(t_0,t)\hat{f}^{\dagger}_{j,\mathrm{S}}\underbrace{\hat{U}(t,t_0)\hat{U}(t_0,t)}_{\hat{1}}\hat{f}_{i,\mathrm{S}}\hat{U}(t,t_0) \\
&= \sum_{j,i} a_{ji}\hat{f}^{\dagger}_{j,\mathrm{H}}(t)\hat{f}_{i,\mathrm{H}}(t)\ . \qquad (8.59)
\end{aligned}$$

[If the Schrödinger operator is time-dependent we have to replace $a_{ji}(t) \to a^H_{ji}(t) = U(t_0,t)a_{ji}(t)U(t;t_0)$.] Ensemble averaging over the equilibrium density operator, $\hat{\rho}(t_0)$, yields:

$$\left\langle \hat{A}_{\mathrm{H}} \right\rangle (t) = \sum_{j,i} a_{ji} \left\langle \hat{f}^{\dagger}_{j,\mathrm{H}}(t)\hat{f}_{i,\mathrm{H}}(t) \right\rangle = \sum_{j,i} a_{ji} n_{ji}(t) = \left\langle \hat{A} \right\rangle (t). \qquad (8.60)$$

Thus, if we know the time-dependent 1pRDM, we can compute all non-equilibrium observables of one-particle type which is our goal. One way to do this is to derive the equation of motion for the 1pRDM $n_{ji}(t)$ which follows e.g. from the BBGKY-hierarchy, as we discussed in chapter 6.

The alternative we consider here is the NEGF formalism which is based on two main ideas. First, we generalize the expectation value of the creation and annihilation operator product in Eq. (8.60) to a contour function, cf. Eq. (8.34):

$$\left\langle \hat{f}^{\dagger}_{j,\mathrm{H}}(z)\hat{f}_{i,\mathrm{H}}(z) \right\rangle = \frac{1}{Z_0}\mathrm{Tr}\left\{ \mathrm{e}^{\beta\mu\hat{N}_{\mathrm{S}}}\hat{T}_{\mathcal{C}}\left\{ \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{\mathcal{C}}\mathrm{d}\bar{z}\,\hat{H}_{\mathrm{S}}(\bar{z})}\hat{f}^{\dagger}_{j,\mathrm{S}}|_z\hat{f}_{i,\mathrm{S}}|_z \right\} \right\}\ , (8.61)$$

and second, we further generalize this function by also *allowing for different contour time arguments*. For a better analysis of the resulting function later on, it is convention to add another contour time-ordering operator and interchange the creation and annihilation operator, which leads to a so called contour-ordered function. After multiplying by $-\frac{\mathrm{i}}{\hbar}$, we arrive at the definition

of the **contour-ordered, one-particle nonequilibrium Green function** (1pNEGF):

$$G_{ij}^{(1)}(z,z') \;:=\; -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\hat{f}_{i,\mathrm{H}}(z)\hat{f}_{j,\mathrm{H}}^{\dagger}(z')\right\rangle . \tag{8.62}$$

To make the relation between Eq. (8.61) and the definition (8.62) more obvious, we again write the averaging explicitly:

$$\begin{aligned} G_{ij}^{(1)}(z,z') &= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_{\mathrm{S}}}\hat{T}_{\mathcal{C}}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{\mathcal{C}}\mathrm{d}\bar{z}\,\hat{H}_{\mathrm{S}}(\bar{z})}\hat{T}_{\mathcal{C}}\left\{\hat{f}_{i,\mathrm{S}}|_z\hat{f}_{j,\mathrm{S}}^{\dagger}|_{z'}\right\}\right\}\right\} \\ &= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_{\mathrm{S}}}\hat{T}_{\mathcal{C}}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_{\mathcal{C}}\mathrm{d}\bar{z}\,\hat{H}_{\mathrm{S}}(\bar{z})}\hat{f}_{i,\mathrm{S}}|_z\hat{f}_{j,\mathrm{S}}^{\dagger}|_{z'}\right\}\right\}, \end{aligned} \tag{8.63}$$

where we have taken advantage of the fact that a time-ordered product does not change under the action of a time-ordering operator, i.e. $\hat{T}_{\mathcal{C}}\hat{T}_{\mathcal{C}} = \hat{T}_{\mathcal{C}}$. Until now, the 1pNEGF, Eq. (8.62), seems to be just an even more complex object than the 1pRDM. The main advantage of this two-time formalism lies in the new possibilities of calculating the 1pNEGF directly from its own equation of motion.

From now on, we will drop the subscripts S and H, i.e. $\hat{f}_i|_z$ and $\hat{f}_i$ are Schrödinger operators whereas $\hat{f}_i(z)$ denotes a Heisenberg operator. We will now express the 1pNEGF by two new quantities by explicitly writing out the definition of the time-ordering operator:

$$\begin{aligned} G_{ij}^{(1)}(z,z') &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\,\hat{f}_i(z)\,\hat{f}_j^{\dagger}(z')\right\rangle = \\ &= \theta_{\mathcal{C}}(z-z')\,G_{ij}^{(1)>}(z,z') + \theta_{\mathcal{C}}(z'-z)\,G_{ij}^{(1)<}(z,z')\;, \end{aligned} \tag{8.64}$$

where the lesser and greater components[25] are,

$$\begin{aligned} G_{ij}^{(1)>}(z,z') &:= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(z)\,\hat{f}_j^{\dagger}(z')\right\rangle\;, \\ G_{ij}^{(1)<}(z,z') &:= \mp\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_j^{\dagger}(z')\,\hat{f}_i(z)\right\rangle\;. \end{aligned} \tag{8.65}$$

Note that $G^{(1)<}$ carries a negative (positive) sign for bosons (fermions)[26], which is motivated by the equal time (anti-)commutation relations[27]

$$[\hat{f}_i(z),\hat{f}_j^{\dagger}(z)]_{\mp} = \delta_{ij}\;, \qquad [\hat{f}_i^{(\dagger)}(z),\hat{f}_j^{(\dagger)}(z)]_{\mp} = 0\;. \tag{8.66}$$

[25] The greater and lesser components are also called correlation functions.

[26] There exist also "anomalous" Green functions containing two annihilation or two creation operators that are relevant for quantum coherence phenomena such as superfluidity or superconductivity [66, 67] which will not be considered here.

[27] Writing $\hat{f}_j^{(\dagger)}(z_2)$ means that the equation is true for both $\hat{f}_j^{\dagger}(z_2)$ and $\hat{f}_j(z_2)$ respectively.

Since we have (by convention) not separated in Eq. (8.64) a singular contribution proportional to $\delta(z-z')$, we will lateron encounter a discontinuity at equal times in the 1pNEGF.

Furthermore, in agreement with Eq. (8.64) and (8.65), we have to redefine our contour time-ordering operator for bosonic and fermionic creation and annihilation operators:

$$\hat{T}_{\mathcal{C}}\left\{\hat{f}_1^{(\dagger)}(z_1)\,\ldots\,\hat{f}_n^{(\dagger)}(z_n)\right\} := \sum_{\mathcal{P}}(\pm 1)^P\theta_{\mathcal{C}}(z_{\mathcal{P}(1)}-z_{\mathcal{P}(2)})\,\ldots\,\theta_{\mathcal{C}}(z_{\mathcal{P}(n-1)}-z_{\mathcal{P}(n)}) \times\ \hat{f}_{\mathcal{P}(1)}^{(\dagger)}(z_{\mathcal{P}(1)})\,\ldots\,\hat{f}_{\mathcal{P}(n)}^{(\dagger)}(z_{\mathcal{P}(n)})\ , \tag{8.67}$$

where P denotes the number of pair permutations (the parity) of field operators in $\mathcal{P}$. In other words, from now on, we will have a sign change whenever we commute two fermionic field operators [creation (annihilation) with creation (annihilation) or creation with annihilation] to obtain a proper contour ordered product. Thus, interchanging an operator $\hat{A}(z)$ consisting of an equal number of creation and annihilation operators (e.g. $\hat{n}_{ij}(z)=\hat{f}_i^\dagger(z)\hat{f}_j(z)$) with a single field operator will not cause a sign change. For example, for fermions (for bosons there is no change in signs) it is

$$\begin{aligned}\hat{T}_{\mathcal{C}}\{\hat{f}_i(z_1)\hat{f}_j^{(\dagger)}(z_2)\hat{n}_{kl}(z_3)\} =&\theta_{\mathcal{C}}(z_1-z_2)\theta_{\mathcal{C}}(z_2-z_3)\hat{f}_i(z_1)\hat{f}_j^{(\dagger)}(z_2)\hat{n}_{kl}(z_3)\\ &+\theta_{\mathcal{C}}(z_1-z_3)\theta_{\mathcal{C}}(z_3-z_2)\hat{f}_i(z_1)\hat{n}_{kl}(z_3)\hat{f}_j^{(\dagger)}(z_2)\\ &+\theta_{\mathcal{C}}(z_3-z_1)\theta_{\mathcal{C}}(z_1-z_2)\hat{n}_{kl}(z_3)\hat{f}_i(z_1)\hat{f}_j^{(\dagger)}(z_2)\\ &-\theta_{\mathcal{C}}(z_3-z_1)\theta_{\mathcal{C}}(z_1-z_2)\hat{f}_j^{(\dagger)}(z_2)\hat{f}_i(z_1)\hat{n}_{kl}(z_3)\\ &-\theta_{\mathcal{C}}(z_2-z_3)\theta_{\mathcal{C}}(z_3-z_1)\hat{f}_j^{(\dagger)}(z_2)\hat{n}_{kl}(z_3)\hat{f}_i(z_1)\\ &-\theta_{\mathcal{C}}(z_3-z_2)\theta_{\mathcal{C}}(z_2-z_1)\hat{n}_{kl}(z_3)\hat{f}_j^{(\dagger)}(z_2)\hat{f}_i(z_1)\ ,\end{aligned} \tag{8.68}$$

where, in the last three terms, $\hat{f}_i(z_1)$ and $\hat{f}_j^{(\dagger)}(z_2)$ have been interchanged, which caused the sign change. In agreement with the above definitions, we further have:

$$\begin{aligned}\hat{T}_{\mathcal{C}}\left\{\hat{f}_i(z_1)\hat{f}_j^{(\dagger)}(z_2)\hat{n}_{kl}(z_3)\right\} =&\hat{T}_{\mathcal{C}}\left\{\hat{f}_i(z_1)\hat{n}_{kl}(z_3)\hat{f}_j^{(\dagger)}(z_2)\right\}\\ =&\hat{T}_{\mathcal{C}}\left\{\hat{n}_{kl}(z_3)\hat{f}_i(z_1)\hat{f}_j^{(\dagger)}(z_2)\right\}\ ,\end{aligned} \tag{8.69}$$

and

$$\hat{T}_{\mathcal{C}}\left\{\hat{f}_i(z_1)\hat{f}_j^{(\dagger)}(z_2)\hat{n}_{kl}(z_3)\right\} = \pm\hat{T}_{\mathcal{C}}\left\{\hat{f}_j^{(\dagger)}(z_2)\hat{f}_i(z_1)\hat{n}_{kl}(z_3)\right\}\ . \tag{8.70}$$

Relations (8.68)–(8.70) are of utmost importance in the following sections, especially when it comes to the derivation of the *Contour Keldysh-Kadanoff-Baym Equations (KBE)*, which represent the main equations of the NEGF-formalism.

Note that the time-ordering operator defined in Eq. (8.67) is linear, i.e. for arbitrary operators $\hat{A}$, $\hat{B}$, $\hat{C}$ in Fock-space, it is

$$\hat{T}_{\mathcal{C}}\left\{(\hat{A}+\hat{B})\hat{C}\right\} = \hat{T}_{\mathcal{C}}\left\{\hat{A}\hat{C}\right\} + \hat{T}_{\mathcal{C}}\left\{\hat{B}\hat{C}\right\} \ , \tag{8.71}$$

and, since any operator in Fock-space possesses a series expansion of the form

$$\hat{A} = \sum_i \left(a_i \hat{f}_i + b_i \hat{f}_i^\dagger\right) + \sum_{ij}\left(a_{ij}\hat{f}_i\hat{f}_j^\dagger + b_{ij}\hat{f}_i^\dagger\hat{f}_j^\dagger + c_{ij}\hat{f}_i\hat{f}_j + d_{ij}\hat{f}_i^\dagger\hat{f}_j\right) + \dots \ , \tag{8.72}$$

the definition (8.67) is sufficient to define the time-ordering for arbitrary Fock operators.

Equal time limite of the 1pNEGF. In fact, the 1pNEGF has not been defined for equal times until now, since we have not defined $\hat{T}_{\mathcal{C}}$ for equal times. To reproduce the 1pRDM (8.61) in the equal time case, we proceed as follows:

$$\begin{aligned}\pm \mathrm{i}\hbar G_{ij}^{(1)}(z,z^+) &:= \pm\mathrm{i}\hbar \lim_{\epsilon\to 0} G_{ij}^{(1)}(z,z+\epsilon) \\ &= \pm\mathrm{i}\hbar G_{ij}^{(1),<}(z,z) = (\pm)\mathrm{i}\hbar(\mp)\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_j^\dagger(z)\,\hat{f}_i(z)\right\rangle = n_{ji}(z). \end{aligned} \tag{8.73}$$

Thus, we use the trick with the time argument z^+ to enforce the desired order of the two field operators.

As an illustration, we consider the coordinate representation of the 1pNEGF, i.e. we replace $|i\rangle \to |\mathbf{r}\rangle$, $\langle \mathbf{r}|i\rangle = \Phi_i(\mathbf{r})$, $\hat{f}_i(z) \to \hat{\Psi}(\mathbf{r},z) = \sum_i \Phi_i(\mathbf{r})\hat{f}_i(z)$:

$$\begin{aligned} G^{(1)}(\mathbf{r},z,\mathbf{r}',z') &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\hat{\Psi}(\mathbf{r},z)\hat{\Psi}^\dagger(\mathbf{r}',z')\right\rangle & (8.74)\\ &= -\frac{\mathrm{i}}{\hbar}\sum_{i,j}\Phi_i(\mathbf{r})\Phi_j^*(\mathbf{r}')\left\langle \hat{T}_{\mathcal{C}}\hat{f}_i(z)\hat{f}_j^\dagger(z')\right\rangle \\ &= \sum_{i,j}\Phi_i(\mathbf{r})\Phi_j^*(\mathbf{r}')G_{ij}^{(1)}(z,z'). & (8.75)\end{aligned}$$

Now let us consider how important quantities can be computed from the 1pNEGF. The total spatial and current density are given by (for bosons/fermions of mass m and no external vector potential applied),

$$\begin{aligned} n(\mathbf{r},z) &= \pm\mathrm{i}\hbar\, G^{(1)}(\mathbf{r}z,\mathbf{r},z^+) \ , & (8.76)\\ \mathbf{j}(\mathbf{r},z) &= \pm\mathrm{i}\hbar\left\{\frac{\hbar}{2m\mathrm{i}}\left(\nabla_{\mathbf{r}}-\nabla_{\mathbf{r}'}\right) G^{(1)}(\mathbf{r}\,z,\mathbf{r}',z^+)\right\}_{\mathbf{r}'=\mathbf{r}} \ . \end{aligned}$$

From the last section [cf. Eq. (8.47) and (8.55)], we know the relation between these contour observables and the real-time observables, e.g., for the contour spatial density, is

$$\begin{aligned} n(\mathbf{r}, t_-) &= n(\mathbf{r}, t), \quad \forall \quad t_- \in [t_{0-}, \infty], \\ n(\mathbf{r}, t_+) &= n(\mathbf{r}, t), \quad \forall \quad t_+ \in [\infty, t_{0+}], \\ n(\mathbf{r}, t_{0+} - \mathrm{i}\hbar\tau) &= n(\mathbf{r}, t_0), \quad \forall \quad \tau \in [0, \beta] \, . \end{aligned} \tag{8.77}$$

It can be shown that not only observables of one-particle type can be calculated from the 1pNEGF, but also the interaction energy can be computed from its dynamics.

Finally, another important quantity is the spectral function defined by:

$$A_{ij}(z, z') = \mathrm{i}\hbar \left\{ G_{ij}^{(1),>}(z, z') - G_{ij}^{(1),<}(z, z') \right\} \, , \tag{8.78}$$

which gives access to the local density of states and the addition, and removal energies. Another important quantity that can be obtained from the single-particle NEGF is the mean interaction energy which is given by (in momentum representation)

$$\langle \hat{V}_{12} \rangle(t) = \pm \, i \, \frac{\mathcal{V}}{4} \int \frac{d\vec{p}}{(2\pi\hbar)^3} \left\{ (i \, \partial_t - i \, \partial_{t'}) - \frac{p^2}{m} \right\} G^<(\vec{p}, t, t')|_{t=t'} \, , \tag{8.79}$$

where $\mathcal{V}$ denotes the volume, and the definition of $G^<$ for real time arguments will be introduced below. Recall that, with density operators we needed the two-particle density operator to compute expectation values of two-particles observables such as the mean interaction energy. Together with the spectral function, this example demonstrates the advantage of the two-time formalism.

For completeness, we give the definition of the **N-particle contour ordered NEGF**:

$$\begin{aligned} &G^{(n)}_{i_1,i_2,\ldots,i_n,j_1,j_2,\ldots,j_n}(z_1, \ldots, z_n, z'_1, \ldots, z'_n) := \\ &\left(-\frac{\mathrm{i}}{\hbar} \right)^n \left\langle \hat{T}_\mathcal{C} \left\{ \hat{f}_{i_1}(z_1), \ldots, \hat{f}_{i_n}(z_n), \hat{f}^\dagger_{j_n}(z'_n), \ldots, \hat{f}^\dagger_{j_1}(z'_1) \right\} \right\rangle \, . \end{aligned} \tag{8.80}$$

8.2.4 Matrix Representation of the Green Function

Instead of the prevailing definition (8.62), also matrix representations with respect to the contour time arguments of the 1pNEGF have emerged [68, 69]. These representations are needed for the solution of the equations of motion of

the 1pNEGF, which we will derive later on. As there are generally nine possibilities to distribute the two time arguments along the three contour branches a), b) and c) of Fig. 8.2, we will have to deal with 3 by 3 matrices of the form

$$G_{ij}^{(1)}(z,z') \cong \begin{bmatrix} G_{ij}^{(1)}(t_-,t'_-) & G_{ij}^{(1)}(t_-,t'_+) & G_{ij}^{(1)}(t_-,t'_|) \\ G_{ij}^{(1)}(t_+,t'_-) & G_{ij}^{(1)}(t_+,t'_+) & G_{ij}^{(1)}(t_+,t'_|) \\ G_{ij}^{(1)}(t_|,t'_-) & G_{ij}^{(1)}(t_|,t'_+) & G_{ij}^{(1)}(t_|,t'_|) \end{bmatrix} = \mathbf{G}_{ij}^{(1)}(z,z') \ . \quad (8.81)$$

The first equality has to be understood in the way that the contour 1pNEGF is completely defined by the components of the matrix on the r.h.s. From now on, the bold notation $\mathbf{G}_{ij}^{(1)}(z,z')$ refers to the 1pNEGF in matrix representation[28]. In the following, we will analyze this matrix and express its components in terms of some new quantities that depend only on the corresponding real times. For that purpose it is useful to keep in mind Fig. 8.2.

We will start with $G_{ij}^{(1)}(t_+,t'_-)$, where the first argument lies on the lower and the second on the upper branch. Since t_+ and t'_- are contour times it is $t_+ > t'_-$:

$$\begin{aligned} G_{ij}^{(1)}(t_+,t'_-) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\{\hat{f}_i(t_+)\hat{f}_j^\dagger(t'_-)\}\right\rangle = -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t_+)\hat{f}_j^\dagger(t'_-)\right\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t)\hat{f}_j^\dagger(t')\right\rangle := G_{ij}^{(1)>}(t,t') \ . \end{aligned} \quad (8.82)$$

First, we have applied the contour time ordering operator and afterwards inserted the definition of the contour Heisenberg operators (cf. Eq. 8.28). The second line in Eq. (8.82) defines one of the real-time correlation functions, which must not be confused with the contour correlation function (cf. Eq. 8.65), for these are completely different quantities [$\theta_{\mathcal{C}}(z-z')G_{ij}^{(1)>}(z,z')$ possesses itself a matrix representation of the form of Eq. (8.81))]. We will now

[28]Note that the Green function possesses a matrix representation in two ways, first, concerning the spin-orbitals i and j and second, concerning the contour time.

carry on in the same way with the rest of the components,

$$
\begin{aligned}
G_{ij}^{(1)}(t_-,t'_+) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\{\hat{f}_i(t_-)\hat{f}_j^\dagger(t'_+)\}\right\rangle = -\frac{\mathrm{i}}{\hbar}(\pm)\left\langle \hat{f}_j^\dagger(t'_+)\hat{f}_i(t_-)\right\rangle \\
&= \mp\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_j^\dagger(t')\hat{f}_i(t)\right\rangle := G_{ij}^{(1)<}(t,t'), \qquad (8.83)\\
G_{ij}^{(1)}(t_-,t'_-) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\{\hat{f}_i(t_-)\hat{f}_j^\dagger(t'_-)\}\right\rangle = -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}\{\hat{f}_i(t)\hat{f}_j^\dagger(t')\}\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\left(\Theta(t-t')\left\langle \hat{f}_i(t)\hat{f}_j^\dagger(t')\right\rangle \pm \Theta(t'-t)\left\langle \hat{f}_i(t)\hat{f}_j^\dagger(t')\right\rangle\right) \\
&= \Theta(t-t')G_{ij}^{(1)>}(t,t') + \Theta(t'-t)G_{ij}^{(1)<}(t,t') \\
&=: G_{ij}^{(1)c}(t,t') \qquad (8.84)\\
G_{ij}^{(1)}(t_+,t'_+) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}}\{\hat{f}_i(t_+)\hat{f}_j^\dagger(t'_+)\}\right\rangle = -\frac{\mathrm{i}}{\hbar}\left\langle \hat{\tilde{T}}\{\hat{f}_i(t)\hat{f}_j^\dagger(t')\}\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\left(\Theta(t'-t)\left\langle \hat{f}_i(t)\hat{f}_j^\dagger(t')\right\rangle \pm \Theta(t-t')\left\langle \hat{f}_i(t)\hat{f}_j^\dagger(t')\right\rangle\right) \\
&= \Theta(t'-t)G_{ij}^{(1)>}(t,t') + \Theta(t-t')G_{ij}^{(1)<}(t,t') \\
&=: G_{ij}^{(1)a}(t,t'). \qquad (8.85)
\end{aligned}
$$

The components $G_{ij}^{(1)c}(t,t')$ and $G_{ij}^{(1)a}(t,t')$ are called causal (c) and anti-causal (a) Green function. Obviously, only two of these four components are independent since the causal and anti-causal Green function are defined by the correlation functions. Moreover, it is common to express the components in terms of the retarded (R) and advanced (A) Green functions,

$$
\begin{aligned}
G_{ij}^{(1),\mathrm{R/A}}(t,t') &:= \pm\Theta(\pm[t-t'])\left\{G_{ij}^{(1),>}(t,t') - G_{ij}^{(1),<}(t,t')\right\}\ , \qquad (8.86)\\
G_{ij}^{(1)c}(t,t') &= \Theta(t-t')G_{ij}^{(1)>}(t,t') + \Theta(t'-t)G_{ij}^{(1)<}(t,t') \\
&= G_{ij}^{(1),\mathrm{R}}(t,t') + \underbrace{[\Theta(t-t')+\Theta(t'-t)]}_{1}G_{ij}^{(1),<}(t,t') \\
&= G_{ij}^{(1),<}(t,t') + G_{ij}^{(1),\mathrm{R}}(t,t')\ , \qquad (8.87)\\
G_{ij}^{(1)a}(t,t') &= G_{ij}^{(1),>}(t,t') - G_{ij}^{(1),\mathrm{R}}(t,t')\ . \qquad (8.88)
\end{aligned}
$$

Consider now the four components with one argument on the upper (or lower)

branch and the other on the imaginary branch,

$$
\begin{aligned}
G^{(1)}_{ij}(t_|, t'_-) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}} \hat{f}_i(t_|)\hat{f}^\dagger_j(t'_-)\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\hat{f}^\dagger_j(t')\right\rangle =: G^{(1)\ulcorner}(t_0 - \mathrm{i}\hbar\tau, t') \qquad (8.89)\\
G^{(1)}_{ij}(t_|, t'_+) &= G^{(1)\ulcorner}(t_0 - \mathrm{i}\hbar\tau, t') \qquad (8.90)\\
G^{(1)}_{ij}(t_-, t'_|) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}} \hat{f}_i(t_-)\hat{f}^\dagger_j(t'_|)\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}(\pm)\left\langle \hat{f}^\dagger_j(t_0 - \mathrm{i}\hbar\tau')\hat{f}_i(t)\right\rangle := G^{(1)\urcorner}_{ij}(t, t_0 - \mathrm{i}\hbar\tau') \qquad (8.91)\\
G^{(1)}_{ij}(t_+, t'_|) &= G^{(1)\urcorner}_{ij}(t, t_0 - \mathrm{i}\hbar\tau')\ , \qquad (8.92)
\end{aligned}
$$

where, again, only two of these four components are independent. The superscripts $\ulcorner$ and $\urcorner$ are quite intuitive when reading them from left to right (regarding the position of the arguments on the contour). Finally, we have the Matsubara Green function (MGF) with both arguments on the imaginary branch[29],

$$
\begin{aligned}
G^{(1)}_{ij}(t_|, t'_|) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{T}_{\mathcal{C}} \hat{f}_i(t_|)\hat{f}^\dagger_j(t'_|)\right\rangle = -\frac{\mathrm{i}}{\hbar}\left\langle \hat{\tilde{T}}_I \hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\hat{f}^\dagger_j(t_0 - \mathrm{i}\hbar\tau')\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\Big\{\Theta(\tau - \tau')\left\langle \hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\hat{f}^\dagger_j(t_0 - \mathrm{i}\hbar\tau')\right\rangle \\
&\qquad\qquad \pm \Theta(\tau' - \tau)\left\langle \hat{f}^\dagger_j(t_0 - \mathrm{i}\hbar\tau')\hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\right\rangle\Big\} \\
&= \Theta(\tau - \tau')G^{(1)>}_{ij}(t_{0+} - \mathrm{i}\hbar\tau, t_{0+} - \mathrm{i}\hbar\tau') \\
&\qquad + \Theta(\tau' - \tau)G^{(1)<}_{ij}(t_{0+} - \mathrm{i}\hbar\tau, t_{0+} - \mathrm{i}\hbar\tau') \\
&=: G^{(1)\mathrm{M}}_{ij}(t_0 - \mathrm{i}\hbar\tau, t_0 - \mathrm{i}\hbar\tau'). \qquad (8.93)
\end{aligned}
$$

Having obtained these relations, the matrix representation, Eq. (8.81), of the 1pNEGF can now be rewritten as follows: The four components with real arguments $(c, <, >, a)$ form the non-equilibrium block, the Matsubara Green (M) function the equilibrium "block" and the four functions with mixed arguments $(\urcorner, \ulcorner)$ the coupling elements, which are the linkage between equilibrium and non-equilibrium.

In matrix representation, we map the contour time-dependent 1pNEGF on to nine functions depending on real (physical) times and arguments $\tau \in [0, \beta]$.

[29] One has to be careful with the time-ordering on the imaginary branch. If $\tau > \tau'$ then $t_0 - \mathrm{i}\hbar\tau < t_0 - \mathrm{i}\hbar\tau'$ which is anti-chronologically ordered, because the contour extends along the negative imaginary axis. Therefore, we have a chronological time ordering with respect to $\tau \in [0, \beta]$.

Collecting the obtained results for the components [Eqs. (8.82)–(8.93)], we know there can be no more than five independent components/functions. In Section 8.2.6, we will show that

$$G_{ij}^{(1),\mathrm{M}}(t_0 - \mathrm{i}\tau, t_0 - \mathrm{i}\hbar\tau') = G_{ij}^{(1),\lceil}(t_0 - \mathrm{i}\hbar(\tau - \tau'), t_0), \tag{8.94}$$

and, therefore, we are left with only four independent components, e.g., one can choose $G_{ij}^{(1)<}(t,t')$, $G_{ij}^{(1)>}(t,t')$, $G_{ij}^{(1)\rceil}(t,t')$ and $G_{ij}^{(1)\lceil}(t,t')$ or $G_{ij}^{(1)\mathrm{R}}(t,t')$, $G_{ij}^{(1)\mathrm{A}}(t,t')$, $G_{ij}^{(1)\rceil}(t,t')$ and $G_{ij}^{(1)\lceil}(t,t')$, as a linear independent subset.

Actually, to simplify the calculus on the contour, there exist different matrix representations which are connected by linear transformations called "Keldysh rotations", see Ref. [65] and Ref. [68]. These different representations are often over-complete. As an illustration the *rak*-representation will is given below (omitting the arguments):

$$\mathbf{L} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix} \qquad \mathbf{M} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\mathbf{G}_{rak} := \mathbf{LMGL}^\dagger = \begin{bmatrix} G^{\mathrm{R}} & G^K & \sqrt{2}G^{\rceil} \\ 0 & G^{\mathrm{A}} & 0 \\ 0 & \sqrt{2}G^{\lceil} & G_{ij}^{\mathrm{M}} \end{bmatrix},$$

where G^K is the Keldysh Green function defined by:

$$G_{ij}^{(1)K}(t,t') := G_{ij}^{(1)>}(t,t') + G_{ij}^{(1)<}(t,t') \,. \tag{8.95}$$

When using the adiabatic switching instead of the equilibrium computation within the Grand ensemble to prepare a proper initial state at time $t = t_0$, one has to deal only with the non-equilibrium block, for which another important representation exists (Langreth and Wilkins):

$$\tilde{\mathbf{L}} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \qquad \tilde{\mathbf{M}} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\mathbf{G}_{LW} := \mathbf{LMG}_{2\times 2}\mathbf{L}^{-1} = \begin{bmatrix} G^{\mathrm{R}} & G^{<} \\ 0 & G^{\mathrm{A}} \end{bmatrix} .$$

Finally, the matrix representation of the contour step function $\theta_{\mathcal{C}}(z - z')$ and the contour delta function $\delta_{\mathcal{C}}(z - z') := \frac{d}{dz}\theta_{\mathcal{C}}(z - z')$ shall be given. By definition

these are

$$\theta_{\mathcal{C}}(z-z') = \begin{bmatrix} \Theta(t-t') & 0 & 0 \\ 1 & \Theta(t'-t) & 0 \\ 1 & 1 & \Theta[\mathrm{i}\hbar(\tau-\tau')] \end{bmatrix}, \tag{8.96}$$

$$\delta_{\mathcal{C}}(z-z') = \begin{bmatrix} \delta(t-t') & 0 & 0 \\ 0 & -\delta(t-t') & 0 \\ 0 & 0 & \delta[\mathrm{i}\hbar(\tau-\tau')] \end{bmatrix}. \tag{8.97}$$

8.2.5 Langreth-Wilkins Rules

Actually, the 1pNEGF is a member of a larger class of two-time contour ordered functions, which belong to a space referred to as Keldysh space. These functions are of the general form:

$$F_{ij}(z,z') = F^{\delta}_{ij}(z)\delta_{\mathcal{C}}(z-z') + \theta_{\mathcal{C}}(z-z')F^{>}_{ij}(z,z') + \theta_{\mathcal{C}}(z'-z)F^{<}_{ij}(z,z') \,. \tag{8.98}$$

In contrast to the self energy $\Sigma(z,z')$, which we will introduce later on, by definition, the Green function has been defined without a singular contribution. Obviously, any function on Keldysh space possesses a matrix representation similar to that of the Green function, Eq. (8.81). Using the matrix representation of the contour delta function, one only has to add the proper singular term in the definition of the diagonal components (F^c, F^a, F^R, F^A).

In the following part, we will have to deal repeatedly with the following product of two contour ordered functions $A_{ij}(z,z')$ and $B_{ij}(z,z')$ defined by:

$$\{AB\}_{ij}(z,z') := \int_{\mathcal{C}} \mathrm{d}\bar{z} \sum_k A_{ik}(z,\bar{z})B_{kj}(\bar{z},z') \,. \tag{8.99}$$

It is straightforward to show that this product again belongs to Keldysh space and, therefore, possesses a matrix representation denoted by $\mathbf{C}(z,z')$. Now, we will express the components of $\mathbf{C}(z,z')$ in terms of the matrix elements of $\mathbf{A}(z,z')$ and $\mathbf{B}(z,z')$. For a simplified notation, we use the Einstein summation convention and omit the spin-orbital arguments of the functions. Thus, we are left with,

$$C(z,z') = \int_{\mathcal{C}} \mathrm{d}\bar{z}\, A(z,\bar{z})B(\bar{z},z') \,. \tag{8.100}$$

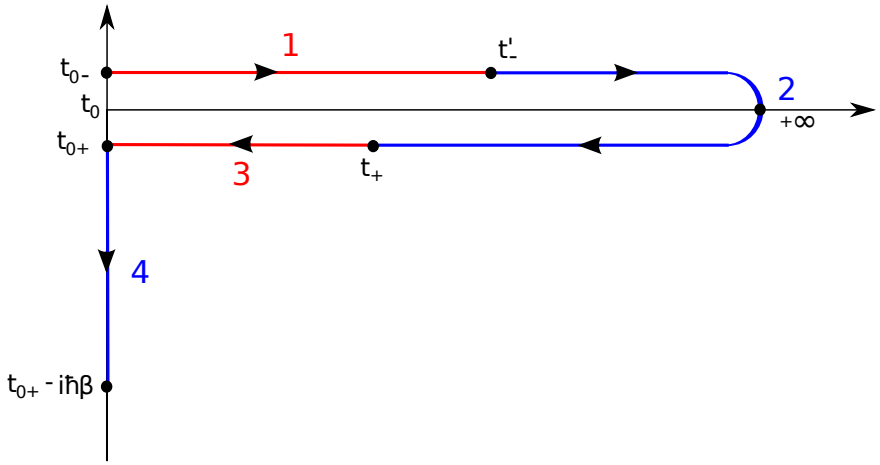

Abbildung 8.3: Illustration of the four parts of the integration in the calculation of $C(t_+, t'_-) = C^>(t, t')$.

As an illustration, we do the whole calculation for the component[30] $C^>(t, t')$:

$$
\begin{aligned}
C^>(t,t') = C(t_+,t'_-) &= \int_{\mathcal{C}} \mathrm{d}\bar{z}\, A(t_+,\bar{z})B(\bar{z},t'_-) \qquad (8.101)\\
&= \int_{\mathcal{C}} \mathrm{d}\bar{z}\, \left[A^\delta(t_+)\delta_{\mathcal{C}}(t_+-\bar{z}) + \theta_{\mathcal{C}}(t_+-\bar{z})A^>(t_+,\bar{z}) + \theta_{\mathcal{C}}(\bar{z}-t_+)A^<(t_+,\bar{z})\right]\\
&\quad \times \left[B^\delta(t'_-)\delta_{\mathcal{C}}(\bar{z}-t'_-) + \theta_{\mathcal{C}}(\bar{z}-t'_-)B^>(\bar{z},t'_-) + \theta_{\mathcal{C}}(t'_- -\bar{z})B^<(\bar{z},t'_-)\right] .
\end{aligned}
$$

The two singular contributions in Eq. (8.101) are evaluated trivially since they contain a contour delta function:

$$
\begin{aligned}
\int_{\mathcal{C}} \mathrm{d}\bar{z}\, A^\delta(t_+)\delta_{\mathcal{C}}(t_+-\bar{z})B(\bar{z},t'_-) &= A^\delta(t_+)B(t_+,t'_-) = A^\delta(t)B^>(t,t')\\
\int_{\mathcal{C}} \mathrm{d}\bar{z}\, A(t_+,\bar{z})B^\delta(t'_-)\delta_{\mathcal{C}}(\bar{z}-t'_-) &= B^\delta(t')A^>(t,t') \; . \qquad (8.102)
\end{aligned}
$$

For the remaining four terms, each with two step functions, we can either evaluate all the terms separately or we can decompose the contour integral in Eq. (8.101) into four parts, as shown in Fig. 8.3, and identify the corresponding contour correlation functions on each integration part, which is a little faster[31],

[30] Again, do not confuse real time correlation functions $F^{>/<}(t,t')$ with contour correlation funcitons $F^{>/<}(z,z')$.

[31] The evaluation of the step functions leads to the same decomposition.

$$
\begin{aligned}
C(t_+,t'_-) &= \underbrace{\int_{t_{0-}}^{t'_-} d\bar{t}_- A^>(t_+,\bar{t}_-)B^<(\bar{t}_-,t'_-)}_{1} + \underbrace{\int_{t'_-}^{t_+} d\bar{z} A^>(t_+,\bar{z})B^>(\bar{z},t'_-)}_{2} \\
&+ \underbrace{\int_{t_+}^{t_{0+}} d\bar{t}_+ A^<(t_+,\bar{t}_+)B^>(\bar{t}_+,t'_-)}_{3} + \underbrace{\int_{t_{0+}}^{t_{0+}-\mathrm{i}\hbar\beta} d\bar{z} A^<(t_+,\bar{z})B^>(\bar{z},t'_-)}_{4} \\
&+ A^\delta(t)B^>(t,t') + B^\delta(t')A^>(t,t') \; . \qquad (8.103)
\end{aligned}
$$

Next, we use the definitions of the real-time matrix elements [cf. Eqs. (8.82)-(8.93)] to convert the contour integrals into real-time integrals,

$$
\begin{aligned}
C^>(t,t') = &\int_{t_0}^{t'} d\bar{t} A^>(t,\bar{t})B^<(\bar{t},t') + \int_{t'}^{t} d\bar{t} A^>(t,\bar{t})B^>(\bar{t},t') \\
&+ \int_{t}^{t_0} d\bar{t} A^<(t,\bar{t})B^>(\bar{t},t') + \int_{t_0}^{t_0-\mathrm{i}\hbar\beta} d\bar{\gamma} A^\rceil(t,\bar{\gamma})B^\lceil(\bar{\gamma},t') \\
&+ A^\delta(t)B^>(t,t') + B^\delta(t')A^>(t,t') \; . \qquad (8.104)
\end{aligned}
$$

After splitting the integration of the second term into

$$
\int_{t'}^{t_0} d\bar{t} A^>(t,\bar{t})B^>(\bar{t},t') + \int_{t_0}^{t} d\bar{t} A^>(t,\bar{t})B^>(\bar{t},t') \; ,
$$

we can recast Eq. (8.104) as

$$
\begin{aligned}
C^>(t,t') = &- \int_{t_0}^{t'} d\bar{t} \left\{ A^>(t,\bar{t}) \left[B^>(\bar{t},t') - B^<(\bar{t},t') \right] \right\} + B^\delta(t')A^>(t,t') \\
&+ \int_{t_0}^{t} d\bar{t} \left\{ \left[A^>(t,\bar{t}) - A^<(t,\bar{t}) \right] B^>(\bar{t},t') \right\} + A^\delta(t)B^>(t,t') \\
&+ \int_{t_0}^{t_0-\mathrm{i}\hbar\beta} d\bar{\gamma} A^\rceil(t,\bar{\gamma})B^\lceil(\bar{\gamma},t') \; . \qquad (8.105)
\end{aligned}
$$

With the definition of the retarded and advanced component,

$$
F^{\mathrm{R/A}}(t,t') := F^\delta(t)\delta(t-t') \pm \Theta(\pm[t-t']) \left\{ F^>(t,t') - F^<(t,t') \right\} \; , \qquad (8.106)
$$

and a transformation of the integration variable in the third term ($\bar{\gamma} \to \bar{\tau} =$

Tabelle 8.1: Langreth-Wilkins rules for the two different types of multiplication of two contour-ordered functions $A(z,z')$ and $B(z,z')$. The result $C(z,z')$ is again a function on the Keldysh space and has the indicated components. The operations denoted by $\star$ and $\circ$ are defined by Eqs. (8.108) and (8.109).

	$C(z,z') = A(z,z')\,B(z',z)$	$C(z,z') = \int_{\mathcal{C}} \mathrm{d}\bar{z}\, A(z,\bar{z})\,B(\bar{z},z')$
C^{M}	$A^{\mathrm{M}}\,B^{\mathrm{M}}$	$A^{\mathrm{M}} \star B^{\mathrm{M}}$
$C^{\lceil}$	$A^{\lceil}\,B^{\rceil}$	$A^{\lceil} \circ B^{\mathrm{A}} + A^{\mathrm{M}} \star B^{\lceil}$
$C^{\rceil}$	$A^{\rceil}\,B^{\lceil}$	$A^{\mathrm{R}} \circ B^{\rceil} + A^{\rceil} \star B^{\mathrm{M}}$
$C^{>}$	$A^{>}\,B^{<}$	$A^{\mathrm{R}} \circ B^{>} + A^{>} \circ B^{\mathrm{A}} + A^{\rceil} \star B^{\lceil}$
$C^{<}$	$A^{<}\,B^{>}$	$A^{\mathrm{R}} \circ B^{<} + A^{<} \circ B^{\mathrm{A}} + A^{\rceil} \star B^{\lceil}$
C^{R}	$A^{\mathrm{R}}\,B^{>} + A^{>}\,B^{\mathrm{A}}$	$A^{\mathrm{R}} \circ B^{\mathrm{R}}$
C^{A}	$A^{\mathrm{A}}\,B^{<} + A^{<}\,B^{\mathrm{R}}$	$A^{\mathrm{A}} \circ B^{\mathrm{A}}$

$\frac{\bar{\gamma}-t_0}{-\mathrm{i}\hbar}$), we end up with,

$$
\begin{aligned}
C^{>}(t,t') = &\int_{t_0}^{\infty} d\bar{t} A^{>}(t,\bar{t}) \underbrace{\left[B^{\delta}(t')\delta(\bar{t}-t') - \Theta(t'-\bar{t})B^{>}(\bar{t},t') - B^{<}(\bar{t},t')\right]}_{B^{\mathrm{A}}(\bar{t},t')} \\
&+ \int_{t_0}^{\infty} d\bar{t} \underbrace{\left[A^{\delta}(t)\delta(\bar{t}-t) + \Theta(t-\bar{t})A^{>}(t,\bar{t}) - A^{<}(t,\bar{t})\right]}_{A^{\mathrm{R}}(t,\bar{t})} B^{>}(\bar{t},t') \\
&- \mathrm{i}\hbar \int_0^{\beta} d\bar{\tau} A^{\rceil}(t, t_0 - \mathrm{i}\hbar\bar{\tau}) B^{\lceil}(t_0 - \mathrm{i}\hbar\bar{\tau}, t') \\
= &\{A^{>} \circ B^{\mathrm{A}}\}(t,t') + \{A^{\mathrm{R}} \circ B^{>}\}(t,t') + \{A^{\rceil} \star B^{\lceil}\}(t,t') \;, \qquad (8.107)
\end{aligned}
$$

where, in the last line, a common short hand notation was introduced:

$$
\{f \circ g\}(t,t') := \int_{t_0}^{\infty} \mathrm{d}\bar{t}\, f(t,\bar{t})\, g(\bar{t},t') \;, \qquad (8.108)
$$

$$
\{f \star g\}(t,t') := -\mathrm{i}\hbar \int_0^{\beta} \mathrm{d}\bar{\tau}\, f(t, t_0 - \mathrm{i}\hbar\bar{\tau})\, g(t_0 - \mathrm{i}\hbar\bar{\tau}, t') \;. \qquad (8.109)
$$

In combination with the proper components[32] f and g, this notation is also used for imaginary arguments ($t_0 - \mathrm{i}\hbar\tau$ and $t_0 - \mathrm{i}\hbar\tau'$).

The derivation of the remaining matrix elements of $\mathbf{C}(z,z')$ can be done in the same way as presented here. The result for all components is called

[32] Meaning, they have to be defined for imaginary arguments.

Langreth-Wilkins rules [64] and is shown in the third column of Tab. 8.1. If one uses the special matrix representation

$$\mathbf{F}(z,z') = \begin{bmatrix} F^{\mathrm{R}} & F^{<} & F^{\rceil} \\ 0 & F^{\mathrm{A}} & 0 \\ 0 & F^{\lceil} & F^{\mathrm{M}} \end{bmatrix} , \tag{8.110}$$

for the Keldysh functions $A(z,z')$ and $B(z,z')$, then the Langreth-Wilkins rules follow trivially from common matrix multiplication: Therefore, this matrix representation allows us to treat functions on Keldysh space like normal matrices, when calculating products of the form (8.100). One only has to insert the proper operations $\circ$ or $\star$ into the components of the resulting matrix. Of course, this is not true for other matrix representations!

When dealing with Green functions, there is another product of two Keldysh functions that frequently occurs:

$$C(z,z') = A(z,z')B(z',z) . \tag{8.111}$$

The second column of Tab. (8.1) shows the matrix elements of $\mathbf{C}(z,z')$, which are trivial, except for the advanced and retarded components. Assuming $t \neq t'$ we have

$$\begin{aligned} C^{\mathrm{R}}(t,t') &= \theta(t-t')\Big[A^{>}(t,t')B^{<}(t',t) - A^{>}(t,t')B^{<}(t',t)\Big] \\ &= \theta(t-t')\Big[A^{>}(t,t')B^{<}(t',t) - A^{>}(t,t')B^{>}(t',t) \\ &\qquad + A^{>}(t,t')B^{>}(t',t) - A^{>}(t,t')B^{<}(t',t)\Big] \\ &= A^{>}(t,t')B^{\mathrm{A}}(t',t) + A^{\mathrm{R}}(t,t')B^{>}(t,t') . \end{aligned} \tag{8.112}$$

8.2.6 Properties of the Nonequilibrium Green function

In this section, first, some important properties of the contour 1pNEGF will be derived. After that, we will find the properties of its individual Keldysh matrix elements.

1. Relations for equal contour time arguments. From the definition of the contour 1pNEGF and the equal-time (anti-) commutation relations of the creation and annihilation operators, we know that there exists a discontinuity

at equal contour times,

$$\begin{aligned} G_{ij}^{(1)>}(z,z) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(z)\hat{f}_j^\dagger(z)\right\rangle \\ &= -\frac{\mathrm{i}}{\hbar}\left(\left\langle \pm\hat{f}_j^\dagger(z)\hat{f}_i(z)+\delta_{ij}\right\rangle\right) \\ &= \mp\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_j^\dagger(z)\hat{f}_i(z)\right\rangle - \frac{\mathrm{i}}{\hbar}\delta_{ij} \\ &= G_{ij}^{(1)<}(z,z) - \frac{\mathrm{i}}{\hbar}\delta_{ij} \end{aligned}$$

$$\iff \quad G_{ij}^{(1)>}(z,z) - G_{ij}^{(1)<}(z,z) = -\frac{\mathrm{i}}{\hbar}\delta_{ij} \tag{8.113}$$

$$\iff \quad \lim_{\epsilon\to 0} G_{ij}^{(1)}(z+\epsilon,z) - G_{ij}^{(1)}(z,z) = -\frac{\mathrm{i}}{\hbar}\delta_{ij}\ . \tag{8.114}$$

2. Kubo-Martin-Schwinger (KMS) condition. The following relations hold:

$$\begin{aligned} G_{ij}^{(1)}(t_{0-},z') &= \pm\mathrm{e}^{\beta\mu}G_{ij}^{(1)}(t_{0+}-\mathrm{i}\hbar\beta,z')\ , \\ G_{ij}^{(1)}(z',t_{0-}) &= \pm\mathrm{e}^{-\beta\mu}G_{ij}^{(1)}(z',t_{0+}-\mathrm{i}\hbar\beta) \quad \forall \quad z'\in\mathcal{C}\ , \end{aligned} \tag{8.115}$$

or, equivalently,

$$\begin{aligned} G_{ij}^{(1)<}(t_{0-},z') &= \pm\mathrm{e}^{\beta\mu}G_{ij}^{(1)>}(t_{0+}-\mathrm{i}\hbar\beta,z') \\ G_{ij}^{(1)>}(z',t_{0-}) &= \pm\mathrm{e}^{-\beta\mu}G_{ij}^{(1)<}(z',t_{0+}-\mathrm{i}\hbar\beta) \quad \forall \quad z'\in\mathcal{C}\ , \end{aligned} \tag{8.116}$$

The proof is based on the following operator identities:

$$\hat{f}_i\mathrm{e}^{\beta\mu\hat{N}} = \mathrm{e}^{\beta\mu(\hat{N}+1)}\hat{f}_i\ , \tag{8.117}$$

$$\hat{f}_i^\dagger\mathrm{e}^{\beta\mu\hat{N}} = \mathrm{e}^{\beta\mu(\hat{N}-1)}\hat{f}_i^\dagger. \tag{8.118}$$

The proof of Eqs. (8.117, 8.118) is simple. Let $\hat{N}|N\rangle = N|N\rangle$. Since $\hat{f}_i$ annihilates a particle in the spin orbital i, we find the following two relations[33],

$$\begin{aligned} \hat{f}_i\mathrm{e}^{\beta\mu\hat{N}}|N\rangle &= \mathrm{e}^{\beta\mu N}\hat{f}_i|N\rangle = \mathrm{e}^{\beta\mu N}c|N-1\rangle \\ \mathrm{e}^{\beta\mu(\hat{N}+1)}\hat{f}_i|N\rangle &= \mathrm{e}^{\beta\mu(\hat{N}+1)}c|N-1\rangle = \mathrm{e}^{\beta\mu N}c|N-1\rangle\ . \end{aligned}$$

This proves Eq. (8.117), and the identity (8.118) follows in the same way. With that, the KMS-conditions follow directly from the definition of the 1pNEGF [cf. Eq. (8.63)]. We have[34]

[33] c is the normalization constant for bosons or fermions (including the phase factor).

[34] In this proof we again use the subscript S to emphasise Schrödinger operators.

$$
\begin{aligned}
G^{(1)}_{ij}(t_{0-},z') &= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}}\hat{T}_\mathcal{C}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_\mathcal{C}\mathrm{d}\bar{z}\,\hat{H}_\mathrm{S}(\bar{z})}\hat{f}_{i,\mathrm{S}}|_{t_{0-}}\hat{f}^\dagger_{j,\mathrm{S}}|_{z'}\right\}\right\} \\
&= (\pm)\left(-\frac{\mathrm{i}}{\hbar}\right)\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}}\hat{T}_\mathcal{C}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_\mathcal{C}\mathrm{d}\bar{z}\,\hat{H}_\mathrm{S}(\bar{z})}\hat{f}^\dagger_{j,\mathrm{S}}|_{z'}\right\}\hat{f}_{i,\mathrm{S}}\right\} \quad (8.119) \\
&= (\pm)\left(-\frac{\mathrm{i}}{\hbar}\right)\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu(\hat{N}_\mathrm{S}+1)}\hat{f}_{i,\mathrm{S}}\hat{T}_\mathcal{C}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_\mathcal{C}\mathrm{d}\bar{z}\,\hat{H}_\mathrm{S}(\bar{z})}\hat{f}^\dagger_{j,\mathrm{S}}|_{z'}\right\}\right\} \quad (8.120) \\
&= (\pm)\mathrm{e}^{\beta\mu}\left(-\frac{\mathrm{i}}{\hbar}\right)\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}}\hat{T}_\mathcal{C}\left\{\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\int_\mathcal{C}\mathrm{d}\bar{z}\,\hat{H}_\mathrm{S}(\bar{z})}\hat{f}_{i,\mathrm{S}}|_{t_{0+}-\mathrm{i}\hbar\beta}\hat{f}^\dagger_{j,\mathrm{S}}|_{z'}\right\}\right\} \\
&= (\pm)\mathrm{e}^{\beta\mu}G^{(1)}_{ij}(t_{0+}-\mathrm{i}\hbar\beta,z').
\end{aligned}
$$

Here, we took advantage of the fact that t_{0-} is the earliest time on $\mathcal{C}$ (Eq. 8.119). Thereby, we have a sign change for fermions from the definition of the time-ordering operator. Second, the cyclic invariance of the trace and Eq. (8.117) were used in Eq. (8.120). Finally, we could reinsert the annihilation operator under the time ordering operator since $(t_{0+}-\mathrm{i}\hbar\beta)$ is the latest contour time[35].

The proof of the second KMS-condition [second line of Eq. (8.115)] and also for higher Green functions works the same way, e.g., it is

$$
\begin{aligned}
&G^{(n)}_{i_1,i_2,\ldots,i_n,j_1,j_2,\ldots,j_n}(z_1,t_{0-},z_3\ldots,z_n,z'_1,z'_2,z'_3,\ldots,z'_n) \\
&= \pm\mathrm{e}^{\beta\mu}G^{(n)}_{i_1,i_2,\ldots,i_n,j_1,j_2,\ldots,j_n}(z_1,t_{0+}-\mathrm{i}\hbar\beta,z_3\ldots,z_n,z'_1,z'_2,z'_3,\ldots,z'_n)\,. \quad (8.121)
\end{aligned}
$$

3. Time transposition symmetries. Now, we will give some useful relations of the matrix elements that are related to an exchange of the two time arguments.

A.) We begin with the real-time correlation functions, for which the relation

$$
G^{(1)\gtrless}_{ij}(t,t') = -\left[G^{(1)\gtrless}_{ji}(t',t)\right]^*\,, \quad (8.122)
$$

holds. Therefore, in practice[36], we have to calculate the correlation functions $G^{(1)\gtrless}_{ij}(t,t')$ only in one half of the time plane, e.g., only for $t \geq t'$ since for $t < t'$ we can use the value of $-\left[G^{(1)\gtrless}_{ji}(t',t)\right]^*$. We will prove this relation for

[35] Recall that the field operators are Schrödinger operators, and we only need to make sure that the ordering of the operators under $\hat{T}_\mathcal{C}$ remains unchanged.

[36] Of course, we always have to calculate the Green functions $\mathbf{G}_{ij}(z,z')$ (matrix with respect to time) for all basis indices $i,j \in 1\ldots N_B$, where N_B is the basis size (approximation).

the greater component:

$$G_{ij}^{(1)>}(t,t') = -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t)\hat{f}_j^\dagger(t')\right\rangle = -\left(-\frac{\mathrm{i}}{\hbar}\right)^*\left\langle\left[\hat{f}_j(t')\hat{f}_i^\dagger(t)\right]^\dagger\right\rangle = \\ = \left[-\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_j(t')\hat{f}_i^\dagger(t)\right\rangle\right]^* = -\left[G_{ji}^{(1)>}(t',t)\right]^*. \tag{8.123}$$

B.) From this we also obtain a symmetry relation for the retarded and advanced function defined by Eq. (8.86):

$$G_{ij}^{(1)R}(t,t') = \left[G_{ji}^{(1)A}(t',t)\right]^*, \tag{8.124}$$

which is straightforwardly proven by using the definition (8.86) and the symmetry properties of $G^{\gtrless}$, Eq. (8.122).

C.) Further, there is a similar relation for the two mixed elements with real and imaginary time arguments:

$$\mp G_{ij}^{(1)\lceil}(t_0 - \mathrm{i}\hbar\tau, t') = \left[G_{ji}^{(1)\rceil}(t', t_0 - \mathrm{i}\hbar(\beta-\tau))\right]^*. \tag{8.125}$$

For the proof, we will start from the r.h.s of Eq. (8.125) and show the equalitiy to the l.h.s:

$$\left[G_{ji}^{(1)\rceil}(t', t_0 - \mathrm{i}\hbar(\beta-\tau))\right]^* = \left[\mp\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i^\dagger(t_0 - \mathrm{i}\hbar(\beta-\tau))\hat{f}_j(t')\right\rangle\right]^* \\ = \pm\frac{\mathrm{i}}{\hbar}\left\langle\left[\hat{f}_i^\dagger(t_0 - \mathrm{i}\hbar(\beta-\tau))\hat{f}_j(t')\right]^\dagger\right\rangle \\ = \pm\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_j^\dagger(t')\left[\hat{f}_i^\dagger(t_0 - \mathrm{i}\hbar(\beta-\tau))\right]^\dagger\right\rangle. \tag{8.126}$$

Remembering that the evolution operator along the imaginary axis is not unitary [cf. Eq. (8.28)], we have to be careful with the hermitian conjugate of a Heisenberg operator, if it has a complex time argument. It is

$$\left[\hat{f}_i^\dagger(t_0 - \mathrm{i}\hbar(\beta-\tau))\right]^\dagger = \left[\hat{U}_0(t_0, t_0 - \mathrm{i}\hbar(\beta-\tau))\hat{f}_{i,\mathrm{S}}^\dagger\hat{U}_0(t_0 - \mathrm{i}\hbar(\beta-\tau), t_0)\right]^\dagger \\ = \left[\mathrm{e}^{\hat{H}_\mathrm{S}(t_0)(\beta-\tau)}\hat{f}_{i,\mathrm{S}}^\dagger\,\mathrm{e}^{-\hat{H}_\mathrm{S}(t_0)(\beta-\tau)}\right]^\dagger \\ = \mathrm{e}^{-\hat{H}_\mathrm{S}(t_0)(\beta-\tau)}\hat{f}_{i,\mathrm{S}}\,\mathrm{e}^{\hat{H}_\mathrm{S}(t_0)(\beta-\tau)} \\ = \hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0)\underbrace{\hat{U}_0(t_0, t_0 - \mathrm{i}\hbar\tau)\hat{f}_{i,\mathrm{S}}\hat{U}_0(t_0 - \mathrm{i}\hbar\tau, t_0)}_{\hat{f}_i(t_0 - \mathrm{i}\hbar\tau)} \\ \times\hat{U}_0(t_0, t_0 - \mathrm{i}\hbar\beta) \\ \left(\neq \hat{f}_i(t_0 - \mathrm{i}\hbar(\beta-\tau))\right). \tag{8.127}$$

Inserting this into Eq. (8.126) and again making use of the cyclic invariance of the trace, we find

$$\begin{aligned}
\left[G_{ji}^{(1)\rceil}(t', t_0 - \mathrm{i}\hbar(\beta - \tau))\right]^* &= \pm\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}}\hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0)\hat{f}_j^\dagger(t')\right. \\
&\qquad \left.\times \hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0)\hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\hat{U}_0(t_0, t_0 - \mathrm{i}\hbar\beta)\right\} \\
&= \pm\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}}\underbrace{\hat{U}_0(t_0, t_0 - \mathrm{i}\hbar\beta)\hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0)}_{\hat{1}}\right. \\
&\qquad \left.\times \hat{f}_j^\dagger(t')\hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0)\hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\right\} \\
&= \pm\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}_\mathrm{S}}\hat{U}_0(t_0 - \mathrm{i}\hbar\beta, t_0)\hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\hat{f}_j^\dagger(t')\right\} \\
&= \pm\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t_0 - \mathrm{i}\hbar\tau)\hat{f}_j^\dagger(t')\right\rangle \\
&= \mp G_{ij}^{(1)\lceil}(t_0 - \mathrm{i}\hbar\tau, t') \; . \qquad (8.128)
\end{aligned}$$

Now, we investigate the Matsubara Green function. First, the MGF is connected to the real time correlation functions in the following way:

$$\begin{aligned}
G_{ij}^{(1)\mathrm{M}}(t_0 - \mathrm{i}\hbar 0, t_0 - \mathrm{i}\hbar 0^+) &= -\frac{\mathrm{i}}{\hbar}\lim_{\epsilon\to 0} G_{ij}^{(1)\mathrm{M}}(t_0 - \mathrm{i}\hbar 0, t_0 - \mathrm{i}\hbar\epsilon) \\
&= -\frac{\mathrm{i}}{\hbar}\lim_{\epsilon\to 0}\left[\Theta(0-\epsilon)\left\langle \hat{f}_i(t_0 - \mathrm{i}\hbar 0)\hat{f}_j^\dagger(t_0 - \mathrm{i}\hbar\epsilon)\right\rangle\right. \\
&\qquad \left. + \Theta(\epsilon - 0)\left\langle \hat{f}_j^\dagger(t_0 - \mathrm{i}\hbar\epsilon)\hat{f}_i(t_0 - \mathrm{i}\hbar 0)\right\rangle\right] \\
&= -\frac{\mathrm{i}}{\hbar}\lim_{\epsilon\to 0}\left\langle \hat{f}_j^\dagger(t_0 - \mathrm{i}\hbar\epsilon)\hat{f}_i(t_0 - \mathrm{i}\hbar 0)\right\rangle \\
&= G_{ij}^{(1)<}(t_0, t_0) \; , \qquad (8.129)
\end{aligned}$$

and naturally,

$$G_{ij}^{(1)\mathrm{M}}(t_0 - \mathrm{i}\hbar 0^+, t_0 - \mathrm{i}\hbar 0) = G_{ij}^{(1)>}(t_0, t_0) \; , \qquad (8.130)$$

holds. Second, the MGF dependents only on the difference of the imaginary part of the complex arguments. Without loss of generality, we assume $\tau \geq \tau'$,

it is,

$$\begin{aligned}
G_{ij}^{(1)\mathrm{M}}(t_0-\mathrm{i}\hbar\tau,t_0-\mathrm{i}\hbar\tau') &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t_0-\mathrm{i}\hbar\tau)\hat{f}_j^\dagger(t_0-\mathrm{i}\hbar\tau')\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}}\hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\hat{U}_0(t_0,t_0-\mathrm{i}\hbar\tau)\hat{f}_i\right. \\
&\quad \left.\times \underbrace{\hat{U}_0(t_0-\mathrm{i}\hbar\tau,t_0-\mathrm{i}\hbar\tau')}_{=\hat{U}_0(t_0-\mathrm{i}\hbar(\tau-\tau'),t_0)}\hat{f}_j\hat{U}_0(t_0-\mathrm{i}\hbar\tau',t_0)\right\} \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}}\hat{U}_0(t_0-\mathrm{i}\hbar\tau',t_0)\hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\right. \\
&\quad \left.\times \hat{U}_0(t_0,t_0-\mathrm{i}\hbar\tau)\hat{f}_i\hat{U}_0(t_0-\mathrm{i}\hbar(\tau-\tau'),t_0)\hat{f}_j\right\} \qquad (8.131) \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}}\hat{U}_0(t_0-\mathrm{i}\hbar\beta,t_0)\right. \\
&\quad \left.\times \hat{U}_0(t_0,t_0-\mathrm{i}\hbar(\tau-\tau'))\hat{f}_i\hat{U}_0(t_0-\mathrm{i}\hbar(\tau-\tau'),t_0)\hat{f}_j\right\} \qquad (8.132) \\
&= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t_0-\mathrm{i}\hbar(\tau-\tau'))\hat{f}_j^\dagger(t_0)\right\rangle \\
&= G_{ij}^{(1)\ulcorner}(t_0-\mathrm{i}\hbar(\tau-\tau'),t_0)\ .
\end{aligned}$$

From Eq. (8.131) to Eq. (8.132), we used the fact that

$$\left[\hat{U}_0(t_1,t_2),\hat{U}_0(t_3,t_4)\right]_- = 0\ . \qquad (8.133)$$

The same derivation for $\tau \leq \tau'$ yields[37]

$$G_{ij}^{(1)\mathrm{M}}(t_0-\mathrm{i}\hbar\tau,t_0-\mathrm{i}\hbar\tau') = G_{ij}^{(1)\urcorner}(t_0,t_0+\mathrm{i}\hbar(\tau-\tau'))\ . \qquad (8.134)$$

Therefore, we can redefine the MGF by a continuous function depending on $\bar{\tau}=\tau-\tau'$ only,

$$G_{ij}^{(1)\mathrm{M}}(t_0-\mathrm{i}\hbar\tau,t_0-\mathrm{i}\hbar\tau') = G_{ij}^{(1)\mathrm{M}}(\bar{\tau}) := \begin{cases} G_{ij}^{(1)\ulcorner}(t_0-\mathrm{i}\hbar\bar{\tau},t_0), & \text{for} \quad \bar{\tau}\geq 0 \\ G_{ij}^{(1)\urcorner}(t_0,t_0+\mathrm{i}\hbar\bar{\tau}), & \text{for} \quad \bar{\tau}<0\ . \end{cases} \qquad (8.135)$$

4. Summary of symmetry relations. Let us summarize all properties of the 1pNEGF and its matrix elements, which we found until now, because

[37] In this case it is not possible to express $G^{(1)\mathrm{M}}$ by $G_{ij}^{(1)\ulcorner}$.

those play an important role in the NEGF-formalism:

$$
\begin{aligned}
G_{ij}^{(1)>}(z,z) - G_{ij}^{(1)<}(z,z) &= -\frac{\mathrm{i}}{\hbar}\,\delta_{ij} \qquad \text{(at equal times!)}\,, && (8.136)\\
G^{(1)}(t_{0-},z') &= \pm \mathrm{e}^{\beta\mu} G^{(1)}(t_{0+} - \mathrm{i}\hbar\beta, z'), \quad \forall \quad z' \in \mathcal{C} && \text{a)}\\
G^{(1)}(z,t_{0-}) &= \pm \mathrm{e}^{-\beta\mu} G^{(1)}(z, t_{0+} - \mathrm{i}\hbar\beta), \quad \forall \quad z \in \mathcal{C} && \text{b)}\,,\\
G_{ij}^{(1)\mathrm{M}}(t_0 - \mathrm{i}\hbar 0, t_0 - \mathrm{i}\hbar 0^+) &= G_{ij}^{(1)<}(t_0,t_0) && \text{c)}\,,\\
G_{ij}^{(1)\mathrm{M}}(t_0 - \mathrm{i}\hbar 0^+, t_0 - \mathrm{i}\hbar 0) &= G_{ij}^{(1)>}(t_0,t_0)\,,\\
G_{ij}^{(1)\mathrm{M}}(t_0 - \mathrm{i}\hbar\tau, t_0 - \mathrm{i}\hbar\tau') &= G_{ij}^{(1)\mathrm{M}}(\bar{\tau}) && \text{d)}\,,\\
G_{ij}^{(1)\gtrless}(t,t') &= -[G_{ji}^{(1)\gtrless}(t',t)]^*\,,\\
G_{ij}^{(1)R}(t,t') &= \left[G_{ji}^{(1)A}(t',t)\right]^*\,,\\
G_{ij}^{(1)\ulcorner}(t_0 - \mathrm{i}\hbar\tau, t') &= \mp\left[G_{ji}^{(1)\urcorner}(t', t_0 - \mathrm{i}\hbar(\beta-\tau))\right]^*\,.
\end{aligned}
$$

Further[38], we can explicitly write down the KMS-conditions a) and b) for the matrix elements (by inserting $t_-^{(\prime)}, t_+^{(\prime)}, t_\urcorner^{(\prime)}$ for $z^{(\prime)}$), which yields the following relations (omitting arguments i and j):

$$
\begin{aligned}
G^<(t_0,t') &= \pm \mathrm{e}^{\beta\mu} G^\ulcorner(t_0 - \mathrm{i}\hbar\beta, t')\,, && (8.137)\\
G^\urcorner(t_0, t_0 - \mathrm{i}\hbar\tau') &= \pm \mathrm{e}^{\beta\mu} G^{\mathrm{M}}(t_0 - \mathrm{i}\hbar\beta, t_0 - \mathrm{i}\hbar\tau')\\
&= \pm \mathrm{e}^{\beta\mu} G^{\mathrm{M}}(\beta - \tau') \underset{\beta-\tau'\geq 0}{=} \pm \mathrm{e}^{\beta\mu} G^\ulcorner(t_0 - \mathrm{i}\hbar(\beta-\tau'), t_0)\,, && (8.138)\\
G^>(t,t_0) &= \pm \mathrm{e}^{-\beta\mu} G^\urcorner(t, t_0 - \mathrm{i}\hbar\beta)\,, && (8.139)\\
G^\ulcorner(t_0 - \mathrm{i}\hbar\tau, t_0) &= \pm \mathrm{e}^{-\beta\mu} G^{\mathrm{M}}(t_0 - \mathrm{i}\hbar\tau, t_0 - \mathrm{i}\hbar\beta)\\
&= \pm \mathrm{e}^{-\beta\mu} G^{\mathrm{M}}(\tau - \beta) \underset{\tau-\beta\leq 0}{=} \pm \mathrm{e}^{-\beta\mu} G^\urcorner(t_0, t_0 + \mathrm{i}\hbar(\tau-\beta))\,. && (8.140)
\end{aligned}
$$

5. Fourier series representation of the Matsubara Green function. Matsubara frequencies. Inserting $G^\urcorner(t_0, t_0 - \mathrm{i}\hbar\tau') = G^{\mathrm{M}}(t_0 - \mathrm{i}\hbar 0, t_0 - \mathrm{i}\hbar\tau') = G^{\mathrm{M}}(\bar{\tau} = -\tau')$ into Eq. (8.138), we see that the MGF is periodic in terms of the relative variable $\bar{\tau}$ with a periodicity length of β[39]:

$$
G_{ij}^{\mathrm{M}}(\bar{\tau}) = \pm \mathrm{e}^{\beta\mu} G_{ij}^{\mathrm{M}}(\bar{\tau} + \beta)\,. \tag{8.141}
$$

[38] From now on, we will drop the superscript "(1)", i.e., it is always the 1pNEGF. If we refer to the 2pNEGF, we will point this out explicitly.

[39] with this notation of the argument the true time follows by multiplying with $\hbar$

Therefore, the MGF possesses a discrete Fourier series of the form (τ now denotes a relative variable)[40]:

$$G_{ij}^{\mathrm{M}}(\tau) = \frac{1}{-\mathrm{i}\hbar\beta} \sum_m g_{ij}(z_m) \mathrm{e}^{-\mathrm{i}z_m(\mathrm{i}\hbar\tau)} \ . \tag{8.142}$$

The z_m's are called *Matsubara frequencies* and are determined by Eq. (8.141). We have

$$\begin{aligned} & G_{ij}^{\mathrm{M}}(0) \stackrel{!}{=} \pm \mathrm{e}^{\beta\mu} G_{ij}^{\mathrm{M}}(\beta) \\ \Leftrightarrow \quad & \frac{1}{-\mathrm{i}\hbar\beta} \sum_m g_{ij}(z_m) \mathrm{e}^0 \stackrel{!}{=} \pm \mathrm{e}^{\beta\mu} \frac{1}{-\mathrm{i}\hbar\beta} \sum_m g_{ij}(z_m) \mathrm{e}^{-\mathrm{i}z_m(\mathrm{i}\hbar\beta)} \quad \forall m \\ \Leftrightarrow \quad & \pm 1 \stackrel{!}{=} \mathrm{e}^{-\mathrm{i}(z_m(\mathrm{i}\hbar\beta)+\mathrm{i}\beta\mu)} \\ \Leftrightarrow \quad & m\pi = z_m \mathrm{i}\hbar\beta + \mathrm{i}\beta\mu \ , \end{aligned} \tag{8.143}$$

and finally[41]

$$z_m = \frac{m\pi}{\mathrm{i}\hbar\beta} - \frac{\mu}{\hbar}, \quad \text{with} \quad m = \begin{cases} \pm 0, \pm 2, \pm 4 \ldots , & \text{for bosons.} \\ \pm 1, \pm 3, \pm 5 \ldots , & \text{for fermions.} \end{cases} \tag{8.144}$$

The Fourier representation of the MGF can be useful, if we want to solve the equation of motion of the MGF (which we will find later on). Instead of solving the equation for the continuous variable τ, we only have to find the Fourier-coefficients $g(z_m)$ at the discrete Matsubara frequencies.

8.3 Equilibrium Spectral Function. Kadanoff-Baym Ansatz (KBA)

In this section, we will assume the system to be in *equilibrium*, also for times $t \geq t_0$ (i.e. the external potential $\hat{v}$ in the Hamiltonian (8.1) does not depend on time and $\partial_t \hat{H} \equiv 0$.). Then always $\left\langle \hat{A} \right\rangle (t) = \left\langle \hat{A} \right\rangle (t_0)$, and thus, there is no evolution along the real time axis, but there may be a time-dependence along

[40] It is convention to factor out the constant $\frac{1}{-\mathrm{i}\hbar\beta}$ from the Fourier coefficients $g(z_m)$.

[41] The different sign of $\frac{\mu}{\hbar}$ compared to that in the book of Kadanoff and Baym comes from the definition of the relative variable $\bar{\tau} := \tau - \tau' \sim$ second minus first argument of the GF, where in that book it is defined the other way round. The present definition coincides with the one used in Ref. [BB13].

the imaginary axis. Therefore, in equilibrium, the only independent matrix element of the 1pNEGF is the MGF. Still, it is advantageous to investigate the other matrix elements as well. For example, the additional assumption of a spatially homogeneous system (i.e. the external potential $\hat{v}$ has no space dependence[42]), will bring us to the *Kadanoff-Baym-Ansatz*, which can serve as a first approximation for the solution of the equations of motion later on. To simplify the notation, we will set $t_0 = 0$ in this section.

8.3.1 Equilibrium correlation functions $G^{\gtrless}$

First, let us examine one of the mixed elements in the equilibrium case[43], it is

$$\begin{aligned}
G^{\ulcorner}(-\mathrm{i}\hbar\tau, t') &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(-\mathrm{i}\hbar\tau)\hat{f}_j^\dagger(t')\right\rangle \\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}}\hat{U}_0(-\mathrm{i}\hbar\beta,0)\hat{U}_0(0,-\mathrm{i}\hbar\tau)\right. \\
&\qquad\left.\times\hat{f}_i\underbrace{\hat{U}_0(-\mathrm{i}\hbar\tau,0)\hat{U}_0(0,t')}_{\hat{U}_0(-\mathrm{i}\hbar\tau-t',0)}\hat{f}_j^\dagger\hat{U}_0(t',0)\right\} \qquad (8.145)\\
&= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}}\hat{U}_0(-\mathrm{i}\hbar\beta,0)\underbrace{\hat{U}_0(t',0)\hat{U}_0(0,-\mathrm{i}\hbar\tau)}_{\hat{U}_0(-\mathrm{i}\hbar\tau-t',0)}\right. \\
&\qquad\left.\times\hat{f}_i\hat{U}_0(-\mathrm{i}\hbar\tau-t',0)\hat{U}_0(0,0)\hat{f}_j^\dagger\hat{U}_0(0,0)\right\} \\
&= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(-\mathrm{i}\hbar\tau-t')\hat{f}_j^\dagger(0)\right\rangle \\
&= G^{\ulcorner}(-\mathrm{i}\hbar\tau-t',0) \qquad (8.146)
\end{aligned}$$

Starting from Eq. (8.145) and again using the cyclic invariance of the trace, we can arrange the arguments in another way:

$$\begin{aligned}
G^{\ulcorner}(-\mathrm{i}\hbar\tau, t') &= -\frac{\mathrm{i}}{\hbar}\frac{1}{Z_0}\mathrm{Tr}\left\{\mathrm{e}^{\beta\mu\hat{N}}\hat{U}_0(-\mathrm{i}\hbar\beta,0)\hat{U}_0(0,0)\hat{f}_i\hat{U}_0(0,0)\right. \\
&\qquad\left.\times\underbrace{\hat{U}_0(-\mathrm{i}\hbar\tau,0)\hat{U}_0(0,t')}_{\hat{U}_0(0,\mathrm{i}\hbar\tau+t')}\hat{f}_j^\dagger\underbrace{\hat{U}_0(t',0)\hat{U}_0(0,-\mathrm{i}\hbar\tau)}_{\hat{U}_0(\mathrm{i}\hbar\tau+t',0)}\right\} \\
&= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(t_0)\hat{f}_j^\dagger(\mathrm{i}\hbar\tau+t')\right\rangle \\
&= G^{\ulcorner}(0,\mathrm{i}\hbar\tau+t')\ .
\end{aligned}$$

[42] In combination with thermodynamic equilibrium, the external potential can thus only be a constant.

[43] Since the Hamiltonian is time-independent, we also use $\hat{U}_0$ for the evolution operator along the real axis.

Together with Eq. (8.146), it is

$$G^{\lceil}_{ij}(-\mathrm{i}\hbar\tau, t') = G^{\lceil}_{ij}(-\mathrm{i}\hbar\tau - t', 0) = G^{\lceil}_{ij}(0, \mathrm{i}\hbar\tau + t') \ . \tag{8.147}$$

and it becomes obvious that the superscripts $\rceil$ and $\lceil$ do not make any sense in the equilibrium case. The only important thing that has to be specified is the order of the creation and annihilation operators. Hence, we define the following Green functions for the equilibrium case:

$$\begin{aligned} \bar{G}^{>}_{ij}(x, x') &:= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}_i(x)\hat{f}^{\dagger}_j(x')\right\rangle \ , \\ \bar{G}^{<}_{ij}(x, x') &:= \mp\frac{\mathrm{i}}{\hbar}\left\langle \hat{f}^{\dagger}_j(x')\hat{f}_i(x)\right\rangle , \quad \forall \quad x, x' \in \mathcal{M} := [-\mathrm{i}\hbar\beta, 0] \cup [0, \infty] \ , \end{aligned} \tag{8.148}$$

and we will refer to them as *Equilibrium Correlation Functions* (ECFs)[44] [45]. The ECFs depend only on the difference variable $\bar{x} := x - x'$, and they fulfill the following relations:

$$\begin{aligned} \bar{G}^{\gtrless}_{ij}(x, x') &= \bar{G}^{\gtrless}_{ij}(x - x', 0) = \bar{G}^{\gtrless}_{ij}(\bar{x}, 0) \\ &= \bar{G}^{\gtrless}_{ij}(0, -\bar{x}) := \bar{G}^{\gtrless}_{ij}(\bar{x}) \ . \end{aligned} \tag{8.149}$$

Making use of the general property of the equilibrium evolution operator:

$$\begin{aligned} \hat{U}_0(x, 0)\hat{U}_0(0, x') = \hat{U}_0(x, x') &= \hat{U}_0(x - x', 0) \ , \\ &= \hat{U}_0(0, -(x - x')), \quad \forall \quad x, x' \in \mathcal{M} \ , \end{aligned}$$

the proof of Eq. (8.149) is similar to that of relation (8.147). Trivially, the ECFs also fulfill the KMS-conditions

$$\begin{aligned} \bar{G}^{<}_{ij}(0, x') &= \pm \mathrm{e}^{\beta\mu}\bar{G}^{>}_{ij}(-\mathrm{i}\hbar\beta, x'), \\ \bar{G}^{>}_{ij}(x, 0) &= \pm \mathrm{e}^{-\beta\mu}\bar{G}^{<}_{ij}(x, -\mathrm{i}\hbar\beta), \end{aligned} \tag{8.150}$$

and we can rewrite these in terms of the ECFs depending only on the relative variable [cf. definition (8.149)]. It is

$$\begin{aligned} \bar{G}^{<}_{ij}(\bar{x}) &= \bar{G}^{<}_{ij}(0, -\bar{x}) = \pm \mathrm{e}^{\beta\mu}\bar{G}^{>}_{ij}(-\mathrm{i}\hbar\beta, -\bar{x}) \\ &= \pm \mathrm{e}^{\beta\mu}\bar{G}^{>}_{ij}(-\mathrm{i}\hbar\beta + \bar{x}, 0) = \pm \mathrm{e}^{\beta\mu}\bar{G}^{>}_{ij}(\bar{x} - \mathrm{i}\hbar\beta) \ . \end{aligned} \tag{8.151}$$

[44] Naturally, the values of the ECF completely define all matrix elements of the 1pNEGF including the MGF.

[45] Note that the whole GF-formalism in the beginning of the book of Kadanoff and Baym deals with the equilibrium case only. Therefore, the anti-chronological time ordering operator does not exist in that approach and, as a consequence, there is no need to introduce a contour. As a matter of fact it becomes quite hard to properly translate the equations of that book into those valid for the contour formalism. One way is to introduce the ECFs as presented here, because we cannot deal with the symbols $\lceil$ and $\rceil$, when it comes to the Fourier transform of the ECFs.

Multiplying Eq. (8.151) by $\pm e^{-\beta\mu}$, one finds

$$\begin{aligned}\bar{G}^{<}_{ij}(\bar{x}) &= \pm e^{\beta\mu}\bar{G}^{>}_{ij}(\bar{x}-i\hbar\beta)\ ,\\ \bar{G}^{>}_{ij}(\bar{x}) &= \pm e^{-\beta\mu}\bar{G}^{<}_{ij}(\bar{x}+i\hbar\beta)\ .\end{aligned} \tag{8.152}$$

Even though these relations include the periodicity of the MGF [cf. Eq. (8.141)], one should not think of the ECFs as being periodic with respect to the relative variable $\bar{x}$, which becomes clear, if we keep in mind the values that $\bar{x}$ can assume:

$$\bar{x} \in [-\infty - i\hbar\beta, \infty + i\hbar\beta]\ .$$

8.3.2 Equilibrium Correlation functions in frequency space. KBA

Now we define the Fourier transform of the real-time ECFs (i.e. $\underline{\bar{x} = t \in \mathbb{R}}$) with respect to the relative time as follows:

$$\begin{aligned}\bar{G}^{>}_{ij}(\omega) :&= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\bar{G}^{>}_{ij}(t) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\left\langle \hat{f}_i(t)\hat{f}^{\dagger}_j(0)\right\rangle = -\frac{i}{\hbar}\left\langle \hat{f}_i(\omega)\hat{f}^{\dagger}_j(0)\right\rangle\\ \bar{G}^{<}_{ij}(\omega) :&= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\bar{G}^{<}_{ij}(t) = \mp\frac{i}{\hbar}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\left\langle \hat{f}^{\dagger}_j(0)\hat{f}_i(t)\right\rangle = \mp\frac{i}{\hbar}\left\langle \hat{f}^{\dagger}_j(0)\hat{f}_i(\omega)\right\rangle\end{aligned} \tag{8.153}$$

With that, we can formulate the KMS-condition (8.152) in Fourier space[46]:

$$\begin{aligned}\bar{G}^{<}_{ij}(\omega) &= \int_{-\infty}^{\infty} dt\, e^{i\omega t}\bar{G}^{<}_{ij}(t)\\ &= \pm e^{\beta\mu}\int_{-\infty}^{\infty} dt\, e^{i\omega t}\bar{G}^{>}_{ij}(t-i\hbar\beta)\\ &= \pm e^{\beta(\mu-\hbar\omega)}\int_{-\infty-i\hbar\beta}^{\infty-i\hbar\beta} d\tilde{t}\, e^{i\omega\tilde{t}}\bar{G}^{>}_{ij}(\tilde{t})\\ &\approx \pm\, e^{\beta(\mu-\hbar\omega)}\int_{-\infty}^{\infty} d\tilde{t}\, e^{i\omega\tilde{t}}\bar{G}^{>}_{ij}(\tilde{t}) = \pm e^{\beta(\mu-\hbar\omega)}\bar{G}^{>}_{ij}(\omega)\ ,\end{aligned} \tag{8.154}$$

[46] Of course, if $\bar{x}$ is real, the ECFs coincide with the real time correlation functions of the contour formalism, but in that formalism $G^{>}_{ij}(t - i\hbar\beta)$ is not defined (the real time correlation functions, by definition, only allow for real time arguments). Moreover, in the contour formalism the KMS for the real time correlation function takes the form of Eq. (8.137). Therefore, in the derivation of the Kadanoff-Baym-Ansatz, one would have to define the Fourier transform of the coupling elements.

where in the third line we have made the substitution

$$\tilde{t} = t - \mathrm{i}\hbar\beta, \quad d\tilde{t} = dt, \quad \tilde{t}(\pm\infty) = \pm\infty - \mathrm{i}\hbar\beta \; . \tag{8.155}$$

The KMS-conditions in Fourier space thus read

$$\begin{aligned} \bar{G}^{<}_{ij}(\omega) &= \pm \mathrm{e}^{\beta(\mu-\hbar\omega)} \bar{G}^{>}_{ij}(\omega) \; , \\ \bar{G}^{>}_{ij}(\omega) &= \pm \mathrm{e}^{-\beta(\mu-\hbar\omega)} \bar{G}^{<}_{ij}(\omega) \; . \end{aligned} \tag{8.156}$$

In correspondence to the contour spectral function, we define the Fourier transform of the real-time, equilibrium spectral function:

$$\bar{a}_{ij}(\omega) := \mathrm{i}\hbar \left\{ \bar{G}^{>}_{ij}(\omega) - \bar{G}^{<}_{ij}(\omega) \right\} . \tag{8.157}$$

Using the boundary condition (8.156), we can now express the ECFs in frequency space by this spectral function. For the lesser ECF, we have

$$\begin{aligned} \bar{a}_{ij}(\omega) &= \mathrm{i}\hbar \left[\pm \mathrm{e}^{-\beta(\mu-\hbar\omega)} - 1 \right] \bar{G}^{<}_{ij}(\omega) \\ &= \pm \mathrm{i}\hbar \underbrace{\left[\frac{1}{\mathrm{e}^{\beta(\hbar\omega-\mu)} \mp 1} \right]^{-1}}_{[f^{\mathrm{EQ}}(\hbar\omega;\beta,\mu)]^{-1}} \bar{G}^{<}_{ij}(\omega) \\ \Leftrightarrow \quad \mathrm{i}\hbar \bar{G}^{<}_{ij}(\omega) &= \pm \bar{a}_{ij}(\omega) f^{\mathrm{EQ}}(\hbar\omega;\beta,\mu) \; . \end{aligned} \tag{8.158}$$

Recasting the greater ECF with the other boundary condition eventually yields

$$\begin{aligned} \mathrm{i}\hbar \bar{G}^{<}_{ij}(\omega) &= \pm \bar{a}_{ij}(\omega) f^{\mathrm{EQ}}(\hbar\omega;\beta,\mu) \; , \\ \mathrm{i}\hbar \bar{G}^{>}_{ij}(\omega) &= \bar{a}_{ij}(\omega) \left[1 \pm f^{\mathrm{EQ}}(\hbar\omega;\beta,\mu) \right] \; , \end{aligned} \tag{8.159}$$

where we have recovered the Bose/Fermi distribution f^{EQ}, i.e. the average occupation number in the GKE of a mode (one-particle state) with energy $\hbar\omega$. The lesser ECF is, obviously, proportional to the mean occupation of the mode with $\hbar\omega$, whereas the greater function is proportional to the mean hole occupation of that mode, thereby including the Pauli principle and the Bose enhancement, respectively. Until now, we only made the assumption of the system to be in thermodynamic equilibrium. Hence, the information about the correlations and an eventually applied, external potential depending on space must be contained in the spectral function. In equilibrium, we indeed only need to find the spectral function.

8.3.3 Spatially homogeneous system

Now, we additionally assume a homogeneous system (apart from a constant, there is no external potential at all.). In that case, it will be useful to switch from the discrete to the coordinate representation (neglecting the spin) [cf. Eq. (8.74)], i.e.,

$$\hat{H} = -\int d^3r \hat{\Psi}^\dagger(\mathbf{r}) \frac{\hbar^2\nabla^2}{2m} \hat{\Psi}(\mathbf{r}) + \frac{1}{2}\int d^3r \int d^3r' \hat{\Psi}^\dagger(\mathbf{r})\hat{\Psi}^\dagger(\mathbf{r}')w(r,r')\hat{\Psi}(\mathbf{r}')\hat{\Psi}(\mathbf{r}) \ ,$$

$$\begin{aligned} \bar{G}^{>}_{ij}(\omega) \to \bar{G}^{>}(\mathbf{r},\mathbf{r}',\omega) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{\Psi}(\mathbf{r},\omega)\hat{\Psi}^\dagger(\mathbf{r}',0)\right\rangle \ , \\ \bar{G}^{<}_{ij}(\omega) \to \bar{G}^{<}(\mathbf{r},\mathbf{r}',\omega) &= \pm\frac{\mathrm{i}}{\hbar}\left\langle \hat{\Psi}^\dagger(\mathbf{r}',0)\hat{\Psi}(\mathbf{r},\omega)\right\rangle \ , \end{aligned} \tag{8.160}$$

where

$$\hat{\Psi}(\mathbf{r},\omega) = \int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}\omega t}\hat{\Psi}(\mathbf{r},t) \ .$$

Further, we introduce relative and center of mass coordinates:

$$\mathbf{R} := \frac{\mathbf{r}+\mathbf{r}'}{2} \qquad \bar{\mathbf{r}} := \mathbf{r}-\mathbf{r}' \ .$$

As a consequence of the spatial homogeneity, the Hamiltonian is translational invariant and thus, the ECFs depend only on the relative coordinates, it is

$$\bar{G}^{\gtrless}(\mathbf{r},\mathbf{r}',\omega) = \bar{G}^{\gtrless}\left(\mathbf{R}+\frac{1}{2}\bar{\mathbf{r}},\mathbf{R}-\frac{1}{2}\bar{\mathbf{r}},\omega\right) = \bar{G}^{\gtrless}(\mathbf{R},\bar{\mathbf{r}},\omega) \underset{\text{homogen.}}{=} \bar{G}^{\gtrless}(\bar{\mathbf{r}},\omega) \ , \tag{8.161}$$

with[47]

$$\begin{aligned} \bar{G}^{>}(\bar{\mathbf{r}},\omega) &= -\frac{\mathrm{i}}{\hbar}\left\langle \hat{\Psi}(\bar{\mathbf{r}},\omega)\hat{\Psi}^\dagger(\bar{\mathbf{r}},0)\right\rangle \ , \\ \bar{G}^{<}(\bar{\mathbf{r}},\omega) &= \mp\frac{\mathrm{i}}{\hbar}\left\langle \hat{\Psi}^\dagger(\bar{\mathbf{r}},0)\hat{\Psi}(\bar{\mathbf{r}},\omega)\right\rangle \ . \end{aligned} \tag{8.162}$$

[47] First, one has to actually show that Eq. (8.161) holds. Note that the spatial and time homogeneity, obviously, cannot be treated in the same manner as their mathematical effect on the GF is different. If these two assumptions would be equal, then, for example, it should be $\bar{G}^{>}(\bar{\mathbf{r}},\omega) = -\frac{\mathrm{i}}{\hbar}\left\langle \hat{\Psi}(\bar{\mathbf{r}},\omega)\hat{\Psi}^\dagger(0,0)\right\rangle$. Verify whether this is correct and the derivation of the spectral function for free particles holds.

As in most cases, when dealing with a spatially homogeneous system, it is advantageous to perform a Fourier transform to momentum space with respect to the relative coordinates (**r** now denotes a relative coordinate.):

$$\begin{aligned}\bar{G}^{>}(\mathbf{p},\omega) &= \int d^3r\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathbf{pr}}\, \bar{G}^{>}(\mathbf{r},\omega) = -\frac{\mathrm{i}}{\hbar}\left\langle \hat{\Psi}(\mathbf{p},\omega)\hat{\Psi}^\dagger(\mathbf{p},0)\right\rangle \\ \bar{G}^{<}(\mathbf{p},\omega) &= \int d^3r\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathbf{pr}}\, \bar{G}^{<}(\mathbf{r},\omega) = \mp\frac{\mathrm{i}}{\hbar}\left\langle \hat{\Psi}^\dagger(\mathbf{p},0)\hat{\Psi}(\mathbf{p},\omega)\right\rangle \ . \end{aligned} \tag{8.163}$$

In momentum and frequency space, the relations (8.159) read

$$\begin{aligned}\mathrm{i}\hbar\bar{G}^{<}(\mathbf{p},\omega) &= \pm\bar{a}(\mathbf{p},\omega) f^{\mathrm{EQ}}(\omega;\beta,\mu), \\ \mathrm{i}\hbar\bar{G}^{>}(\mathbf{p},\omega) &= \bar{a}(\mathbf{p},\omega)\left[1 \pm f^{\mathrm{EQ}}(\omega;\beta,\mu)\right], \end{aligned} \tag{8.164}$$

and this is the so-called *Kadanoff-Baym-Ansatz*. It is only an approximation, if used for non-equilibrium and inhomogeneous systems, otherwise it is exact.

8.3.4 Properties of the spectral function: Sum rule. Correlations.

Next, we will investigate the spectral function a little further since, in equilibrium, the system is fully described by it. From the previous definitions [cf. Eq. (8.157)], the spectral function in momentum and frequency space is given by

$$\begin{aligned}\bar{a}(\mathbf{p},\omega) &= \mathrm{i}\hbar\left\{\bar{G}^{>}(\mathbf{p},\omega) - \bar{G}^{<}(\mathbf{p},\omega)\right\} \\ &= \int d^3r \int_{-\infty}^{\infty} dt\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathbf{pr}+\mathrm{i}\omega t}\left(\left\langle \hat{\Psi}(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r},0)\right\rangle \mp \left\langle \hat{\Psi}^\dagger(\mathbf{r},0)\hat{\Psi}(\mathbf{r},t)\right\rangle\right)\end{aligned}$$

and since $\int_{-\infty}^{\infty} d\omega\, \mathrm{e}^{\mathrm{i}\omega t} = 2\pi\delta(t)$, the spectral function fulfils the *sum rule*:

$$\begin{aligned}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\bar{a}(\mathbf{p},\omega) &= \int d^3r \int_{-\infty}^{\infty} dt\, \delta(t)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathbf{pr}}\left(\left\langle \hat{\Psi}(\mathbf{r},t)\hat{\Psi}^\dagger(\mathbf{r},0)\right\rangle \mp \left\langle \hat{\Psi}^\dagger(\mathbf{r},0)\hat{\Psi}(\mathbf{r},t)\right\rangle\right) \\ &= \int d^3r\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\mathbf{pr}} \underbrace{\left(\left\langle \hat{\Psi}(\mathbf{r},0)\hat{\Psi}^\dagger(\mathbf{r},0)\right\rangle \mp \left\langle \hat{\Psi}^\dagger(\mathbf{r},0)\hat{\Psi}(\mathbf{r},0)\right\rangle\right)}_{=\left[\hat{\Psi}(\mathbf{r}),\hat{\Psi}^\dagger(\mathbf{r})\right]_{\mp}=\delta(\mathbf{r})} \\ &= \mathrm{e}^0 = 1\ .\end{aligned}$$

Ideal System: The spectral function of a system of free particles with the Hamiltonian

$$\hat{H} = \int d^3r\, \hat{\Psi}^\dagger(\mathbf{r})\left(-\frac{\hbar^2\nabla^2}{2m}\right)\hat{\Psi}(\mathbf{r}), \tag{8.165}$$

can be computed explicitly. For that purpose, we rewrite the Fourier transform of the lesser ECF as follows

$$\mathrm{i}\hbar\bar{G}^{<}(\mathbf{p},\omega) = \pm\int_{-\infty}^{\infty} dt\, \mathrm{e}^{\mathrm{i}\omega t}\left\langle \hat{\Psi}^{\dagger}(\mathbf{p},0)\hat{\Psi}(\mathbf{p},t)\right\rangle \ . \tag{8.166}$$

When acting on an N-particle state, $\hat{\Psi}(\mathbf{p})$ removes a particle with momentum

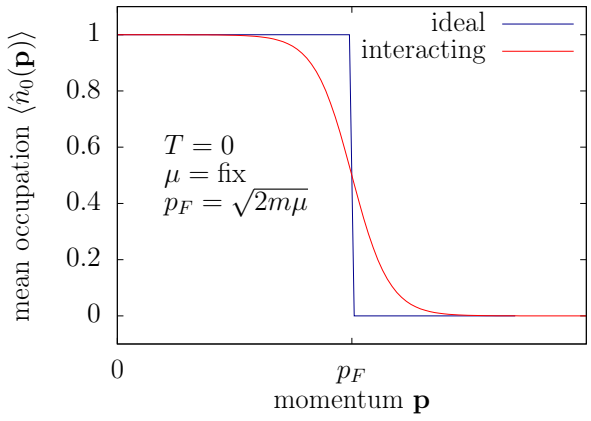

Abbildung 8.4: Equilibrium momentum distribution at zero temperature for an ideal (blue curve) and an interacting (red), homogeneous system of fermions, see also the PIMC result in Fig. 3.2.

$\mathbf{p}$ and thus with energy (free particles) $E_0 = \frac{\mathbf{p}^2}{2m}$. Therefore, the following operator identity holds[48]

$$\begin{aligned}\hat{\Psi}(\mathbf{p},t) &= \hat{U}_0(0,t)\hat{\Psi}(\mathbf{p},0)\hat{U}_0(t,0)\\ &= \mathrm{e}^{+\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{\Psi}(\mathbf{p},0)\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\\ &= \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}E_0 t}\hat{\Psi}(\mathbf{p},0)\ .\end{aligned} \tag{8.167}$$

[48]The proof is similar to that of the identity (8.117). Instead of the eigenstates of the number operator $\hat{N}$, one simply uses the eigenstates $|E\rangle$ of the Hamiltonian with $\hat{H}|E\rangle = E|E\rangle$. Then, it is $\mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{\Psi}(\mathbf{p},0)|E\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}|E-E_0\rangle = \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(E-E_0)t}|E-E_0\rangle$.

Inserting this into Eq. (8.166) and comparing the result with Eq. (8.164) yields an explicit expression for the spectral function of free particles:

$$\begin{aligned} \mathrm{i}\hbar\bar{G}^{<}(\mathbf{p},\omega) &= \pm\int_{-\infty}^{\infty} dt\, \mathrm{e}^{-\frac{\mathrm{i}}{\hbar}(E_0-\hbar\omega)t} \left\langle \hat{\Psi}^{\dagger}(\mathbf{p},0)\hat{\Psi}(\mathbf{p},0)\right\rangle \\ &= \pm 2\pi\hbar\,\delta(\hbar\omega - E_0)\,\langle\hat{n}(\mathbf{p})\rangle \\ &\stackrel{!}{=} \pm\bar{a}(\mathbf{p},\omega) f^{\mathrm{EQ}}(\hbar\omega;\beta,\mu) \\ \Leftrightarrow \quad \bar{a}_0(\mathbf{p},\omega) &= 2\pi\hbar\,\delta(\hbar\omega - E_0)\ . \end{aligned} \tag{8.168}$$

Thereby, since it is $\hbar\omega = \frac{p^2}{2m} = E_0$ (delta function), we immediately identify the momentum distribution function of free (non-interacting) particles:

$$\langle\hat{n}\rangle_0^{\mathrm{EQ}}(\mathbf{p};\beta,\mu) = f^{\mathrm{EQ}}\left(\frac{\mathbf{p}^2}{2m};\beta,\mu\right) = \frac{1}{\mathrm{e}^{\beta\left(\frac{\mathbf{p}^2}{2m}-\mu\right)}\mp 1}\ , \tag{8.169}$$

which is well known from statistical mechanics. Note that in equilibrium the energy distribution is always a Fermi/Bose distribution[49], whereas the momentum distribution is only Fermi/Bose, if the particles are free (non-interacting). Otherwise the correlations will deform the distribution in the vicinity of the Fermi level even at zero temperature (see Fig. 8.4).

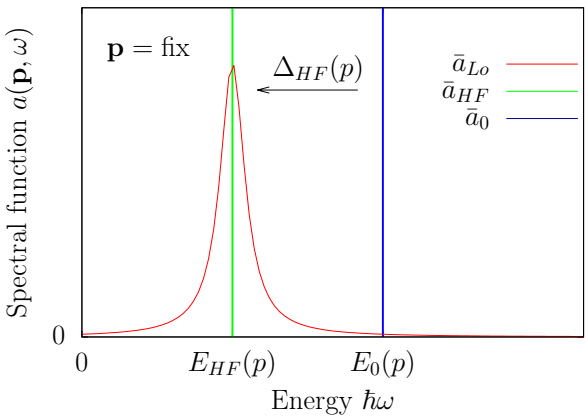

Abbildung 8.5: Equilibrium spectral function for an ideal, homogeneous system (blue delta peak) and an interacting homogeneous system treated either on the Hartree-Fock level (green delta peak) or within the quasi-particle picture using a Lorentzian line shape (red curve).

[49] Because Eq. (8.164) is true for an interacting system.

Further, for an interacting system treated on Hartree-Fock level, the shape of the spectral function still remains a sharp delta peak:

$$\begin{aligned} \bar{a}_{\mathrm{HF}}(\mathbf{p},\omega) &= 2\pi\hbar\delta(\hbar\omega - E_{\mathrm{HF}}(\mathbf{p})) \\ E_{\mathrm{HF}}(\mathbf{p}) &= E_0 - \Delta_{\mathrm{HF}}(\mathbf{p}), \end{aligned} \tag{8.170}$$

where $\Delta_{\mathrm{HF}}(\mathbf{p})$ is the (*real*) Hartree-Fock shift of the one-particle energy.

todo:

1. formula and figure for $\Delta_{\mathrm{HF}}(p)$ for UEG
2. plot energy dispersion in HF
3. extend to Fermi liquid theory, basic ideas

For an interacting system treated beyond Hartree-Fock level, one expects the spectral function to be broadened, which can be approximated by a Lorentzian line shape ("quasi-particle picture"):

$$\bar{a}_{\mathrm{Lo}}(\mathbf{p},\omega) = \frac{2\hbar^2\Gamma(\mathbf{p})}{[\hbar\omega - E_{\mathrm{HF}}(\mathbf{p}) - \Delta_{\mathrm{cor}}(\mathbf{p})]^2 + \Gamma^2(\mathbf{p})} \xrightarrow{\hbar\Gamma(\mathbf{p})\to 0} 2\pi\hbar\delta[\hbar\omega - \Delta E(\mathbf{p})] \,, \tag{8.171}$$

where $\Gamma(\mathbf{p})$ is proportional to the collision rate of particles, that defines the width of the spectral function that determines the quasiparticle lifetime[50], see Fig. (8.5). For a detailed discussion of the equilibrium spectral functions, the reader is referred to [27]. Note that the quasi-particle approximation neglects the frequency dependence of the correlation contributions to the energy shift and width. These effects emerge naturally from the NEGF analysis below.

[50] This can be visualized by plotting the spectral function vs. difference time.

8.4 Keldysh-Kadanoff-Baym Equations (KBE)

In the last section, we have investigated the 1pNEGF for an equilibrium system. Now, we will return to the general case of a non-equilibrium system that is exposed to a time-dependent external perturbation and find the equations of motion for the 1pNEGF. For that purpose, we first will obtain the time-dependent equations of motion for the entire Keldysh (matrix) Green function on the Keldysh contour from which we then will derive the equations of motion for the relevant real-time components, using the Langreth-Wilkins rules.

8.4.1 Derivation of the first equation of the Martin-Schwinger hierarchy

Recall the definition of the 1pNEGF (we skip the superscript "1") which we rewrite as the expectation value of a NEGF operator without ensemble average,

$$
\begin{aligned}
G_{ij}(z,z') &:= \langle \hat{G}_{ij}(z,z') \rangle \,, && (8.172)\\
\hat{G}_{ij}(z,z') &:= -\frac{\mathrm{i}}{\hbar} \hat{T}_{\mathcal{C}}\, \hat{f}_i(z)\, \hat{f}_j^\dagger(z') && (8.173)\\
&= \theta_{\mathcal{C}}(z-z')\, \hat{G}^{>}_{ij}(z,z') + \theta_{\mathcal{C}}(z'-z)\, \hat{G}^{<}_{ij}(z,z') \,,\\
\hat{G}^{>}_{ij}(z,z') &:= -\frac{\mathrm{i}}{\hbar} \hat{f}_i(z)\, \hat{f}_j^\dagger(z') \,,\\
\hat{G}^{<}_{ij}(z,z') &:= \mp\frac{\mathrm{i}}{\hbar} \hat{f}_j^\dagger(z')\, \hat{f}_i(z) \,.
\end{aligned}
$$

Further, to shorten the notation, we choose a different writing of the step and delta functions on the contour:

$$
\theta_{\mathcal{C}}(z-z') := \theta_{\mathcal{C}}(z,z'), \qquad \delta(z-z') := \delta(z,z') \,. \tag{8.174}
$$

Since the contour variable $z \in \mathcal{C}$ is continuous, we can compute the derivative of the 1pNEGF operator with respect to z and z' to find its equation of motion[51]. We start with z:

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\partial}{\partial z}\, \hat{G}_{ij}(z,z') &= \mathrm{i}\hbar\delta_{\mathcal{C}}(z,z')\Big\{ \underbrace{\hat{G}^{>}_{ij}(z,z') - \hat{G}^{<}_{ij}(z,z')}_{\underset{z=z'}{=} -\frac{\mathrm{i}}{\hbar}\delta_{ij}} \Big\} && (8.175)\\
&\quad + \theta_{\mathcal{C}}(z,z')\, \mathrm{i}\hbar\frac{\partial}{\partial z}\, \hat{G}^{>}_{ij}(z,z') + \theta_{\mathcal{C}}(z',z)\, \mathrm{i}\hbar\frac{\partial}{\partial z}\, \hat{G}^{<}_{ij}(z,z')\\
&= \delta_{\mathcal{C}}(z,z')\delta_{ij} + \theta_{\mathcal{C}}(z,z')\frac{\partial \hat{f}_i(z)}{\partial z}\hat{f}_j^\dagger(z') \pm \theta_{\mathcal{C}}(z',z)\hat{f}_j^\dagger(z')\frac{\partial \hat{f}_i(z)}{\partial z} \,.
\end{aligned}
$$

[51] Since the ensemble average is with the unperturbed density operator $\hat{\rho}_0$, the time derivatives of the 1pNEGF and the 1pNEGF operator coincide.

Due to the contour delta function, we could use the discontinuity property of the 1pNEGF operator [cf. Eq. (8.136) a)] in the first line. Now we make use of the equation of motion of the field operators in an arbitrary basis[52] which we obtained in Ch. 5 [cf. Eq. (5.34)]:

$$\begin{aligned}\frac{\partial \hat{f}_i(z)}{\partial z} &= -\frac{\mathrm{i}}{\hbar}\left[\hat{f}_i(z),\hat{H}(z)\right]_- \\ &= -\frac{\mathrm{i}}{\hbar}\left\{\sum_k \underbrace{t_{ik}+v_{ik}(z)}_{h_{ik}(z)}\hat{f}_k(z)+\sum_{j'kl} w_{ij'kl}(z)\hat{f}^\dagger_{j'}(z)\hat{f}_l(z)\hat{f}_k(z)\right\}, \quad (8.176)\end{aligned}$$

where the pair interaction is allowed to be time-dependent, e.g. to simulate an interaction quench or to describe the adiabatic switch-on of correlations. Inserting this into Eq. (8.175) yields:

$$\begin{aligned}&\mathrm{i}\hbar\frac{\partial}{\partial z}\hat{G}_{ij}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} \quad (8.177)\\ &+\sum_k h_{ik}(z)\underbrace{\left\{\theta_{\mathcal{C}}(z,z')\left(-\frac{\mathrm{i}}{\hbar}\right)\hat{f}_k(z)\hat{f}^\dagger_j(z')+\theta_{\mathcal{C}}(z',z)\left(\pm\frac{\mathrm{i}}{\hbar}\right)\hat{f}^\dagger_j(z')\hat{f}_k(z)\right\}}_{\hat{G}_{kj}(z,z')}\\ &\underbrace{-\frac{\mathrm{i}}{\hbar}\sum_{j'kl} w_{ij'kl}(z)\Big\{\theta_{\mathcal{C}}(z,z')\underbrace{\hat{f}^\dagger_{j'}(z)\hat{f}_l(z)}_{\hat{n}_{j'l}(z)}\hat{f}_k(z)\hat{f}^\dagger_j(z')\pm\theta_{\mathcal{C}}(z',z)\hat{f}^\dagger_j(z')\underbrace{\hat{f}^\dagger_{j'}(z)\hat{f}_l(z)}_{\hat{n}_{j'l}(z)\hat{f}_k(z)}\Big\}}_{=:\hat{I}_{ij}(z,z')}.\end{aligned}$$

While, in the second term on the r.h.s., we could re-substitute the 1pNEGF operator, $\hat{G}_{kj}(z,z')$, the last term is more complicated involving averages over four operators. This term is also called operator collision term, $\hat{I}_{ij}(z,z')$, and we identified the 1pRDM operators $\hat{n}_{j'l}(z)$ within the four operator products. In order to identify the contour-ordered two-particle nonequilibrium Green function (2pNEGF) operator [cf. Eq. (8.80)]

$$\hat{G}^{(2)}_{ij,kl}(t_1,t_2;t_1',t_2') = -\frac{1}{\hbar^2}\hat{T}_{\mathcal{C}}\,\hat{f}_i(t_1)\,\hat{f}_j(t_2)\,\hat{f}^\dagger_l(t_2')\,\hat{f}^\dagger_k(t_1'), \quad (8.178)$$

in the collision term, we introduce the generalized (two-time but instantaneous) two-body interaction,

$$\hat{w}(z,\bar{z}) := \delta_{\mathcal{C}}(z,\bar{z})\,\hat{w}(z) \quad \Rightarrow \quad w_{ij'kl}(z.\bar{z}) = \delta_{\mathcal{C}}(z,\bar{z})w_{ij'kl}(z). \quad (8.179)$$

[52] Since it is $\left[\hat{f}_i(t_0--\frac{\mathrm{i}}{\hbar}\tau),\hat{H}(t_0--\frac{\mathrm{i}}{\hbar}\tau)\right]_- = \hat{U}_0(t_0,t_0--\frac{\mathrm{i}}{\hbar}\tau)\left[\hat{f}_i,\hat{H}\right]_-\hat{U}_0(t_0--\frac{\mathrm{i}}{\hbar}\tau,t_0)$ and $\hat{U}_0$ fulfils the group property, one readily checks that the equation of motion not only holds for real times t, but also for imaginary times $t_0-\mathrm{i}\hbar\tau$, $\tau\in[0,\beta]$ and thus also for contour Heisenberg operators.

With that, we rewrite the collision term as

$$\hat{I}_{ij}(z,z') = -\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z,\bar{z})\Big\{\theta_{\mathcal{C}}(z,z')\hat{n}_{j'l}(\bar{z})\hat{f}_k(z)\hat{f}_j^\dagger(z') \pm \theta_{\mathcal{C}}(z',z)\hat{f}_j^\dagger(z')\hat{n}_{j'l}(\bar{z})\hat{f}_k(z)\Big\}\,,$$

and we notice that $\hat{n}_{j'l}(\bar{z})$ is always left of $\hat{f}_k(z)$. Therefore, we write

$$\begin{aligned}
\hat{I}_{ij}(z,z') &= -\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\lim_{\epsilon\to 0}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z+\epsilon,\bar{z})\Big\{\theta_{\mathcal{C}}(z,z')\hat{n}_{j'l}(z+\epsilon)\hat{f}_k(z)\hat{f}_j^\dagger(z') \pm \theta_{\mathcal{C}}(z',z)\hat{f}_j^\dagger(z')\hat{n}_{j'l}(z+\epsilon)\hat{f}_k(z)\Big\} \\
&= -\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\Big\{\theta_{\mathcal{C}}(z,z')\hat{n}_{j'l}(z^+)\hat{f}_k(z)\hat{f}_j^\dagger(z') \pm \theta_{\mathcal{C}}(z',z)\hat{f}_j^\dagger(z')\hat{n}_{j'l}(z^+)\hat{f}_k(z)\Big\} \qquad (8.180)\\
&= -\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\hat{T}_{\mathcal{C}}\Big\{\hat{n}_{j'l}(z^+)\hat{f}_k(z)\hat{f}_j^\dagger(z')\Big\} \qquad (8.181)\\
&= -\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\hat{T}_{\mathcal{C}}\Big\{\hat{n}_{j'l}(\bar{z})\hat{f}_k(z)\hat{f}_j^\dagger(z')\Big\} \qquad (8.182)\\
&= -\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\hat{T}_{\mathcal{C}}\Big\{\hat{f}_k(z)\hat{n}_{j'l}(\bar{z})\hat{f}_j^\dagger(z')\Big\}\,. \qquad (8.183)
\end{aligned}$$

From line (8.180) to (8.181), we used that, by definition, z^+ is greater than z on $\mathcal{C}$ and thus, there are only two cases left for the time ordering of the three arguments: First, $z^+ > z > z'$ and second, $z' > z^+ > z$. The sign change for fermions, in the second term, is due to the interchange of $\hat{f}_k(z)$ and $\hat{f}_j(z')$ [cf. Eq. (8.68)]. In line (8.182) we could change the argument of the 1pRD operator, for it is $z^+ = \bar{z}$ under the integral (delta function in $w_{ij'kl}$) and finally, we took advantage of the fact that the 1pRD operator commutes with the field operators under the time-ordering operator, cf. Eq. (8.69). After recasting the 1pRD operator as

$$\hat{n}_{j'l}(\bar{z}) = \hat{f}_{j'}^\dagger(\bar{z})\hat{f}_l(\bar{z}) = \pm\hat{T}_{\mathcal{C}}\Big\{\hat{f}_l(\bar{z})\hat{f}_{j'}^\dagger(\bar{z}^+)\Big\}\,,$$

we can identify the 2pNEGF operator:

$$\begin{aligned}\hat{I}_{ij}(z,z') &= \mp\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\hat{T}_{\mathcal{C}}\left\{\hat{f}_k(z)\hat{T}_{\mathcal{C}}\left\{\hat{f}_l(\bar{z})\hat{f}^\dagger_{j'}(\bar{z}^+)\right\}\hat{f}^\dagger_j(z')\right\}\\ &= \mp\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\underbrace{\hat{T}_{\mathcal{C}}\left\{\hat{f}_k(z)\hat{f}_l(\bar{z})\hat{f}^\dagger_{j'}(\bar{z}^+)\hat{f}^\dagger_j(z')\right\}}_{=-\hbar^2\hat{G}^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^+)}\\ &= \pm\mathrm{i}\hbar\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\hat{G}^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^+)\ . \end{aligned} \tag{8.184}$$

Together with Eq. (8.177), and after performing the ensemble averaging, we arrive at the first equation of motion of the 1pNEGF, the first equation of the Martin-Schwinger hierarchy:

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial}{\partial z}G_{ij}(z,z') &= \delta_{\mathcal{C}}(z,z')\delta_{ij} + \sum_k h_{ik}(z)G_{kj}(z,z')\\ &\quad \pm \mathrm{i}\hbar\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})G^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^+)\ . \end{aligned} \tag{8.185}$$

8.4.2 Adjoint of the first equation of the Martin-Schwinger hierarchy

The second equation of motion is obtained in a similar way. We just have to compute the derivative of the 1pNEGF operator with respect to z':

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial}{\partial z'}\hat{G}_{ij}(z,z') &= -\mathrm{i}\hbar\delta_{\mathcal{C}}(z,z')\Big\{\underbrace{\hat{G}^{>}_{ij}(z,z') - \hat{G}^{<}_{ij}(z,z')}_{\underset{z=z'}{=}-\frac{\mathrm{i}}{\hbar}\delta_{ij}}\Big\}\\ &\quad + \theta_{\mathcal{C}}(z,z')\hat{f}_i(z)\frac{\partial\hat{f}^\dagger_j(z')}{\partial z'} \pm \theta_{\mathcal{C}}(z',z)\frac{\partial\hat{f}^\dagger_j(z')}{\partial z'}\hat{f}_i(z)\ . \end{aligned}$$

After inserting the equation of motion of the creation operator $\hat{f}^\dagger_j(z')$,

$$\frac{\partial\hat{f}^\dagger_j(z')}{\partial z'} = \frac{\mathrm{i}}{\hbar}\Big\{\sum_k h_{kj}(z')\hat{f}^\dagger_k(z') + \sum_{j'kl} w_{kljj'}(z')\hat{f}^\dagger_k(z')\hat{f}^\dagger_l(z')\hat{f}_{j'}(z')\Big\}\ ,$$

which is the adjoint equation of (8.176), with $z \to z'$ ($h^*_{jk} = h_{kj}$, $w^*_{jj'kl} = w_{kljj'}$), we have

$$\begin{aligned}
&\mathrm{i}\hbar\frac{\partial}{\partial z'}\,G_{ij}(z,z') = -\delta_{\mathcal{C}}(z,z')\delta_{ij} \qquad (8.186)\\
&-\sum_k h_{kj}(z')\underbrace{\left\{\theta_{\mathcal{C}}(z,z')\left(-\frac{\mathrm{i}}{\hbar}\right)\hat{f}_i(z)\hat{f}^\dagger_k(z') + \theta_{\mathcal{C}}(z',z)\left(\mp\frac{\mathrm{i}}{\hbar}\right)\hat{f}^\dagger_k(z')\hat{f}_i(z)\right\}}_{=\hat{G}_{ik}(z,z')}\\
&+\frac{\mathrm{i}}{\hbar}\sum_{j'kl} w_{kljj'}(z')\Big\{\theta_{\mathcal{C}}(z,z')\hat{f}_i(z)\hat{f}^\dagger_k(z')\underbrace{\hat{f}^\dagger_l(z')\hat{f}_{j'}(z')}_{\hat{n}_{lj'}(z')}\\
&\qquad\qquad \pm\theta_{\mathcal{C}}(z',z)\hat{f}^\dagger_k(z')\underbrace{\hat{f}^\dagger_l(z')\hat{f}_{j'}(z')}_{=\hat{n}_{lj'}(z')}\hat{f}_i(z)\Big\}\,.
\end{aligned}$$

Again, we could identify the 1pNEGF operator in the first line, and we defined the last line as the negative of the second collision operator, $\tilde{I}_{ij}(z,z')$. Using the generalized two-body interaction [Eq. (8.179)], we rewrite this collision term in a similar way as we did with the first one to re-substitute the 2pNEGF operator:

$$\begin{aligned}
-\tilde{I}_{ij}(z,z') = \frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{kljj'}(z',\bar{z})\Big\{&\theta_{\mathcal{C}}(z,z')\hat{f}_i(z)\hat{f}^\dagger_k(z')\hat{n}_{lj'}(\bar{z})\\
&\pm\theta_{\mathcal{C}}(z',z)\hat{f}^\dagger_k(z')\hat{n}_{lj'}(\bar{z})\hat{f}_i(z)\Big\}\,.
\end{aligned}$$

Now, the 1pRD operator $\hat{n}_{lj'}(\bar{z})$ is always to the right of $\hat{f}_k(z')$ and, therefore, we can write

$$\begin{aligned}
-\tilde{I}_{ij}(z,z') &= \frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{kljj'}(z'^{-},\bar{z})\hat{T}_{\mathcal{C}}\left\{\hat{f}_i(z)\hat{f}^\dagger_k(z')\hat{n}_{lj'}(\bar{z})\right\}\\
&= \frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{kljj'}(z'^{-},\bar{z})\hat{T}_{\mathcal{C}}\left\{\hat{f}_i(z)\hat{n}_{lj'}(\bar{z})\hat{f}^\dagger_k(z')\right\}\\
&= \frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{kljj'}(z'^{-},\bar{z})\hat{T}_{\mathcal{C}}\left\{\hat{f}_i(z)(\pm)\hat{T}_{\mathcal{C}}\left\{\hat{f}_{j'}(\bar{z})\hat{f}^\dagger_l(\bar{z}^+)\right\}\hat{f}^\dagger_k(z')\right\}\\
&= \pm\frac{\mathrm{i}}{\hbar}\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{kljj'}(z'^{-},\bar{z})\underbrace{\hat{T}_{\mathcal{C}}\left\{\hat{f}_i(z)\hat{f}_{j'}(\bar{z})\hat{f}^\dagger_l(\bar{z}^+)\hat{f}^\dagger_k(z')\right\}}_{=-\hbar^2\hat{G}^{(2)}_{ij'kl}(z,\bar{z},z',\bar{z}^+)}
\end{aligned}$$

Inserting this result into Eq. (8.186), performing the ensemble average and then multiplying the whole equation by (-1), yields the second equation of

motion:

$$-\mathrm{i}\hbar\frac{\partial}{\partial z'}G_{ij}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} + \sum_k G_{ik}(z,z')h_{kj}(z') \pm \mathrm{i}\hbar\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, G^{(2)}_{ij'kl}(z,\bar{z},z',\bar{z}^+)\, w_{kljj'}(z'^-,\bar{z})\,, \tag{8.187}$$

where the Green functions now appear to the left (this yields proper matrix multiplication).

It is convenient to write both equations of motion [Eqs. (8.185) and (8.187)] in the following way:

$$\sum_k\left\{\mathrm{i}\hbar\frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z)\right\}G_{kj}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} \pm \pm\mathrm{i}\hbar\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z})\, G^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^+)\,, \tag{8.188}$$

$$\sum_k G_{ik}(z,z')\left\{-\mathrm{i}\hbar\frac{\partial}{\partial z'}\delta_{kj} - h_{kj}(z')\right\} = \delta_{\mathcal{C}}(z,z')\delta_{ij} \pm \pm\mathrm{i}\hbar\sum_{j'kl}\int_{\mathcal{C}} d\bar{z}\, G^{(2)}_{ij'kl}(z,\bar{z},z',\bar{z}^+)\, w_{kljj'}(z'^-,\bar{z})\,. \tag{8.189}$$

These equations form the extremely important equations of motion for the two-time contour Nonequilibrium Green functions. Obviously, these equations for G are not closed but couple to the two-particle Green functions. More generally, these equations form the first of a chain of coupled equations for the N-particle NEGF. This chain (or hierarchy) is called *Martin-Schwinger hierarchy* (MSH) [56]. We will not write down the higher order equations but mention that the first equation leads to the *Keldysh-Kadanoff-Baym-Equations* (KBE). In these equations, the two-particle NEGF is eliminated in favor of the selfenergy, as we will discuss in detail in Sec. 8.6.

Before we discuss the properties of the MSH, we notice, that the second equation is the adjoint of the first one, i.e., we adjoin the first equation and then interchange $i \leftrightarrow j$ and $z \leftrightarrow z'$. In doing this, special care must be taken with the infinitesimal larger times z^+ and $\bar{z}^+$. For example, it is

$$\begin{aligned}\left[G^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^+)\right]^* &= -\frac{1}{\hbar^2}\left\langle\hat{T}_{\mathcal{C}}\left\{\left[\hat{f}_k(z)\hat{f}_l(\bar{z})\hat{f}^\dagger_{j'}(\bar{z}^+)\hat{f}^\dagger_j(z')\right]^\dagger\right\}\right\rangle \\ &= \mp\frac{1}{\hbar^2}\left\langle\hat{T}_{\mathcal{C}}\left\{\left[\hat{f}_k(z)\hat{n}_{j'l}(\bar{z})\hat{f}^\dagger_j(z')\right]^\dagger\right\}\right\rangle \\ &= \mp\frac{1}{\hbar^2}\left\langle\hat{T}_{\mathcal{C}}\left\{\hat{f}_j(z')\hat{n}^\dagger_{j'l}(\bar{z})\hat{f}^\dagger_k(z)\right\}\right\rangle,\end{aligned} \tag{8.190}$$

and, since

$$\hat{n}^{\dagger}_{j'l}(\bar{z}) = \hat{f}^{\dagger}_{l}(\bar{z})\hat{f}_{j'}(\bar{z}) = \pm\hat{T}_{\mathcal{C}}\left\{\hat{f}_{j'}(\bar{z})\hat{f}^{\dagger}_{l}(\bar{z}^{+})\right\} ,$$

we further have

$$\begin{aligned}\left[G^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^{+})\right]^{*} &= -\frac{1}{\hbar^{2}}\left\langle\hat{T}_{\mathcal{C}}\left\{\hat{f}_{j}(z')\hat{f}_{j'}(\bar{z})\hat{f}^{\dagger}_{l}(\bar{z}^{+})(\bar{z})\hat{f}^{\dagger}_{k}(z)\right\}\right\rangle \\ &= G^{(2)}_{jj'kl}(z',\bar{z};z,\bar{z}^{+}) ,\end{aligned} \tag{8.191}$$

which, after interchanging $i \leftrightarrow j$ and $z \leftrightarrow z'$, leads to the correct 2pNEGF in the collision term of the second equation[53].

8.4.3 Properties of the Martin-Schwinger hierarchy

Let us now briefly discuss the properties of the Martin-Schwinger hierarchy.

i. The entire hierarchy is, of course, equivalent to the full many-body problem. Therefore, the solution for the 1pNEGF yields the exact dynamics of the system in equilibrium and non-equilibrium (provided the exact 2pNEGF is used on the r.h.s.).

ii. The first equations of the MSH are a set of coupled (non-Markovian[54]) integro-differential equations and are valid for imaginary and real times defined on the round-trip Keldysh contour $\mathcal{C}$. Thereby, the second equation in (8.188) is just the adjoint of the first one with the times interchanged, i.e., $t \leftrightarrow t'$, as we discussed above.

iii. The boundary (respectively, initial) conditions for the first equation of the MSH are given by the Kubo-Martin-Schwinger (KMS) relations formulated as properties a) and b) in Eq. (8.136), cf. [56, Kub57]. If the equilibrium Matsubara Green function of the system is known, sufficient KMS conditions are expressions c) and d) in Eq. (8.136).

[53]Note that we have to *first* perform the limit $\bar{z}^{+} = \lim_{\epsilon\to 0}(\bar{z}+\epsilon)$, under the time-ordering operator, before adjoining the product of field operators in line (8.190). Otherwise we would have ended up with

$$\left[G^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^{+})\right]^{*} = G^{(2)}_{jj'kl}(z',\bar{z}^{+};z,\bar{z}) , \tag{8.192}$$

which is, obviously, not the correct result. Therefore, when complex conjugating the collision term of the first KBE equation, we first must perform the contour time integral and then perform both time limits under $\hat{T}_{\mathcal{C}}$. This will finally gives rise to the z'^{-} in the generalized two-body interaction.

[54]This means they involve a time integral that reflects memory effects.

iv. As discussed above, Eqs. (8.188) are not closed, i.e., they do not uniquely define the 1pNEGF without further knowledge. Instead, these equations require the 2pNEGF which, in turn, satisfies its own equation of motion– the Bethe-Salpeter equation, cf. Refs. [72, 73]. Generally, the equation of motion for $G^{(n)}$ ($n \geq 2$) requires information about $G^{(n-1)}$ and $G^{(n+1)}$, cf. Refs. [73, 74]. The entire chain of equations for all $G^{(n)}$ forms the Martin-Schwinger hierarchy.

v. In the special case of equal time arguments, $t = t'$, the MSH reduces to the BBGKY (Bogolyubov-Born-Green-Kirkwood-Yvon) hierarchy for the reduced density operators, cf., e.g., [Bon98]. The special case of the dynamics of single-time quantities will be studied in Section 8.9 below.

8.5 Decoupling of the Martin-Schwinger hierarchy

Since an exact solution of the hierarchy is, in general, not possible, approximations for the two-particle Green function are necessary. We start by discussing the simplest ones.

8.5.1 One-particle case

In the case of an isolated particle, of course, $G^{(2)} = 0$, and the equations become modified versions of the time-dependent Schrödinger equation,

$$\sum_k \left\{ \mathrm{i}\hbar \frac{\partial}{\partial z} \delta_{ik} - h_{ik}(z) \right\} G_{kj}(z, z') = \delta_{\mathcal{C}}(z, z') \delta_{ij} \,, \tag{8.193}$$

$$\sum_k G_{ik}(z, z') \left\{ -\mathrm{i}\hbar \frac{\partial}{\partial z'} \delta_{kj} + h_{kj}(z') \right\} = \delta_{\mathcal{C}}(z, z') \delta_{ij} \,, \tag{8.194}$$

where the main differences are the formulation on the Keldysh contour and the appearance of the delta functions on the right. The consequences of this modification will be discussed below, in Sec. 8.7.

8.5.2 Mean field (Hartree) approximation

For any many-particle system, the neglect of $G^{(2)}$ is not justified. Even in the case of non-interacting particles or particles that are very far from each other

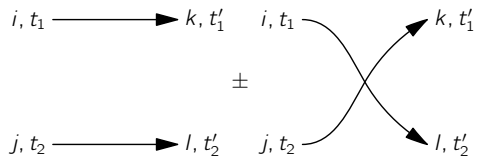

Abbildung 8.6: Hartree-Fock: the simplest conserving approximation for the two-particle Green function $G^{(2)}_{ij,kl}(t_1, t_2; t_1', t_2')$, cf. Eq. (8.199). The sign refers to bosons (+) and fermions (−).

$G^{(2)}$ remains finite and assumes the limiting form of the case of independent particles:

$$G^{(2)}_{ij,kl}(t_1, t_2; t_1', t_2') = G_{ik}(t_1, t_1')G_{jl}(t_2, t_2') \,. \tag{8.195}$$

The corresponding diagram is sketched in the left part of Fig. 8.6. When this expression is inserted into the collision integral I on the right of Eq. (8.185), we obtain again an effective single-particle equation with a one-particle hamiltonian that is modified by an additional potential energy term Σ^{H}:

$$\sum_k \left\{ i\hbar \frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z) - \Sigma^{\mathrm{H}}_{ik}(z) \right\} G_{kj}(z, z') = \delta_{\mathcal{C}}(z, z')\delta_{ij} \,, \tag{8.196}$$

$$\Sigma^{\mathrm{H}}_{ik}(z) = \pm i\hbar \sum_{j'l} \int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(\bar{z}^+, \bar{z}) G_{lj'}(\bar{z}, \bar{z}^+) \,. \tag{8.197}$$

This result is nothing but the standard Hartree mean field (recall that the Green function with identical time arguments is directly related to the density matrix). As we will see below, this function is closely related to the Hartree selfenergy which is defined as a two-time function

$$\Sigma^{\mathrm{H}}_{ik}(z, z') = \Sigma^{\mathrm{H}}_{ik}(z)\delta_{\mathcal{C}}(z, z') \,. \tag{8.198}$$

Note that the contour integral in (8.197) is, in fact, not present because $w(z, z')$ contains a contour delta function.

8.5.3 Hartree-Fock approximation

We now extend the result for the ideal two-particle NEGF, Eq. (8.195) to the quantum case of particles with spin. This gives rise to exchange effects and to permutations of identical particles which we discussed before for the many-particle wave function and for the two-particle density operator. Consequently,

also the ideal two-particle NEGF acquires an additional exchange contribution, the Fock Green function,

$$G^{(2)\mathrm{HF}}_{ij,kl}(t_1,t_2;t_1',t_2') = G_{ik}(t_1,t_1')G_{jl}(t_2,t_2') \pm G_{il}(t_1,t_2')G_{jk}(t_2,t_1')\,, \qquad (8.199)$$

where the sign differs for bosons and fermions. As in the case of the two-particle wave function, this ideal 2-particle NEGF can be written in form of a Slater permanent/determinant. Inserting the ansatz (8.199) into the collision integral we obtain

$$\begin{aligned} I^F_{ij}(z,z') &= \sum_k (+i\hbar) \sum_{j'l} \int_{\mathcal{C}} d\bar{z}\, w_{ij',kl}(z^+,\bar{z}) G_{kj'}(z,z^+) G_{lj}(\bar{z},z') = \\ &:= \sum_k \Sigma^{\mathrm{F}}_{ik}(z,\bar{z}) G_{kj}(z,z')\,, \qquad (8.200) \\ \Sigma^{\mathrm{F}}_{ik}(z,\bar{z}) &= i\hbar \sum_{j'l} w_{j'i,lk}(z,\bar{z}) G_{li}(z,\bar{z})\,, \qquad (8.201) \end{aligned}$$

where we introduced the Fock selfenergy. It is a function of two times, however, due to the delta function in the potential, it is also time local.

Hartree-Fock approximation again translates into an effective single-particle problem with an effective 1-particle hamiltonian, but involves operator for Σ^{HF}. Details will be given below, in Sec. 8.6.

8.5.4 Correlation effects in $G^{(2)}$

The general form of two-particle NEGF can be written as an ideal part (Hartree-Fock) plus an addition, the correlation part of the 2pNEGF:

$$\begin{aligned} G^{(2)}_{ijkl}(t_1,t_2;t_1',t_2') &= G^{(2)\mathrm{HF}}_{ijkl}(t_1,t_2;t_1',t_2') + \mathcal{G}_{ijkl}(t_1,t_2;t_1',t_2')\,, \qquad (8.202) \\ &= G^{(2)\mathrm{H}}_{ijkl}(t_1,t_2;t_1',t_2') + L_{ijkl}(t_1,t_2;t_1',t_2')\,. \qquad (8.203) \end{aligned}$$

Here the first line contains the correlated part of the 2pNEGF which resembles the two-particle correlation operator (correlated part of the two-particle RDO). The second line contains an alternative definition: here only the Hartree part is separated, so the remainder contains Fock and correlation contributions. The function L is, therefore, called exchange-correlation function. It is closely related to the exchange correlation functional of density functional theory.

We already saw for the Hartree and Fock approximations that the collision integral can be rewritten as an integral over an effective potential energy. This structure of the collision integral suggests to look for a similar representation also for the general case. This leads to the introduction of the one-particle selfenergy which we discuss in the next section.

8.6 Selfenergy. Keldysh-Kadanoff-Baym equations

In order to transform the KBEs (8.188), (8.189) into a closed form avoiding the MS hierarchy, we have to express the 2pNEGF in terms of the 1pNEGF. However, in the presence of correlations, this can be done only by summing over an infinite number of contributions. For this reason, we generally have to resort to approximations when dealing with nonequilibrium Green functions. Highly useful expansions are provided by many-body perturbation theory (MBPT). To give details in this regard and to cover topics such as "self-consistency" and "conserving approximations" is the task of Section 8.8.

8.6.1 Definition of the selfenergy

We now formally rewrite the contour integrals in Eqs. (8.188), (8.189) as convolutions and include all interaction effects into a new one-particle quantity–the "self-energy" (1pSE) Σ:

$$\pm \mathrm{i}\hbar \sum_{j'kl} \int_{\mathcal{C}} d\bar{z}\, w_{ij'kl}(z^+,\bar{z}) G^{(2)}_{kljj'}(z,\bar{z};z',\bar{z}^+) \;\equiv\; \sum_k \int_{\mathcal{C}} \mathrm{d}\bar{z}\, \Sigma_{ik}(z,\bar{z})\, G_{kj}(\bar{z},z') \;, \tag{8.204}$$

$$\pm \mathrm{i}\hbar \sum_{j'kl} \int_{\mathcal{C}} d\bar{z}\, G^{(2)}_{ij'kl}(z,\bar{z},z',\bar{z}^+)\, w_{kljj'}(z'^-,\bar{z}) \;\equiv\; \sum_k \int_{\mathcal{C}} \mathrm{d}\bar{z}\; G_{ik}(z,\bar{z})\, \Sigma_{kj}(\bar{z},z') \;, \tag{8.205}$$

These equations define the self-energy as a functional of the 1pNEGF and the generalized two-body interaction w on the roundtrip contour, i.e. $\Sigma_{ij}(z,z') = \Sigma_{ij}[G,w](z,z')$. It is, thereby, assumed that the selfenergy is the same in both equations, which can be proven, in particular, for conserving approximations. Note that, on the l.h.s. we could remove the contour integral, due to the delta function in the potential. We keep it only in order to simplify selfenergy derivations below.

With this substitution we obtain the Keldysh-Kadanoff-Baym equations

(KBE) – two formally closed equations for the two-time 1pNEGF:

$$\sum_k \left\{ \mathrm{i}\hbar \frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z) \right\} G_{kj}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} + \tag{8.206}$$
$$+ \sum_k \int_{\mathcal{C}} \mathrm{d}\bar{z}\, \Sigma_{ik}(z,\bar{z})\, G_{kj}(\bar{z},z') \ ,$$
$$\sum_k G_{ik}(z,z') \left\{ -\mathrm{i}\hbar \frac{\partial}{\partial z'}\delta_{kj} + h_{kj}(z') \right\} = \delta_{\mathcal{C}}(z,z')\delta_{ij} + \tag{8.207}$$
$$+ \sum_k \int_{\mathcal{C}} \mathrm{d}\bar{z}\ G_{ik}(z,\bar{z})\, \Sigma_{kj}(\bar{z},z') \ .$$

8.6.2 Hartree and Fock selfenergies

Using the Hartree and Fock approximations for the two-particle NEGF and the definition of the selfenergy, Eq. 8.206, we immediately identify the corresponding Hartree and Fock selfenergies where the contour integrations have been performed: Inserting the HF approximation for $G^{(2)}$ into the first KBE, we obtain,

$$\left\{ \mathrm{i}\hbar \frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z) \right\} G_{kj}(z,z') - \delta_{\mathcal{C}}(z-z')\,\delta_{ij} = \tag{8.208}$$
$$= \pm \mathrm{i}\hbar \int_{\mathcal{C}} \mathrm{d}\bar{z}\, w_{ij'kl}(z,\bar{z}) \left\{ G_{lj'}(\bar{z},\bar{z}^+)\, G_{kj}(z,z') \pm G_{lj}(\bar{z},z')\, G_{kj'}(z,\bar{z}^+) \right\} \ ,$$
$$\equiv \int_{\mathcal{C}} \mathrm{d}\bar{z}\, \Sigma^{\mathrm{HF}}_{ik}(z,\bar{z}) G_{kj}(\bar{z},z') \tag{8.209}$$

where we sum over repeating subscripts. If we express the integral on the r.h.s. in the form of ((8.206)), we easily verify that the selfenergy has the form,

$$\Sigma^{\mathrm{HF}}_{ij}(z,z') = \Sigma^{\mathrm{H}}_{ij}(z,z') + \Sigma^{\mathrm{F}}_{ij}(z,z') \ , \tag{8.210}$$

where we identify the two contributions as

$$\begin{aligned} \Sigma^{\mathrm{H}}_{ik}(z,\bar{z}) &= \pm \mathrm{i}\hbar\, \delta_{\mathcal{C}}(z-\bar{z})\, w_{ij'kl}(z)\, G_{lj'}(z,z^+) \ , \\ \Sigma^{\mathrm{F}}_{ik}(z,\bar{z}) &= \mathrm{i}\hbar\, w_{ij'lk}(z,\bar{z})\, G_{lj'}(z,\bar{z}) \ . \end{aligned} \tag{8.211}$$

The first term is the Hartree self-energy that involves the density matrix, $\pm i\hbar G_{lj'}(z,z^+) = n_{lj'}(z)$, whereas the second term (the Fock contribution) accounts for exchange effects, i.e., for the Pauli exclusion principle, in the case

of fermions. Moreover, as $w(t-t')$ involves a contour delta function, we directly observe that the HF approximation leads to a regular (time-local) self-energy and, thus, neglects correlation effects. Improvements of (8.199) beyond Hartree-Fock are obtained by vertex corrections, e.g. Ref. [76], and will be discussed in the following. An important necessary criterion for the construction of approximations is that they retain the symmetries and conservation laws of the original (exact) Hamiltonian.

Basis representations.
Before we do this we briefly discuss how the above results depend on the chosen single-particle basis. so far we considered a general basis where single-particle and two-particle quantities are represented by two-dimensional and four-dimensional matrices, respectively.

1. First we consider a more compact notation where orbital and time indices are combined such as $1=(i_1,s_1,t_1)$. With a generalized interaction potential [Joo22], $w(12;1'2')=\delta_{\mathcal{C}}(z_1,z_2)\delta_{\mathcal{C}}(z_1,z_{2'})\delta_{\mathcal{C}}(z_1,z_{1'})w_{i_1i_2i'_1i'_2}(z_1)$ we can rewrite the Hartree and Fock selfenergies as

$$\Sigma^{\mathrm{HF}}(1,1')=\pm i\hbar\int w(1\underline{2};1'\underline{3})G(\underline{32})+i\hbar\int w(1\underline{2};\underline{3}1')G(\underline{32})\,, \quad (8.212)$$

   where integration over underlined times and summation over underlined orbital indices is implied. Note that we exchanged the orbital indices of the potential in the Fock term which allowed us to use the same notation for the Green function. The corresponding Feynman diagrams are presented in Ref. [Joo22]

2. Consider now a diagonal basis (for example the coordinate representation) where the potential is of the form $w_{ijkl}(z)=\delta_{ik}\delta_{jl}w(z)$. Then we obtain for the Hartree and the Fock selfenergies

$$\Sigma^{\mathrm{H}}_{i_1,i'_1}(z_1,z'_1)=\pm i\hbar\delta_{\mathcal{C}}(z_1,z'_1)\delta_{i_1,i'_1}\sum_{i_2}w_{i_1,i_2}G_{i_2i_2}(z_1,z_1^+)\,, \quad (8.213)$$

$$\Sigma^{\mathrm{F}}_{ij}(z_1,z_2)=i\hbar\delta_{\mathcal{C}}(z_1,z_2)w_{ij}(z_1)G_{ij}(z_1,z_1^+)\,. \quad (8.214)$$

   A detailed analysis of many different representations can be found in the review [SHSB20].

8.6.3 Correlation and exchange-correlation selfenergies

As the two-particle NEGF, also the full selfenergy contains a Hartree-Fock and a correlation contribution

$$\Sigma_{ik}(z,z')=\Sigma^{\mathrm{HF}}_{ik}(z,z')+\Sigma^{\mathrm{cor}}_{ik}(z,z')\,. \quad (8.215)$$

While the Hartree-Fock selfenergy is time-diagonal (or time-local), i.e. $\Sigma^{\mathrm{HF}}(z,z') \propto \delta_{\mathcal{C}}(z-z')$, the correlation part is non-diagonal. Whereas the former makes the KBEs trivial to solve as they become Markovian (the contour integral over the selfenergy can be taken), the latter preserves the non-Markovian structure and accounts for memory effects, that are related to correlations.

8.7 Inverse Green Function. Nonequilibrium Dyson equation

One of the main advantages of the two-time formalism is that the partial differential equations for the 1pNEGF are easily converted into integral equations for which effective approximations via iteration schemes exist.

8.7.1 Inverse Green function

We first demonstrate this for the non-interacting case where $\Sigma \to 0$, cf. Sec. 8.5.1. Then Eq. (8.206) has the form of a linear equation with a delta inhomogeneity (here on the Keldysh contour) which is solved by the *mathematical Green function* of this equation which we will call G_0. Obviously, G_0 can be used to explicitly construct the solution of Eq. (8.206) with an arbitrary inhomogeneity (i.e. for $\Sigma \neq 0$).

The inverse Green function of the ideal system is obtained as

$$\sum_k \left\{ \mathrm{i}\hbar \frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z) \right\} G_{0,kj}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} \tag{8.216}$$

$$:= \int_{\mathcal{C}} \mathrm{d}\bar{z} \sum_k G^{-1}_{0,ik}(z,\bar{z}) G_{0,kj}(\bar{z},z') \,,$$

$$\text{with} \quad G^{-1}_{0,ik}(z,\bar{z}) \equiv \left\{ \mathrm{i}\hbar \frac{\partial}{\partial z}\delta_{ik} - h_{ik}(z) \right\} \delta_{\mathcal{C}}(z,\bar{z}) \,. \tag{8.217}$$

Now we take into account the selfenergy term on the r.h.s. of Eq. (8.206) which we move to the left allowing us to define the inverse of the correlated Green

function:

$$\int_{\mathcal{C}} \mathrm{d}\bar{z} \sum_k \left\{ \left[\mathrm{i}\hbar \frac{\partial}{\partial z} \delta_{ik} - h_{ik}(z) \right] \delta_{\mathcal{C}}(z,\bar{z}) - \Sigma_{ik}(z,\bar{z}) \right\} G_{kj}(z,z') = \delta_{\mathcal{C}}(z,z')\delta_{ij} \tag{8.218}$$

$$:= \int_{\mathcal{C}} \mathrm{d}\bar{z} \sum_k G^{-1}_{ik}(z,\bar{z}) G_{kj}(\bar{z},z') \,,$$

$$\text{with} \quad G^{-1}_{ik}(z,\bar{z}) \equiv G^{-1}_{0,ik}(z,\bar{z}) - \Sigma_{ik}(z,\bar{z}) \,, \tag{8.219}$$

where we have expressed the inverse Green function by the inverse of the ideal case[55]. In the special mean field case (Hartree-Fock), with $\Sigma(z,z') \to \Sigma^{\mathrm{HF}}(z,z') \sim \delta_{\mathcal{C}}(z,z')$, the inverse Green function is time-diagonal, as for the ideal system.

8.7.2 Dyson equation

In a similar way as for the inverse, we can express the full Green function G in terms of the ideal Green function G_0. This is achieved by multiplying Eq. (8.206) with $G_{0,li}(z,\bar{z})$, summing over "i" and integrating over $\bar{z}$. We simplify the procedure by rewriting Eq. (8.206) with the combined orbital and time arguments $1, 1'$ etc. and renaming the arguments (recall that integration and summation is implied over underlined arguments):

$$G_0^{-1}(\tilde{1},\underline{\bar{1}}) G(\underline{\bar{1}},1') = \delta_{\mathcal{C}}(\tilde{1},1') + \Sigma(\tilde{1},\underline{\bar{1}}) G(\underline{\bar{1}},1') \,. \tag{8.220}$$

This we multiply by $G_0(1,\tilde{1})$ and integrate/sum over $\underline{\tilde{1}}$ taking into account that $G_0(1,\underline{\tilde{1}}) G_0^{-1}(\underline{\tilde{1}},\underline{\bar{1}}) = \delta_{\mathcal{C}}(1,\underline{\bar{1}})$, with the result

$$G(1,1') = G_0(1,1') + G_0(1,\underline{\tilde{1}}) \Sigma(\underline{\tilde{1}},\underline{\bar{1}}) G(\underline{\bar{1}},1') \,. \tag{8.221}$$

This is the nonequilibrium Dyson equation for the one-particle Green function which is fully equivalent to the Keldysh-Kadanoff-Baym equation. Often the orbital summations and time integrations over repeating indices (time arguments) are suppressed resulting in the matrix form

$$G = G_0 + G_0 \Sigma G \,. \tag{8.222}$$

This is actually a matrix equation on the Keldysh contour for 3×3 (or 2×2) Keldysh matrices where the equations for the different Keldysh components

[55] Instead of the ideal Green function we could also use any other reference function, for example, the Hartree-Fock Green function.

follow straightforward from the Langreth rules, cf. Tab. 8.1:

$$\{\vec{A}\,\vec{B}\}(t,t') = \int_{\mathcal{C}} \mathrm{d}\bar{t}\, \vec{A}(t,\bar{t})\, \vec{B}(\bar{t},t') \; . \tag{8.223}$$

To specify the structure of the integral term on the r.h.s. of Eq. (8.221) in terms of components of the 1pSE and the 1pNEGF, it is necessary to apply the Langreth-Wilkins rules twice. We recall that the operations indicated by $\star$ and $\circ$ are defined by ($x, y \in \{\mathrm{A}, \mathrm{R}, >, <, \rceil, \lceil\}$),

$$\{A^x \circ B^y\}(t,t') = \int_{t_0}^{\infty} \mathrm{d}\bar{t}\, A^x(t,\bar{t})\, B^y(\bar{t},t') \; , \tag{8.224}$$

and,

$$\begin{aligned}
\{A^{\mathrm{M}} \star B^{\mathrm{M}}\}(\tau) &= \int_0^{\beta} \mathrm{d}\bar{\tau}\, A^{\mathrm{M}}(\tau-\bar{\tau})\, B^{\mathrm{M}}(\bar{\tau}) \; , \qquad (8.225)\\
\{A^{\mathrm{M}} \star B^{\lceil}\}(t_0 - \mathrm{i}\tau, t) &= \int_0^{\beta} \mathrm{d}\bar{\tau}\, A^{\mathrm{M}}(\tau-\bar{\tau})\, B^{\lceil}(t_0 - \mathrm{i}\bar{\tau}, t) \; ,\\
\{A^{\rceil} \star B^{\mathrm{M}}\}(t, t_0 - \mathrm{i}\tau) &= \int_0^{\beta} \mathrm{d}\bar{\tau}\, A^{\rceil}(t, t_0 - \mathrm{i}\bar{\tau})\, B^{\mathrm{M}}(\bar{\tau}-\tau) \; ,\\
\{A^{\rceil} \star B^{\lceil}\}(t,t') &= -\mathrm{i}\int_0^{\beta} \mathrm{d}\bar{\tau}\, A^{\rceil}(t, t_0 - \mathrm{i}\bar{\tau})\, B^{\lceil}(t_0 - \mathrm{i}\bar{\tau}, t') \; .
\end{aligned}$$

8.7.3 Equilibrium Limit of the Dyson Equation

The KBEs (8.206), (8.207) are valid for all times z and z' on the contour $\mathcal{C}$. However, if the system Hamiltonian is time-independent (note that this is assumed above for times $t, t' \leq t_0$), the only independent matrix component of the Green function is G^{M}. As a consequence, the contour reduces to its imaginary track, and the KBEs (8.206), (8.207) simplify to the Dyson equation for the Matsubara Green function[56], were we use the result (8.225)

$$\left\{\mathrm{i}\hbar\,\frac{\partial}{\partial\tau}\delta_{ik} - h_{ik}\right\} G^{\mathrm{M}}_{kj}(\tau) = \delta(\tau)\,\delta_{ij} + \int_0^{\beta} \mathrm{d}\bar{\tau}\, \Sigma^{\mathrm{M}}_{ik}(\tau-\bar{\tau})\, G^{\mathrm{M}}_{kj}(\bar{\tau}), \tag{8.226}$$

in which we have applied the transformation,

$$\mathcal{X}_{ij}(\tau-\tau') = -\mathrm{i}\hbar\,\mathcal{X}_{ij}(t_0 - \mathrm{i}\tau, t_0 - \mathrm{i}\tau') \; , \tag{8.227}$$

[56]Summation over k is implied.

to the 1pNEGF ($\mathcal{X} = G^{\mathrm{M}}$) and the 1pSE ($\mathcal{X} = \Sigma^{\mathrm{M}}$). In this notation, the time difference $\tau - \tau'$ generally ranges from $-\beta$ to $+\beta$, and the equilibrium 1pRDM is simply,

$$n_{ij} = G^{\mathrm{M}}_{ij}(0^-) \; . \tag{8.228}$$

Further, the antiperiodicity properties a) and b) of Eq. (8.136) allow us to restrict the solution of Eq. (8.226) to a half interval, e.g., $[-\beta, 0]$ which includes the reduced density matrix at the upper interval boundary[57] [58].

If we include the regular part of the self-energy [e.g. the Hartree-Fock selfenergy],

$$\Sigma^{\mathrm{M}}_{\mathrm{reg},ij}(\tau) = \delta(\tau)\, \Sigma^{\mathrm{M}}_{0,ij} \; , \tag{8.229}$$

into an effectively non-interacting Green function[59] $G^{\mathrm{M}}_0(\tau)$, the Dyson equation attains the form [compare with Eq. (8.221)],

$$G^{\mathrm{M}}_{ij}(\tau) = G^{\mathrm{M}}_{0,ij}(\tau) + \int_0^\beta \mathrm{d}\bar{\tau} \int_0^\beta \mathrm{d}\bar{\bar{\tau}}\, G^{\mathrm{M}}_{0,ik}(\tau - \bar{\tau}) \Sigma^{\mathrm{cor}}_{kl}(\bar{\tau} - \bar{\bar{\tau}})\, G^{\mathrm{M}}_{lj}(\bar{\bar{\tau}}) \, , \tag{8.230}$$

$$\Sigma^{\mathrm{cor}}_{ij}(\tau) = \Sigma^{\mathrm{M}}_{ij}(\tau) - \Sigma^{\mathrm{M}}_{\mathrm{reg},ij}(\tau) \; .$$

It is important to note that here (aside from w) the self-energy Σ^{M}_0 is strictly a functional of the effectively non-interacting Green function, whereas $\Sigma^{\mathrm{M}}(\tau)$ depends on the full Green function and includes, both, a regular and an irregular part.

If the effectively non-interacting Green function $G^{\mathrm{M}}_0(\tau)$ is known, equation (8.230) can be solved by iteration starting from setting $G^{\mathrm{M}}(\tau) = G^{\mathrm{M}}_0(\tau)$ on the r.h.s. Eventually, a self-consistent Matsubara Green function is reached. Together with transformation (8.227) and properties c) and d) of Eq. (8.136), this solution serves as a proper initial condition for the real-time propagation of the 1pNEGF. This means that, in this case, the many-body system will remain stationary in time as far as no external field is applied and the same "conserving" approximation is used for the self-energy, cf. Section 8.8.1.

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[57] Sometimes, $G^{\mathrm{M}}(\tau)$ is considered on the symmetric interval $[-\frac{\beta}{2}, \frac{\beta}{2}]$, see, e.g., [75].

[58] Note that for $\bar{\tau} = \tau - \tau' \in [-\beta, 0]$ it is always $\tau \geq \tau'$ and therefore $G^{M}(\bar{\tau}) = G^{\lceil}(t_0 - \mathrm{i}\hbar\bar{\tau}, t_0)$

[59] The corresponding Dyson equation is obtained by replacing the one-particle energy h_{ij} in Eq. (8.226) by $h_{ij} + \Sigma^{\mathrm{M}}_{0,ij}$ and setting the integration kernel to zero. Sometimes, one refers to G^{M}_0 as the "bare" Green function whereas the full Green function G^{M} is the "dressed" one.

Before considering approximations for the correlation selfenergy we point out that an explicit equilibrium solution of the Dyson equation (8.230) can be obtained via Fourier transform, using the convolution theorem:

$$G^{\mathrm{M}}(\omega) = G_0^{\mathrm{M}}(\omega) + G_0^{\mathrm{M}}(\omega)\Sigma^{\mathrm{cor}}(\omega)G^{\mathrm{M}}(\omega)\,. \tag{8.231}$$

If the Green functions and selfenergy are diagonal in orbital space (e.g. in case of the momentum representation for a uniform system)[60], this can be solved to yield explicitly

$$G^{\mathrm{M}}(\omega,p) = \frac{G_0^{\mathrm{M}}(\omega,p)}{1 - G_0^{\mathrm{M}}(\omega,p)\Sigma^{\mathrm{cor}}(\omega,p)}\,. \tag{8.232}$$

This is, however, only formally an explicit solution because Σ^{cor} also depends on the unknown G^{M}. For this diagonal case, it is also instructive to analyze the inverse Green functions. Applying again the convolution theorem, the definition of the inverse, Eqs. (8.217) and (8.219), becomes

$$G_0^{\mathrm{M},-1}(\omega,p)G_0^{\mathrm{M}}(\omega,p) = 1\,, \tag{8.233}$$

$$G^{\mathrm{M},-1}(\omega,p)G^{\mathrm{M}}(\omega,p) = 1\,, \tag{8.234}$$

i.e. the inverse is just one over the Green function. This can be used to simplify the result (8.232) by multiplying with $G_0^{\mathrm{M}}/G_0^{\mathrm{M}}$,

$$G^{\mathrm{M}}(\omega) = \frac{1}{G_0^{\mathrm{M},-1}(\omega,p) - \Sigma^{\mathrm{cor}}(\omega,p)}\,. \tag{8.235}$$

An explicit result is obtained after performing the time derivative of the Fourier transform of the non-interacting (HF) Green function:

$$G_0^{\mathrm{M},-1}(\omega,p) = \hbar\omega - \epsilon(p)\,, \tag{8.236}$$

$$G^{\mathrm{M},-1}(\omega,p) = \hbar\omega - \epsilon(p) - \Sigma^{\mathrm{cor}}(\omega,p)\,. \tag{8.237}$$

8.8 Many-Body Approximations

One of the key problems in solving the Kadanoff-Baym equations (8.206), (8.207) as well as the Dyson equation (8.226) is that they contain an unknown function – the selfenergy – or, equivalently, the two-particle Green function. These functions are exactly known only in special model cases[61]. Therefore, the standard way to proceed is to perform a truncation of the MS hierarchy through a many-body approximation (MBA). The simplest truncation is, of course, the Hartree-Fock approximation that was discussed in detail above. Now we systematically go beyond that limit.

[60] **Task:** Extend this to the case of a matrix equation for G_{ij}^{M}.

[61] Alternatively, one could use them, as an input, from computer simulations.

8.8.1 Requirements for a Conserving Scheme

If we analyze the HF approximation of the 2pNEGF, we realize that it obeys a specific symmetry: It is invariant under the simultaneous exchange of the first and the second pair of (spatial and temporal) arguments, cf. Eq. (8.199). Also, we find that, when applying the HF approximation to the KBEs (8.206), (8.207), the system's total energy, particle number and momentum are preserved[62]. For this reason, HF is called a "conserving" approximation. In this regard, we note that the 1pNEGF allows us to determine the total energy by (we sum over i and j, i.e., take the trace),

$$\left\langle \hat{H} \right\rangle (t) = -\mathrm{i}\hbar G_{ij}(t,t^+)\, h_{ji}(t) - \frac{\mathrm{i}\hbar}{2} \int_{\mathcal{C}} \mathrm{d}\bar{t}\, \Sigma_{ij}(t,\bar{t})\, G_{ji}(\bar{t},t^+) \;, \tag{8.238}$$

where the first part is the single-particle energy and the second part the interaction energy (including HF). The equilibrium limit of this is,

$$\left\langle \hat{H} \right\rangle = G^{\mathrm{M}}_{ij}(0^-)\, h_{ji} + \frac{1}{2} \int_0^\beta \mathrm{d}\tau\, \Sigma^{\mathrm{M}}_{ij}(-\tau)\, G^{\mathrm{M}}_{ji}(\tau) \;. \tag{8.239}$$

In fact, it has been shown by *Baym* [77] that the symmetry of $G^{(2)}$ in (8.199) is directly linked to important conservation laws and the preservation of particle number. More precisely, an arbitrary MBA is automatically conserving if,

i.) the approximate 1pNEGF simultaneously satisfies the first equation of the MS hierarchy and its adjoint, i.e., Eqs. (8.188), (8.189), and

ii.) the approximation for $G^{(2)}$ satisfies the symmetry,

$$G^{(2)}_{ij,kl}(t_1,t_2;t_1^+,t_2^+) = G^{(2)}_{ji,lk}(t_2,t_1;t_2^+,t_1^+) \;. \tag{8.240}$$

Conditions i.) and ii.) represent important criteria for the development of self-consistent solutions of the KBEs beyond the HF level. Thereby, condition ii.) is simple to verify if the analytical dependence of $G^{(2)}$ on G is known for a chosen approximation. On the other hand, a condition equivalent to ii.) can be formulated for the one-particle self-energy, cf. the discussion on "Φ-derivable" approximations in the following Subsection.

Comment: Note that in single-time reduced density operator theory there are similar conservation conditions. There energy conservation is fulfilled if the three-particle density operator F_{123} is invariant with respect to index changes [Bon98].

[62] For an analysis of conservation laws, we refer to Ref. [27].