

## Chapter 2

# Nonequilibrium Green's Functions

Real-time nonequilibrium Green's functions (NEGFs) naturally appear in the extension of the Matsubara formalism of (equilibrium) quantum many-body theory [55, 56] to situations far from equilibrium. In this respect, the term “one-particle NEGF”, cf. Sect. 2.1.2, is synonymous for the phrase “propagator” as well as for “correlation function”. The great success of NEGFs is, in general, due to the fact that fundamentals of equilibrium theory, e.g., Feynman rules and diagram techniques, can be applied without major conceptual modifications also to nonequilibrium situations.

Nonequilibrium Green's functions are the main ingredients to quantum statistical mechanics and quantum kinetic equations [11], the development of which was pioneered by Martin [57] and Schwinger [58] and was expedited by Kadanoff and Baym [28] in the USA and, in parallel, by Keldysh [59] in the USSR. The main achievements were rendered in the late 1950s and in the 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., Refs. [24–26, 60, 61], and have been applied to give quantum corrections to the Boltzmann equation [62–64]. On the other hand, NEGFs have nowadays<sup>1</sup>, reached the potential to numerically treat time-dependent quantum systems more or less *ab-initio*<sup>2</sup>. 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. For an overview, see Part IV of this monograph.

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<sup>1</sup>Due to the continuously increasing power of computers.

<sup>2</sup>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.

## 2.1 Introduction

Our ultimate goal is the description of time-dependent processes in a fully interacting quantum many-body system of identical particles.

Using second quantization methods and fermionic creation ( $\hat{f}_i^\dagger$ ) and annihilation ( $\hat{f}_i$ ) operators acting on a many-particle state  $|\{n\}\rangle$  in Fock space<sup>3</sup>, see Appendix A, we consider a generic time-dependent many-body Hamiltonian,

$$\hat{H}(t) = \sum_{ij} \langle i|h^{(1)}(t)|j\rangle \hat{f}_i^\dagger \hat{f}_j + \frac{1}{2} \sum_{ij,kl} \langle ij|w^{(2)}|kl\rangle \hat{f}_i^\dagger \hat{f}_j^\dagger \hat{f}_l \hat{f}_k, \quad (2.1)$$

$$h^{(1)}(t) = t^{(1)} + v^{(1)}(t),$$

where  $t^{(1)}$  ( $v^{(1)}$ ) is the kinetic (potential) energy of a single particle,  $w^{(2)}$  denotes the two-body interaction potential, and  $\langle i|h^{(1)}(t)|j\rangle$  and  $\langle ij|w^{(2)}|kl\rangle$  are the corresponding matrix elements, cf. Eq. (A.18). The great advantage of the second quantization formulation is that the anticommutation relations<sup>4</sup>,

$$[\hat{f}_i, \hat{f}_j^\dagger]_+ = \delta_{ij}, \quad [\hat{f}_i, \hat{f}_j]_+ = [\hat{f}_i^\dagger, \hat{f}_j^\dagger]_+ = 0, \quad (2.2)$$

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,

$$\hat{\rho}_{1,ij} = \hat{f}_i^\dagger \hat{f}_j. \quad (2.3)$$

This matrix of operators yields after ensemble averaging the familiar one-particle density matrix  $\rho_{1,ij} = \langle \hat{\rho}_{1,ij} \rangle$ . Below, we will express it in terms of the single-particle Green's function, cf. Eq. (2.15).

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. NEGFs make essential use of the Heisenberg picture (H). In contrast to the Schrödinger picture (S), where the system's state vector  $\Psi_S^{(N)}$  evolves in time and operators of observables are stationary, the Heisenberg picture allows for the operators to develop with time—at simultaneously time-independent states. The transformation between S and H is mediated by the unitary time evolution operator<sup>5</sup> which obeys the Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t'} \hat{U}(t', t) = \hat{H}(t') \hat{U}(t', t), \quad (2.4)$$

<sup>3</sup>  $\hat{f}_i^\dagger$  ( $\hat{f}_i$ ) adds (removes) a particle to (from) a spin orbital  $|i\rangle$ , e.g., Ref. [36].

<sup>4</sup> The anticommutator is defined as  $[\hat{a}, \hat{b}]_+ = \hat{a}\hat{b} + \hat{b}\hat{a}$ . In the case of bosons, the same expressions hold with the commutator  $[\cdot, \cdot]_+ \rightarrow [\cdot, \cdot]_-$ .

<sup>5</sup> In matrix representation, the unitarity is expressed by  $\hat{U}^\dagger \hat{U} = 1$ .

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

$$\hat{U}(t', t) = \hat{T} \exp \left( -\frac{i}{\hbar} \int_t^{t'} d\bar{t} \hat{H}(\bar{t}) \right), \quad (2.5)$$

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

where  $\hat{H}(t)$  is the full Hamiltonian, and  $\hat{T}$  is the standard time-ordering operator<sup>6</sup>. For any operator  $\hat{A}_H$  in the Heisenberg picture, it is,

$$\hat{A}_H(t) = \hat{U}(t_0, t) \hat{A}_S \hat{U}(t, t_0), \quad (2.6)$$

$$i\hbar \frac{\partial}{\partial t} \hat{A}_H(t) = \left[ \hat{A}_H(t), \hat{H}_H(t) \right]_- \quad (\text{Heisenberg equation}). \quad (2.7)$$

The corresponding state vector  $\Psi_H^{(N)}(t_0) = \hat{U}(t_0, t) \Psi_S^{(N)}(t)$  remains constant ( $t_0$  gives only a reference time), and any operator that commutes with the Hamiltonian is a constant of motion, as is obvious from Eq. (2.7).

Using the Heisenberg picture, the creation and annihilation operators in Eqs. (2.1) to (2.3) become explicitly time-dependent, i.e., we replace  $\hat{f}_i \rightarrow \hat{f}_{i,H}(t)$ . The anti-commutation relations of Eq. (2.2) then remain valid in the equal-time limit.

Furthermore, many situations require to properly define the initial state at the 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  $\hat{\rho}$ , cf. Appendix A. 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 [59, 65–67], 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., [67, 68].

Of course, other approaches exist which *a priori* define (non-)correlated nonequilibrium initial states, see, e.g., Refs. [69–71] and references therein.

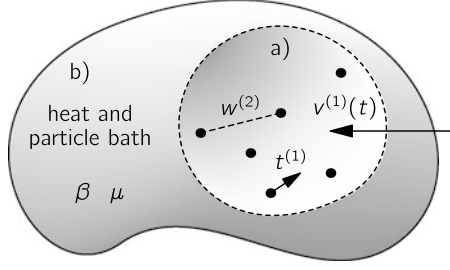
In this article, we mainly follow approach (ii), because the mathematical methods behind nonequilibrium Green's functions are most comprehensively developed along this line. However, strategy (i) is not irrelevant, and we will later emphasize its significance when using the generalized Kadanoff-Baym ansatz (GKBA), see Sect. 2.4.2.

### 2.1.1 Keldysh Contour

From now on, we suppose that the quantum many-body system of Eq. (2.1) [system (a)] exchanges particles and energy with a reservoir at a temperature

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<sup>6</sup>In the interaction (or Dirac) picture (I), we deal with a representation intermediate between S and H, where usually the state vector  $\Psi_I^{(N)}$  carries the time dependence of some time-independent part  $\hat{H}_0$  of the full Hamiltonian  $\hat{H}(t)$ .



**Fig. 2.1** Grand canonical ensemble (GCE) with inverse temperature  $\beta = 1/(k_B T)$  and chemical potential  $\mu$ . 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,  $w^{(2)}$  denotes the two-body interaction between identical particles (here, fermions) with kinetic energy  $t^{(1)}$ , and  $v^{(1)}$  refers to the presence of a time-dependent local potential in (a), cf. Hamiltonian (2.1)

$T = (k_B \beta)^{-1}$  [system (b)]. Physically, this matter of fact is described by the grand canonical ensemble (GCE), see Fig. 2.1, whereby the exact state of the overall system is generally not known, and one has to resort to a mixed state (ensemble) description.

In the GCE, we can evaluate time-dependent averages of an observable  $\hat{A}$  according to<sup>7</sup> (the system is in equilibrium for  $t \leq t_0$ ),

$$\langle \hat{A} \rangle(t) = \frac{1}{Z_0} \text{Tr} \{ e^{-\beta(\hat{H}(t) - \mu \hat{N})} \hat{A}_S \}, \quad (2.8)$$

where  $Z_0 = \text{Tr} \{ e^{-\beta(\hat{H}(t_0) - \mu \hat{N})} \}$  is the partition function,  $\mu$  denotes the one-particle chemical potential and  $\hat{N}$  is the particle number operator. The trace is defined as in Appendix A.4, summing over a complete set of states in the Fock space.

Working out that, for the time-evolution operator of Eq. (2.5), it is  $\hat{U}(t_0 - i\beta, t_0) = e^{-\beta(\hat{H}(t_0) - \mu \hat{N})}$ , i.e., the initial statistical operator acts like an evolution operator in imaginary time, we can rewrite Eq. (2.8) using the cyclic invariance of the trace as<sup>8</sup>,

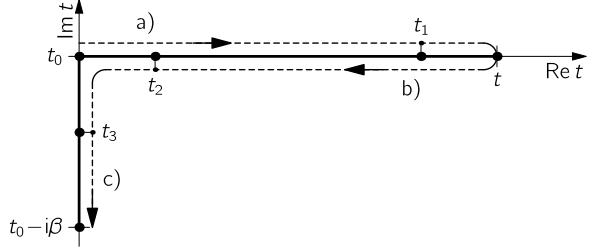
$$\begin{aligned} \langle \hat{A} \rangle(t) &= \frac{1}{Z_0} \text{Tr} \{ \hat{U}(t_0 - i\beta, t_0) \hat{U}(t_0, t) \hat{A}_S \hat{U}(t, t_0) \} \\ &= \frac{1}{Z_0} \text{Tr} \{ \hat{U}(t_0 - i\beta, t_0) \hat{A}_H \}. \end{aligned} \quad (2.9)$$

From right to left, the first line indicates a successive time evolution of the system along a contour: First, it evolves along the real time axis from time  $t_0$  to time  $t$  (where the operator acts) and back from  $t$  to  $t_0$ . Second, an additional evolution

<sup>7</sup>The subscript S in  $\hat{A}_S$  indicates the Schrödinger picture.

<sup>8</sup>We emphasize that, with  $\hat{U}(t_0 - i\beta, t_0) = \hat{\rho}(t_0)$ , it is the time-independent density operator that enters in the trace of Eq. (2.9).

**Fig. 2.2** Complex round-trip Keldysh contour  $\mathcal{C}$  including three different branches denoted (a), (b) and (c). On  $\mathcal{C}$ , time  $t_2$  is later than  $t_1$ , and time  $t_3$  is later than  $t_1$  and  $t_2$ , cf. the arrows



occurs parallel to the imaginary axis from time  $t_0$  to time  $t_0 - i\beta$ . Such a complex time contour is originally due to Keldysh [59], and we refer to it as the contour  $\mathcal{C}$ . For illustration of the round-trip propagation path, see Fig. 2.2.

On the Keldysh contour<sup>9</sup>, we can define a generalized time-ordering operator  $\hat{T}_{\mathcal{C}}$ , which works chronologically (antichronologically) on the upper (lower) branch of the contour and arranges imaginary times which originate from the vertical branch behind purely real times. For a contour-ordered product of operators  $\hat{A}_{1,H}(t_1) \dots \hat{A}_{n,H}(t_n)$  which commute pairwise at equal times, we then have ( $t_1, \dots, t_n \in \mathcal{C}$ ),

$$\begin{aligned} \hat{T}_{\mathcal{C}} \{ \hat{A}_{1,H}(t_1) \dots \hat{A}_{n,H}(t_n) \} &= \sum_{\mathcal{P}} \theta_{\mathcal{C}}(t_{\mathcal{P}(1)} - t_{\mathcal{P}(2)}) \dots \theta_{\mathcal{C}}(t_{\mathcal{P}(n-1)} - t_{\mathcal{P}(n)}) \\ &\quad \times \hat{A}_{\mathcal{P}(1),H}(t_{\mathcal{P}(1)}) \dots \hat{A}_{\mathcal{P}(n),H}(t_{\mathcal{P}(n)}), \end{aligned} \quad (2.10)$$

where  $\theta_{\mathcal{C}}(t - t')$  is the contour step function that equals one for  $t$  later than  $t'$  on  $\mathcal{C}$  and zero otherwise, cf. the arrows in Fig. 2.2.

We now can refine Eq. (2.9) as follows,

$$\langle \hat{A} \rangle(t) = \frac{1}{Z_0} \text{Tr} \left\{ \hat{T}_{\mathcal{C}} \exp \left( -\frac{i}{\hbar} \int_{\mathcal{C}} d\bar{t} \hat{H}(\bar{t}) \right) \hat{A}_S|_t \right\} = \frac{1}{Z_0} \text{Tr} \{ \hat{U}_{\mathcal{C}} \hat{A}_S|_t \} \quad (2.11)$$

with the generalized time-evolution operator  $\hat{U}_{\mathcal{C}}$ .

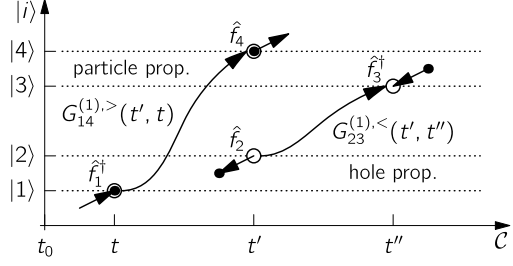
The presence of the Keldysh contour assesses a contour algebra which was described in detail by DuBois [72] and Langreth [73] and which culminates in the application of the Langreth-Wilkins rules [74], see Table 2.1.

### 2.1.2 One-Particle Nonequilibrium Green's Function

The contour-ordered, one-particle nonequilibrium Green's function (1pNEGF) is defined according to (for simplicity, we drop subscripts H and S which indicate the Heisenberg or Schrödinger picture),

<sup>9</sup>Sometimes,  $\mathcal{C}$  is called Schwinger-Keldysh contour.

**Fig. 2.3** The one-particle nonequilibrium Green's functions (correlation functions)  $G^{(1),>}$  and  $G^{(1),<}$  correspond, respectively, to the propagation of a “particle” and a “hole”. The propagation paths are indicated by curved arrows



$$G_{ij}^{(1)}(t, t') = -\frac{i}{\hbar} \langle \hat{T}_{\mathcal{C}} \hat{f}_i(t) \hat{f}_j^\dagger(t') \rangle$$

$$= \theta_{\mathcal{C}}(t - t') G_{ij}^{(1),>}(t, t') + \theta_{\mathcal{C}}(t' - t) G_{ij}^{(1),<}(t, t'), \quad (2.12)$$

where the times  $t$  and  $t'$  are located on the Keldysh contour  $\mathcal{C}$ , and the lesser and greater components<sup>10</sup> are,

$$G_{ij}^{(1),>}(t, t') = -\frac{i}{\hbar} \langle \hat{f}_i(t) \hat{f}_j^\dagger(t') \rangle, \quad (2.13)$$

$$G_{ij}^{(1),<}(t, t') = \frac{i}{\hbar} \langle \hat{f}_j^\dagger(t') \hat{f}_i(t) \rangle.$$

In the GCE, the ensemble average  $\langle \dots \rangle$  is evaluated as in Eq. (2.11), i.e.,

$$G_{ij}^{(1)}(t, t') = -\frac{i}{\hbar Z_0} \text{Tr} \{ \hat{U}_{\mathcal{C}} \hat{f}_i |t\rangle \hat{f}_j^\dagger |t'\rangle \}. \quad (2.14)$$

Here, we restrict ourselves to fermions<sup>11</sup> and, furthermore, do not consider “anomalous” Green’s functions<sup>12</sup> that are relevant for quantum coherence phenomena such as superfluidity or superconductivity [75–77].

In a quasi-particle picture, the greater component of the 1pNEGF describes the propagation of an added particle whereas the lesser component describes the propagation of a removed particle (“hole”), for illustration see Fig. 2.3. Moreover, the 1pNEGF is directly connected to all one-particle observables, as in the equal-time limit, we recover the 1pRDM ( $t$  real and  $\varepsilon > 0$ ),

$$\rho_{1,ij}(t) = -i\hbar G_{ij}^{(1),<}(t, t) = -i\hbar G_{ij}^{(1)}(t, t^+) = -i\hbar \lim_{\varepsilon \rightarrow 0} G_{ij}^{(1)}(t, t + \varepsilon). \quad (2.15)$$

As an illustration, consider the coordinate representation: With  $G^{(1)}(\mathbf{r}t, \mathbf{r}'t') = \sum_{ij} \phi_i^*(\mathbf{r}) \phi_j(\mathbf{r}') G_{ij}^{(1)}(t, t')$  for (spin) orbitals  $|i\rangle = \phi_i(\mathbf{r})$ , the total spatial and current density are given by (for fermions of mass  $m$  and no external vector potential applied),

<sup>10</sup>The greater and lesser components are also called correlation functions.

<sup>11</sup>For bosons,  $G^{(1),<}$  carries the opposite spin.

<sup>12</sup>Containing two annihilation or two creation operators.

$$\begin{aligned}\rho_1(\mathbf{r}, t) &= -i\hbar G^{(1)}(\mathbf{r}t, \mathbf{r}t^+), \\ \mathbf{j}_1(\mathbf{r}, t) &= -i\hbar \left\{ \frac{\nabla_{\mathbf{r}} - \nabla_{\mathbf{r}'}}{2mi} G^{(1)}(\mathbf{r}t, \mathbf{r}'t') \right\}_{t'=t^+}.\end{aligned}\quad (2.16)$$

Furthermore, we define the spectral function,

$$A_{1,ij}(t, t') = i\hbar \{G_{ij}^{(1),>}(t, t') - G_{ij}^{(1),<}(t, t')\}, \quad (2.17)$$

which gives access to the local density of states and the addition, respectively, removal energies.

Instead of the prevailing definition (2.12), also matrix representations of the 1pNEGF have emerged. Useful 2 by 2 matrix notations cover only real-time arguments and are known from Keldysh theory. Thereby, different representations are connected by a linear transformation called “Keldysh rotation”, see Ref. [74]. A common representation is (omitting the arguments),

$$\mathbf{G}_{2 \times 2}^{(1)} = \begin{bmatrix} G^{(1),R} & G^{(1),<} \\ 0 & G^{(1),A} \end{bmatrix}, \quad (2.18)$$

where the retarded (R) and advanced (A) Green’s functions are given by,

$$G^{(1),R/A}(t, t') = \pm \theta_{\mathcal{C}}(\pm[t - t']) \{G^{(1),>}(t, t') - G^{(1),<}(t, t')\}. \quad (2.19)$$

Allowing also for imaginary time arguments, we can extend Eq. (2.18) to a 3 by 3 matrix [78, 79], as there are generally nine possibilities to distribute the arguments along the three contour branches (a), (b) and (c) of Fig. 2.2:

$$\mathbf{G}_{3 \times 3}^{(1)} = \begin{bmatrix} G^{(1),c} & G^{(1),<} & G^{(1),\lceil} \\ G^{(1),>} & G^{(1),a} & G^{(1),\lceil} \\ G^{(1),\lceil} & G^{(1),\lceil} & G^{(1),M} \end{bmatrix}. \quad (2.20)$$

Here, the causal (c) and anticausal (a) Green’s functions are defined by,

$$G^{(1),c/a}(t, t') = \theta_{\mathcal{C}}(\pm[t - t']) G^{(1),>}(t, t') + \theta_{\mathcal{C}}(\pm[t' - t]) G^{(1),<}(t, t'), \quad (2.21)$$

and  $G^{(1),M}(t, t')$  denotes the Matsubara Green’s function for which  $t$  and  $t'$  are on the imaginary track of  $\mathcal{C}$ . Further, the mixed Green’s function  $G^{(1),\lceil}$  (respectively,  $G^{(1),\rceil}$ ) takes a real time as first (second) argument and an imaginary time as second (first) argument. As one generally does not distinguish the origin of the real-time arguments in  $G^{(1),\lceil}$  and  $G^{(1),\rceil}$ , the symbols  $\lceil$  ( $\rceil$ ) are quite intuitive when reading them from left to right [80].

Note that both matrix representations, (2.18) and (2.20), are overcomplete because not all components are independent. Regarding the 3 by 3 matrix, either the four components  $G^{(1),M}$ ,  $G^{(1),\rceil}$ ,  $G^{(1),<}$  and  $G^{(1),>}$  or  $G^{(1),M}$ ,  $G^{(1),\lceil}$ ,  $G^{(1),c}$  and  $G^{(1),a}$  define a linear independent subset<sup>13</sup>.

<sup>13</sup>Provided the system is in a nonequilibrium state. In the case of a 2 by 2 matrix, there are only two independent components,  $G^{(1),>}$  and  $G^{(1),<}$ .

We collect some useful relations<sup>14</sup> ( $t_0$  real,  $\tau, \tau' \in [-\beta, 0]$ ):

$$\begin{aligned}
 G_{ij}^{(1),>}(t, t) - G_{ij}^{(1),<}(t, t) &= -\frac{i}{\hbar} \delta_{ij} \quad (\text{at equal times!}), \\
 G_{ij}^{(1)}(t_0 - i\beta, t') &= -G_{ij}^{(1)}(t_0, t') \quad (\text{a}), \\
 G_{ij}^{(1)}(t, t_0) &= -G_{ij}^{(1)}(t, t_0 - i\beta) \quad (\text{b}), \\
 G_{ij}^{(1),M}(t_0 - i0, t_0 - i0^+) &= G_{ij}^{(1),<}(t_0, t_0) \quad (\text{c}), \\
 G_{ij}^{(1),M}(t_0 - i\tau, t_0 - i\tau') &= G_{ij}^{(1),\lceil}(t_0 - i(\tau - \tau'), t_0) \quad (\text{d}), \\
 G_{ij}^{(1),\geq}(t, t') &= -[G_{ji}^{(1),\geq}(t', t)]^*, \\
 G_{ij}^{(1),\lceil}(t_0 - i\tau, t') &= [G_{ji}^{(1),\lceil}(t', t_0 - i(\beta - \tau))]^*.
 \end{aligned} \tag{2.22}$$

In Eq. (2.22)(a) to (d), the system's Hamiltonian is time independent for times  $t, t' \leq t_0$ , and we assume a thermodynamic equilibrium with temperature  $\beta^{-1}$ . Further, in a matrix representation regarding the basis indices  $i$  and  $j$ , the last two properties read,

$$\begin{aligned}
 G^{(1),\geq}(t, t') &= -[G^{(1),\geq}(t', t)]^\dagger, \\
 G^{(1),\lceil}(t_0 - i\tau, t') &= [G^{(1),\lceil}(t', t_0 - i(\beta - \tau))]^\dagger.
 \end{aligned} \tag{2.23}$$

## 2.2 Equations of Motion

For the derivation of equations of motion for the 1pNEGF, we first consider its time derivative in terms of the greater and lesser components,

$$\begin{aligned}
 \frac{\partial}{\partial t} G_{ij}^{(1)}(t, t') &= \delta_{\mathcal{C}}(t - t') \{ G_{ij}^{(1),>}(t, t') - G_{ij}^{(1),<}(t, t') \} \\
 &\quad + \theta_{\mathcal{C}}(t - t') \frac{\partial}{\partial t} G_{ij}^{(1),>}(t, t') + \theta_{\mathcal{C}}(t' - t) \frac{\partial}{\partial t} G_{ij}^{(1),<}(t, t').
 \end{aligned} \tag{2.24}$$

Due to the contour delta function, the difference between  $G^{(1),>}$  and  $G^{(1),<}$  in the first line will be evaluated only at equal times which gives rise to a factor  $-\frac{i}{\hbar} \delta_{ij}$ , cf. Eq. (2.22). Explicitly writing out the second line yields with Eq. (2.13),

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<sup>14</sup>Properties (a) and (b) are sometimes called Kubo-Martin-Schwinger (KMS) conditions and follow from Eq. (2.14) under the cyclic property of the trace. For bosons, the antiperiodicity turns into periodicity. In expression (c), the second time argument on the l.h.s. is infinitesimally larger on  $\mathcal{C}$  than the first one.



$$\begin{aligned}
& i\hbar \frac{\partial}{\partial t} G_{ij}^{(1)}(t, t') \\
& = \delta_{\mathcal{C}}(t - t') \delta_{ij} \\
& \quad + \theta_{\mathcal{C}}(t - t') \left\langle \left\{ \frac{\partial}{\partial t} \hat{f}_i(t) \right\} \hat{f}_j^{\dagger}(t') \right\rangle - \theta_{\mathcal{C}}(t' - t) \left\langle \hat{f}_j^{\dagger}(t') \left\{ \frac{\partial}{\partial t} \hat{f}_i(t) \right\} \right\rangle, \quad (2.25)
\end{aligned}$$

where the dynamics of the annihilation operators is given by the Heisenberg equation (cf. Eq. (2.7)),

$$i\hbar \frac{\partial}{\partial t} \hat{f}_i(t) = [\hat{f}_i(t), \hat{H}(t)]_{-}. \quad (2.26)$$

Taking advantage of the relations in Eq. (A.11) of Appendix A, we readily evaluate the commutator in Eq. (2.26) as (summation over  $j', k$  and  $l$  is implied),

$$i\hbar \frac{\partial}{\partial t} \hat{f}_i(t) = \langle i | h^{(1)} | k \rangle \hat{f}_k(t) + \langle i j' | w^{(2)} | k l \rangle \hat{f}_{j'}^{\dagger}(t) \hat{f}_l(t) \hat{f}_k(t). \quad (2.27)$$

It follows<sup>15</sup>,

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} G_{ij}^{(1)}(t, t') & = \delta_{\mathcal{C}}(t - t') \delta_{ij} \\
& \quad - \frac{i}{\hbar} \langle i | h^{(1)} | k \rangle \{ \theta_{\mathcal{C}}(t - t') \langle \hat{f}_k(t) \hat{f}_j^{\dagger}(t') \rangle - \theta_{\mathcal{C}}(t' - t) \langle \hat{f}_j^{\dagger}(t') \hat{f}_k(t) \rangle \} \\
& \quad - \frac{i}{\hbar} \langle i j' | w^{(2)} | k l \rangle \{ \theta_{\mathcal{C}}(t - t') \langle \hat{f}_{j'}^{\dagger}(t) \hat{f}_l(t) \hat{f}_k(t) \hat{f}_j^{\dagger}(t') \rangle \\
& \quad - \theta_{\mathcal{C}}(t' - t) \langle \hat{f}_j^{\dagger}(t') \hat{f}_{j'}^{\dagger}(t) \hat{f}_l(t) \hat{f}_k(t) \rangle \}. \quad (2.28)
\end{aligned}$$

While in the second term on the r.h.s. we can resubstitute the 1pNEGF  $G_{kj}^{(1)}(t, t')$ , the last term is more complicated involving averages over four operators. In order to identify these terms with the contour-ordered two-particle nonequilibrium Green's function<sup>16</sup> (2pNEGF),

$$G_{ij,kl}^{(2)}(t, t'; \bar{t}, \bar{t}') = \left( -\frac{i}{\hbar} \right)^2 \langle \hat{T}_{\mathcal{C}} \hat{f}_i(t) \hat{f}_j(t') \hat{f}_l^{\dagger}(\bar{t}') \hat{f}_k^{\dagger}(\bar{t}) \rangle, \quad (2.29)$$

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

$$w^{(2)}(t, t') = \delta_{\mathcal{C}}(t - t') w^{(2)}, \quad (2.30)$$

to be evaluated on the contour  $\mathcal{C}$ . Then, Eq. (2.28) becomes,

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} G_{ij}^{(1)}(t, t') & = \delta_{\mathcal{C}}(t - t') \delta_{ij} + \langle i | h^{(1)} | k \rangle G_{kj}^{(1)}(t, t') \\
& \quad - \frac{i}{\hbar} \int_{\mathcal{C}} d\bar{t} \langle i j' | w^{(2)}(t - \bar{t}) | k l \rangle \{ \theta_{\mathcal{C}}(t - t') \langle \hat{f}_{j'}^{\dagger}(\bar{t}) \hat{f}_l(\bar{t}) \hat{f}_k(t) \hat{f}_j^{\dagger}(t') \rangle \\
& \quad - \theta_{\mathcal{C}}(t' - t) \langle \hat{f}_j^{\dagger}(t') \hat{f}_{j'}^{\dagger}(\bar{t}) \hat{f}_l(\bar{t}) \hat{f}_k(t) \rangle \}. \quad (2.31)
\end{aligned}$$

<sup>15</sup>Again, the notation implies summation over all repeatedly occurring indices.

<sup>16</sup>In the language of quasi-particles, the 2pNEGF is a “particle-hole” propagator.

### 2.2.1 Keldysh-Kadanoff-Baym Equations

With the action of the time-ordering operator  $\hat{T}_{\mathcal{C}}$  (recall Eq. (2.10) in Sect. 2.1), we identify the bracket in the last term of Eq. (2.31) including a prefactor of  $-\hbar^{-2}$  as the 2pNEGF  $G_{lk,jj'}^{(2)}(t, \bar{t}, t'\bar{t}^+)$ , where  $\bar{t}^+$  denotes the limit from above on the contour. The resulting equation determines the dynamics of the one-particle nonequilibrium Green's function with respect to the first time argument  $t$ . Starting in Eq. (2.24) with the time derivative with respect to  $t'$ , we can derive a similar equation for  $\frac{\partial}{\partial t'} G_{ij}^{(1)}(t, t')$ .

Together, these two equations then form the equations of motion for the 1pNEGF, known as the two-time Keldysh-Kadanoff-Baym equations (KBEs)<sup>17</sup> [28]:

$$\begin{aligned} & \left\{ i\hbar \frac{\partial}{\partial t} \delta_{ik} - \langle i | h^{(1)}(t) | k \rangle \right\} G_{kj}^{(1)}(t, t') \\ &= \delta_{\mathcal{C}}(t - t') \delta_{ij} - i\hbar \int_{\mathcal{C}} d\bar{t} \langle ij' | w^{(2)}(t - \bar{t}) | kl \rangle G_{lk,jj'}^{(2)}(t, \bar{t}; t', \bar{t}^+), \\ & G_{ik}^{(1)}(t, t') \left\{ -i\hbar \frac{\partial}{\partial t'} \delta_{kj} - \langle k | h^{(1)}(t') | j \rangle \right\} \\ &= \delta_{\mathcal{C}}(t - t') \delta_{ij} - i\hbar \int_{\mathcal{C}} d\bar{t} G_{li,kj'}^{(2)}(t, \bar{t}; t', \bar{t}^+) \langle kj' | w^{(2)}(t' - \bar{t}) | jl \rangle. \end{aligned} \quad (2.32)$$

A few remarks are in order:

- (i) The KBEs are a set of coupled (non-Markovian<sup>18</sup>) integro-differential equations and are valid for imaginary and real times defined on the round-trip Keldysh contour  $\mathcal{C}$ . Note that the second equation in (2.32) is just the adjoint of the first one with the times interchanged, i.e.,  $t \leftrightarrow t'$ .
- (ii) The boundary (respectively, initial) conditions for the KBEs are given by the Kubo-Martin-Schwinger (KMS) relations formulated as properties (a) and (b) in Eq. (2.22), cf. [57, 81]. If the equilibrium Matsubara Green's function of the system is known, sufficient KMS conditions are expressions (c) and (d) in Eq. (2.22).
- (iii) The KBEs in the form of Eq. (2.32) are not closed, i.e., they do not uniquely define the 1pNEGF without further knowledge. Instead, each KBE requires the 2pNEGF which in turn satisfies the Bethe-Salpeter equation, cf. Refs. [82, 83]. Generally, the equation of motion for  $G^{(n)}$  ( $n \geq 2$ ) requires information about  $G^{(n-1)}$  and  $G^{(n+1)}$ , cf. Refs. [83, 84]. From this point of view, the KBEs represent only the first equations of a complete hierarchy of equations of motion for the NEGFs. This hierarchy is known as the Martin-Schwinger (MS) hierarchy [57].

<sup>17</sup>Summation over  $j, k$  and  $l$  is implied. For bosons, the contour integrals in the KBEs take a prefactor of  $+i\hbar$ .

<sup>18</sup>This means they involve a time integral that reflects memory effects.

- (iv) In the special case of equal time arguments,  $t = t'$ , the MS hierarchy reduces to the BBGKY (Bogolyubov-Born-Green-Kirkwood-Yvon) hierarchy for the reduced density operators, cf., e.g., Ref. [11]. The special case of the dynamics of single-time quantities will be studied in Sect. 4.2.3.

In order to transform the KBEs (2.32) 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's 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 Sect. 2.3.

Formally, we can rewrite the contour integral in the KBEs as a convolution and include all interaction effects into a one-particle self-energy<sup>19</sup> (1pSE)  $\Sigma^{(1)}$ :

$$-i\hbar \int_{\mathcal{C}} d\bar{t} \langle ij' | w^{(2)}(t - \bar{t}) | kl \rangle G_{lk, jj'}^{(2)}(t, \bar{t}; t', \bar{t}^+) = \int_{\mathcal{C}} d\bar{t} \Sigma_{ik}^{(1)}(t, \bar{t}) G_{kj}^{(1)}(\bar{t}, t'), \quad (2.33)$$

$$\Sigma_{ij}^{(1)}(t, t') = \Sigma_{ij}^{(1)}[G^{(1)}, w^{(2)}](t, t').$$

In the course of this, the self-energy becomes a functional of the 1pNEGF and the generalized two-body interaction  $w^{(2)}$ . Often one distinguishes between the regular (“time-diagonal” or “time-local”) part of the self-energy  $\Sigma_{\text{reg}}^{(1)}(t, t') \propto \delta_{\mathcal{C}}(t - t')$  and the irregular part  $\Sigma_{\text{cor}}^{(1)}(t, t')$ . Whereas for the former the KBEs are trivial to solve as they become Markovian (the contour integral vanishes), the latter keeps the non-Markovian structure and accounts for memory effects, i.e., correlations.

Using, e.g., the matrix representation of Eq. (2.18), the KBEs can also be written in form of a Dyson equation (we drop the label “ $2 \times 2$ ” for the Green's functions),

$$\mathbf{G}^{(1)} = \mathbf{G}_0^{(1)} + \mathbf{G}_0^{(1)} \Sigma_{2 \times 2}^{(1)} \mathbf{G}^{(1)}, \quad (2.34)$$

where  $\mathbf{G}_0^{(1)}$  denotes the 1pNEGF of the ideal, non-interacting system. The self-energy matrix  $\Sigma_{2 \times 2}^{(1)}$  has the same components as  $\mathbf{G}^{(1)}$  and  $\mathbf{G}_0^{(1)}$  in Eq. (2.18) and acts as integration kernel. Further, the product in Eq. (2.34) involves by definition the integration over two intermediate time variables. For two functions  $\mathbf{A}$  and  $\mathbf{B}$  in Keldysh space<sup>20</sup>, it is,

$$\{\mathbf{A}\mathbf{B}\}(t, t') = \int_{\mathcal{C}} d\bar{t} \mathbf{A}(t, \bar{t}) \mathbf{B}(\bar{t}, t'). \quad (2.35)$$

To specify the structure of the (collision) integral on the r.h.s. of Eq. (2.33) in terms of components of the 1pSE and the 1pNEGF, one most easily applies the Langreth-Wilkins rules. A tabular summary of these can be found in Table 2.1. The operations indicated by  $\star$  and  $\circ$  are defined by  $(x, y \in \{A, R, >, <, \uparrow, \downarrow\})$ ,

<sup>19</sup>We sum over  $k$ .

<sup>20</sup>I.e., contour-ordered functions  $\mathbf{A}(t, t')$  and  $\mathbf{B}(t, t')$  with  $t, t' \in \mathcal{C}$ .

**Table 2.1** Langreth-Wilkins rules for the multiplication and convolution of two contour-ordered functions **A** and **B**. The result **C** is again a function on the Keldysh space and has the indicated components. The operations denoted by  $\star$  and  $\circ$  are defined by Eqs. (2.36) and (2.37)

	$C(t, t') = A(t, t')B(t', t)$	$C(t, t') = \int_{\mathcal{C}} d\bar{t} A(t, \bar{t})B(\bar{t}, t')$
$C^M$	$A^M B^M$	$A^M \star B^M$
$C^\Gamma$	$A^\Gamma B^\Gamma$	$A^\Gamma \circ B^A + A^M \star B^\Gamma$
$C^\Gamma$	$A^\Gamma B^\Gamma$	$A^R \circ B^\Gamma + A^\Gamma \star B^M$
$C^>$	$A^> B^<$	$A^R \circ B^> + A^> \circ B^A + A^\Gamma \star B^\Gamma$
$C^<$	$A^< B^>$	$A^R \circ B^< + A^< \circ B^A + A^\Gamma \star B^\Gamma$
$C^R$	$A^R B^> + A^> B^A$	$A^R \circ B^R$
$C^A$	$A^A B^< + A^< B^R$	$A^A \circ B^A$

$$\{A^x \circ B^y\}(t, t') = \int_{t_0}^{\infty} d\bar{t} A^x(t, \bar{t})B^y(\bar{t}, t'), \quad (2.36)$$

and,

$$\begin{aligned} \{A^M \star B^M\}(\tau) &= \int_0^\beta d\bar{\tau} A^M(\tau - \bar{\tau})B^M(\bar{\tau}), \\ \{A^M \star B^\Gamma\}(t_0 - i\tau, t) &= \int_0^\beta d\bar{\tau} A^M(\tau - \bar{\tau})B^\Gamma(t_0 - i\bar{\tau}, t), \\ \{A^\Gamma \star B^M\}(t, t_0 - i\tau) &= \int_0^\beta d\bar{\tau} A^\Gamma(t, t_0 - i\bar{\tau})B^M(\bar{\tau} - \tau), \\ \{A^\Gamma \star B^\Gamma\}(t, t') &= -i \int_0^\beta d\bar{\tau} A^\Gamma(t, t_0 - i\bar{\tau})B^\Gamma(t_0 - i\bar{\tau}, t'). \end{aligned} \quad (2.37)$$

### 2.2.2 Equilibrium Limit. Dyson Equation

The KBEs (2.32) are valid for all times  $t$  and  $t'$  on the contour  $\mathcal{C}$ . However, if the Hamiltonian of the system is time independent (note that this is assumed above for times  $t, t' \leq t_0$ ), the only independent matrix component of the Green's function is  $G^{(1),M}$ . As a consequence, the contour reduces to its imaginary track, and the KBEs (2.32) with closure (2.33) simplify to the Dyson equation for the Matsubara Green's function<sup>21</sup>,

<sup>21</sup>Summation over  $k$  is implied.

$$\left\{ i\hbar \frac{\partial}{\partial \tau} \delta_{ik} - \langle i|h^{(1)}|k \rangle \right\} G_{kj}^{(1),M}(\tau) = \delta(\tau) \delta_{ij} + \int_0^\beta d\bar{\tau} \Sigma_{ik}^{(1),M}(\tau - \bar{\tau}) G_{kj}^{(1)}(\bar{\tau}), \quad (2.38)$$

in which we have applied the transformation,

$$\mathcal{X}_{ij}(\tau - \tau') = -i\hbar \mathcal{X}_{ij}(t_0 - i\tau, t_0 - i\tau'), \quad (2.39)$$

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

$$\rho_{1,ij} = G_{ij}^{(1),M}(0^-). \quad (2.40)$$

Further, the antiperiodicity properties (a) and (b) of Eq. (2.22) allow us to restrict the solution of Eq. (2.38) to a half interval, e.g.,  $[-\beta, 0]$  which includes the reduced density matrix at the upper interval boundary<sup>22</sup>.

If we include the regular part of the self-energy,

$$\Sigma_{\text{reg},ij}^{(1),M}(\tau) = \delta(\tau) \Sigma_{0,ij}^{(1),M}, \quad (2.41)$$

in an effectively non-interacting Green's function<sup>23</sup>  $G_0^{(1),M}(\tau)$ , the Dyson equation attains the form (compare with Eq. (2.34)),

$$G_{ij}^{(1),M}(\tau) = G_{0,ij}^{(1),M}(\tau) + \int_0^\beta d\bar{\tau} \int_0^\beta d\bar{\bar{\tau}} \Sigma_{ik}^{(1),K}(\bar{\tau} - \bar{\bar{\tau}}) G_{kj}^{(1),M}(\bar{\bar{\tau}}), \quad (2.42)$$

$$\Sigma_{ij}^{(1),K}(\tau) = \Sigma_{ij}^{(1),M}(\tau) - \Sigma_{\text{reg},ij}^{(1),M}(\tau).$$

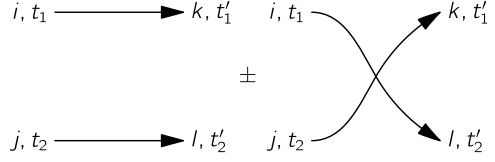
It is important to note that here (aside from  $w^{(2)}$ ) the self-energy  $\Sigma_0^{(1),M}$  is strictly a functional of the effectively non-interacting Green's function, whereas  $\Sigma^{(1),M}(\tau)$  depends on the full Green's function and includes, both, a regular and an irregular part.

If the effectively non-interacting Green's function  $G_0^{(1),M}(\tau)$  is known, Eq. (2.42) can be solved by iteration starting from setting  $G^{(1),M}(\tau) = G_0^{(1),M}(\tau)$  on the r.h.s. Eventually, a self-consistent Matsubara Green's function is reached. Together with transformation (2.39) and properties (c) and (d) of Eq. (2.22), 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 long as no external field is applied and the same “conserving” approximation is used for the self-energy, cf. Sect. 2.3.1.

<sup>22</sup>Sometimes,  $G^{(1),M}(\tau)$  is considered on the symmetric interval  $[-\frac{\beta}{2}, \frac{\beta}{2}]$ , see, e.g., [85].

<sup>23</sup>The corresponding Dyson equation is obtained by replacing the one-particle energy  $\langle i|h^{(1)}|j \rangle$  in Eq. (2.38) by  $\langle i|h^{(1)}|j \rangle + \Sigma_{0,ij}^{(1),M}$  and setting the integration kernel to zero. Sometimes, one refers to  $G_0^{(1),M}$  as the “undressed” (“bare”) Green's function whereas the full Green's function  $G^{(1),M}$  is the “dressed” one.

**Fig. 2.4** Hartree-Fock: the simplest conserving approximation for the two-particle Green's function  $G_{ij,kl}^{(2)}(t_1, t_2; t'_1, t'_2)$ , cf. Eq. (2.43). The sign refers to bosons (+) and fermions (−)



## 2.3 Many-Body Approximations

One of the key problems in solving the Kadanoff-Baym equations (2.32) as well as the Dyson equation (2.38) is the fact that basically exact knowledge of the two-particle Green's function is required due to the presence of the MS hierarchy, cf. Sect. 2.2.1, point (iii). Unfortunately,  $G^{(2)}$  is in general unknown. Therefore, we have to perform a truncation of the hierarchy through a many-body approximation (MBA).

The simplest hierarchy decoupling is achieved in the so-called Hartree-Fock (HF) approximation,

$$G_{ij,kl}^{(2)}(t_1, t_2; t'_1, t'_2) \approx G_{ik}^{(1)}(t_1, t'_1)G_{jl}^{(1)}(t_2, t'_2) + G_{il}^{(1)}(t_1, t'_2)G_{jk}^{(1)}(t_2, t'_1). \quad (2.43)$$

For plasmas, it leads to a quantum mechanical version of the Vlasov equation [83]. In terms of one-particle propagators (representable by arrows) we can illustrate Eq. (2.43) as shown in Fig. 2.4.

Inserting the HF approximation for  $G^{(2)}$  into the first KBE, we obtain (for fermions),

$$\begin{aligned} & \left\{ i\hbar \frac{\partial}{\partial t} \delta_{ik} - \langle i | h^{(1)}(t) | k \rangle \right\} G_{kj}^{(1)}(t, t') \\ &= \delta_{\mathcal{C}}(t - t') \delta_{ij} - i\hbar \int_{\mathcal{C}} d\bar{t} \langle ij' | w^{(2)}(t - \bar{t}) | kl \rangle \{ G_{lj}^{(1)}(t, t') G_{kj'}^{(1)}(\bar{t}, \bar{t}^+) \\ & \quad - G_{il}^{(1)}(t, \bar{t}^+) G_{kj}^{(1)}(t', \bar{t}) \}, \end{aligned} \quad (2.44)$$

where we sum over  $j', k$  and  $l$ . If we express the integral on the r.h.s. in the form of Eq. (2.33) using a 1pSE, we easily verify that,

$$\Sigma_{ij}^{(1),\text{HF}}(t, t') = \Sigma_{ij}^{(1),\text{H}}(t, t') + \Sigma_{ij}^{(1),\text{F}}(t, t'), \quad (2.45)$$

with (retaining the generalized two-body interaction),

$$\begin{aligned} \Sigma_{ij}^{(1),\text{H}}(t, t') &= -i\hbar \delta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \langle ij | w^{(2)}(t - \bar{t}) | kl \rangle G_{kl}^{(1)}(\bar{t}, \bar{t}^+), \\ \Sigma_{ij}^{(1),\text{F}}(t, t') &= i\hbar \langle il | w^{(2)}(t^+ - t') | kj \rangle G_{kl}^{(1)}(t, t'). \end{aligned} \quad (2.46)$$

The first (second) term is the Hartree (Fock) self-energy, whereby the Fock contribution accounts for exchange effects, i.e., for the Pauli exclusion principle in the case of fermions. Moreover, as  $w^{(2)}(t - t')$  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 Eq. (2.43) beyond Hartree-Fock are obtained by vertex corrections, e.g., [86], 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.

### 2.3.1 Requirements for a Conserving Scheme

If we analyze the HF approximation of Eq. (2.43), we realize that the approximate 2pNEGF obeys a specific symmetry: It is invariant under the simultaneous exchange of the first and the second pair of (spatial and temporal) arguments. Also, we find that, when applying the HF approximation to the KBEs (2.32), the system's total energy, particle number and momentum are preserved<sup>24</sup>. 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),

$$\langle \hat{H} \rangle(t) = -i\hbar G_{ij}^{(1)}(t, t^+) \langle j | h^{(1)}(t) | i \rangle - \frac{i\hbar}{2} \int_{\mathcal{C}} d\tilde{t} \Sigma_{ij}^{(1)}(t, \tilde{t}) G_{ji}^{(1)}(\tilde{t}, t^+). \quad (2.47)$$

The equilibrium limit of this is,

$$\langle \hat{H} \rangle = G_{ij}^{(1)\text{M}}(0^-) \langle j | h^{(1)} | i \rangle + \frac{1}{2} \int_0^\beta d\tau \Sigma_{ij}^{(1)\text{M}}(-\tau) G_{ji}^{(1)\text{M}}(\tau). \quad (2.48)$$

In fact, it has been shown by Baym [87] that the symmetry of  $G^{(2)}$  in Eq. (2.43) 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 two KBEs in the form of Eq. (2.32), and
- (ii) the approximation for  $G^{(2)}$  is in line with the symmetry,

$$G_{ij,kl}^{(2)}(t_1, t_2; t_1^+, t_2^+) = G_{ji,lk}^{(2)}(t_2, t_1; t_2^+, t_1^+). \quad (2.49)$$

Conditions (i) and (ii) represent important criteria for the development of self-consistent solutions of the KBEs beyond the HF level. Condition (ii) is simple to verify if the approximate dependence of  $G^{(2)}$  on  $G^{(1)}$  is known. On the other hand, a condition equivalent to (ii) can be formulated for the one-particle self-energy, cf. the discussion on “ $\Phi$ -derivable” approximations in the following subsection.

### 2.3.2 Perturbation Expansions

There exist at least two ways of generating perturbative solutions of the Kadanoff-Baym equations: Either one can apply an iterative procedure using the integral ver-

<sup>24</sup>For an analysis of conservation laws, we refer to Ref. [28].

sion of the equations of motion for  $G^{(1)}$  (Dyson's equation) or one can directly apply self-consistent approximations to the self-energy.

First, we will review the iterative procedure. To this end, we start from taking the functional derivative of the 1pNEGF with respect to the one-particle potential energy  $v^{(1)}(t)$ . Working out the derivative of time-ordered products, cf. Appendix B.1, we can write (omitting spatial and spin degrees of freedom),

$$\frac{\delta G^{(1)}(t, t')}{\delta v^{(1)}(\bar{t})} = G^{(1)}(t, t') G^{(1)}(\bar{t}, \bar{t}^+) - G^{(2)}(t, \bar{t}; t' \bar{t}^+). \quad (2.50)$$

This identity allows us to express the 2pNEGF in the Kadanoff-Baym equations in terms of  $\delta G^{(1)}/\delta v^{(1)}$  [28]. The first equation of motion then reads<sup>25</sup>,

$$\begin{aligned} & \left\{ i\hbar \frac{\partial}{\partial t} - h^{(1)}(t) \right\} G^{(1)}(t, t') \\ &= \delta_{\mathcal{C}}(t - t') - i\hbar \int_{\mathcal{C}} d\bar{t} w^{(2)}(t - \bar{t}) \left\{ G^{(1)}(\bar{t}, \bar{t}^+) - \frac{\delta}{\delta v^{(1)}(\bar{t})} \right\} G^{(1)}(t, t'). \end{aligned} \quad (2.51)$$

Unfortunately, Eq. (2.51) is not suited for a straightforward solution. However, it can be converted into an integral equation using the non-interacting Green's function which obeys,

$$\left\{ i\hbar \frac{\partial}{\partial t} - h^{(1)}(t) \right\} G_0^{(1)}(t, t') = \delta_{\mathcal{C}}(t - t'), \quad (2.52)$$

and has the inverse<sup>26</sup>  $[G_0^{(1)}]^{-1}(t, t') = \delta_{\mathcal{C}}(t - t') \{ i\hbar \frac{\partial}{\partial t'} - h^{(1)}(t') \}$ . Using Eqs. (2.50) and (2.52), we obtain,

$$\begin{aligned} G^{(1)}(t, t') &= G_0^{(1)}(t, t') - i\hbar \int_{\mathcal{C}} d\bar{t} \int_{\mathcal{C}} d\bar{\bar{t}} G^{(1)}(t, \bar{t}) w^{(2)}(\bar{t} - \bar{\bar{t}}) \\ &\quad \times \left\{ G^{(1)}(\bar{\bar{t}}, \bar{\bar{t}}^+) + \frac{\delta}{\delta v^{(1)}(\bar{\bar{t}})} \right\} G^{(1)}(\bar{\bar{t}}, t'), \end{aligned} \quad (2.53)$$

which is a formal solution of Eq. (2.51) and satisfies the KMS conditions.

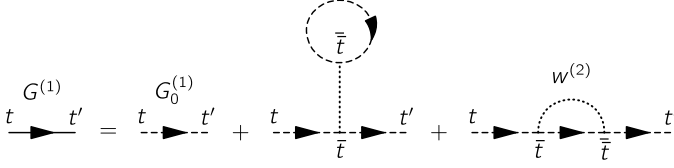
Equation (2.53) is the starting point for expanding the 1pNEGF in a power series regarding the interaction  $w^{(2)}$ . The individual contributions are obtained by iteration. While the zeroth order is just  $G^{(1)} = G_0^{(1)}$ , the first-order expression follows from substituting the non-interacting Green's function on the r.h.s. yielding,

$$\begin{aligned} G^{(1)}(t, t') &= G_0^{(1)}(t, t') - i\hbar \int_{\mathcal{C}} d\bar{t} \int_{\mathcal{C}} d\bar{\bar{t}} G_0^{(1)}(t, \bar{t}) w^{(2)}(\bar{t} - \bar{\bar{t}}) \\ &\quad \times \left\{ G_0^{(1)}(\bar{\bar{t}}, \bar{\bar{t}}^+) + \frac{\delta}{\delta v^{(1)}(\bar{\bar{t}})} \right\} G_0^{(1)}(\bar{\bar{t}}, t'). \end{aligned} \quad (2.54)$$

<sup>25</sup>Note, that  $h^{(1)}(t) = t^{(1)} + v^{(1)}(t)$ .

<sup>26</sup>The inverse Green's function is defined as  $\int_{\mathcal{C}} d\bar{t} [G^{(1)}]^{-1}(t, \bar{t}) G^{(1)}(\bar{t}, t') = \delta_{\mathcal{C}}(t - t')$ .





**Fig. 2.5** Diagrammatic representation of the first-order iteration result of Eq. (2.56) leading to the Hartree-Fock (HF) approximation. The (non-)interacting 1pNEGF is indicated by solid (dashed) arrows. The dotted lines mark the generalized two-body interaction potential  $w^{(2)}$

In contrast to Eq. (2.53), the functional derivative is here simple to evaluate<sup>27</sup>:

$$\frac{\delta G_0^{(1)}(t, t')}{\delta v^{(1)}(\bar{t})} = G_0^{(1)}(t, \bar{t}) G_0^{(1)}(\bar{t}, t'). \quad (2.55)$$

Hence, in the first-order approximation (in  $w^{(2)}$ ), the KBEs obtain the integral form,

$$G^{(1)}(t, t') = G_0^{(1)}(t, t') - i\hbar \int_{\mathcal{C}} d\bar{t} \int_{\mathcal{C}} d\bar{t}^- G_0^{(1)}(t, \bar{t}) w^{(2)}(\bar{t} - \bar{t}^-) \times \{G_0^{(1)}(\bar{t}^-, \bar{t}^+) G_0^{(1)}(\bar{t}, t') - G_0^{(1)}(\bar{t}, \bar{t}^+) G_0^{(1)}(\bar{t}^-, t')\}. \quad (2.56)$$

Comparing the last part of the integrand in Eq. (2.56) to Eq. (2.44), we find that the solution of first order is just the HF approximation expanded to first order in the interaction, cf. Fig. 2.5. Substituting  $G^{(1)}$  for  $G_0^{(1)}$  in the brackets leads to the full HF approximation.

In order to generate higher-order contributions, we reinsert Eq. (2.56) into the initial equation (2.53) and replace the derivative with respect to  $v^{(1)}$  again by Eq. (2.55). Doing so, most of the terms in second order just originate from iterating the Hartree-Fock equation. The additional ones are counted among the lowest-order terms of a many-body approximation beyond Hartree-Fock (the second Born approximation). We note that the exact 1pNEGF follows from accounting for all topologically distinct connected diagrams, for a discussion see, e.g., Ref. [28].

Often, only summations of infinite classes of terms have reasonable convergence properties. Therefore, an expansion of  $G^{(1)}$  in powers of  $w^{(2)}$  and  $G_0^{(1)}$  is not really practical. To overcome this bottleneck, it is a great advantage, that sums of infinite classes are equivalently obtained by expanding the 1pSE in terms of  $w^{(2)}$  and the full, interacting 1pNEGF. Such an approach leads to a self-consistent approximation and, potentially, is conserving (compare with Sect. 2.3.1).

The starting points are the following equations for the 1pSE and the derivative  $\delta G^{(1)}/\delta v^{(1)}$  of Eq. (2.50), which generate higher-order approximations by iterative use<sup>28</sup>:

<sup>27</sup>The result follows from evaluating  $\frac{\delta}{\delta v^{(1)}(\bar{t})} \int_{\mathcal{C}} d\bar{t} [G_0^{(1)}]^{-1}(t, \bar{t}) G_0^{(1)}(\bar{t}, t') = 0$  under the product rule, multiplying by  $G_0^{(1)}$  from the left, integrating over a second time variable and using the definition of the inverse  $[G_0^{(1)}]^{-1}$  as defined below Eq. (2.52).

<sup>28</sup>For the derivations, see Appendix B.2 and Refs. [88, 89].

$$\begin{aligned}\Sigma^{(1)}(t, t') &= i\hbar w^{(2)}(t^+ - t') G^{(1)}(t, t') \\ &\quad - i\hbar \delta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} w^{(2)}(t - \bar{t}) G^{(1)}(\bar{t}, \bar{t}^+) \\ &\quad + i\hbar \int_{\mathcal{C}} d\bar{t} \int_{\mathcal{C}} d\bar{t}' G^{(1)}(t, \bar{t}) w^{(2)}(t^+ - \bar{t}') \frac{\delta \Sigma^{(1)}(\bar{t}, t')}{\delta v^{(1)}(\bar{t})}, \quad (2.57)\end{aligned}$$

$$\begin{aligned}\frac{\delta G^{(1)}(t, t')}{\delta v^{(1)}(\bar{t})} &= G^{(1)}(t, \bar{t}) G^{(1)}(\bar{t}, t') \\ &\quad + \int_{\mathcal{C}} dt_1 \int_{\mathcal{C}} dt_2 G^{(1)}(t, t_1) \frac{\delta \Sigma^{(1)}(t_1, t_2)}{\delta v^{(1)}(\bar{t})} G^{(1)}(t_2, t'). \quad (2.58)\end{aligned}$$

Neglecting the derivative  $\delta \Sigma^{(1)}/\delta v^{(1)}$  on the r.h.s., we arrive again at the HF approximation for the self-energy, i.e., we get  $\Sigma^{(1),\text{HF}}$  which is regular and of first order in the interaction, compare with Eqs. (2.45) and (2.46).

The first iteration of Eq. (2.57) yields [88, 89],

$$\begin{aligned}\Sigma^{(1)}(t, t') &= \Sigma^{(1),\text{HF}} + i\hbar \int_{\mathcal{C}} d\bar{t} \int_{\mathcal{C}} d\bar{t}' G^{(1)}(t, \bar{t}) w^{(2)}(t^+ - \bar{t}') \\ &\quad \times \frac{\delta}{\delta v^{(1)}(\bar{t})} \left\{ \Sigma^{(1),\text{HF}}(\bar{t}, t') \right. \\ &\quad \left. + i\hbar \int_{\mathcal{C}} dt_1 \int_{\mathcal{C}} dt_2 G^{(1)}(\bar{t}, t_1) w^{(2)}(\bar{t}^+ - t_2) \frac{\delta \Sigma^{(1)}(t_1, t')}{\delta v^{(1)}(t_2)} \right\}, \quad (2.59)\end{aligned}$$

where the derivative  $\delta \Sigma^{(1),\text{HF}}/\delta v^{(1)}$  evaluates with Eq. (2.46) and Eq. (2.58) to,

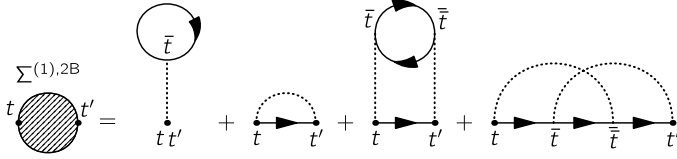
$$\begin{aligned}\frac{\delta \Sigma^{(1),\text{HF}}(\bar{t}, t')}{\delta v^{(1)}(\bar{t})} &= i\hbar \frac{\delta G^{(1)}(\bar{t}, t')}{\delta v^{(1)}(\bar{t})} w^{(2)}(\bar{t}^+ - t') \\ &\quad - i\hbar \int_{\mathcal{C}} dt_1 w^{(2)}(t', t_1) \frac{\delta G^{(1)}(t_1, t_1^+)}{\delta v^{(1)}(\bar{t})} \\ &= i\hbar G^{(1)}(\bar{t}, \bar{t}) G^{(1)}(\bar{t}, t') w^{(2)}(\bar{t}^+ - \bar{t}) \\ &\quad - i\hbar \delta_{\mathcal{C}}(\bar{t} - t') \int_{\mathcal{C}} dt_1 w^{(2)}(t' - t_1) G^{(1)}(t_1, \bar{t}) G^{(1)}(\bar{t}, t_1^+) \\ &\quad + (i\hbar) \times \text{terms} \left\{ w^{(2)}, G^{(1)}, \frac{\delta \Sigma^{(1)}}{\delta v^{(1)}} \right\}. \quad (2.60)\end{aligned}$$

Inserting Eq. (2.59) in Eq. (2.60), we obtain the result,

$$\Sigma^{(1)}(t, t') = \Sigma^{(1),2\text{B}}(t, t') + (i\hbar)^2 \times \text{terms} \left\{ w^{(2)}, G^{(1)}, \frac{\delta \Sigma^{(1)}}{\delta v^{(1)}} \right\},$$

where we have introduced the second Born (2B) self-energy as,

$$\begin{aligned}\Sigma^{(1),2\text{B}}(t, t') - \Sigma^{(1),\text{HF}}(t, t') &= (i\hbar)^2 \int_{\mathcal{C}} d\bar{t} \int_{\mathcal{C}} d\bar{t}' G^{(1)}(t, \bar{t}) w^{(2)}(t^+ - \bar{t}') G^{(1)}(\bar{t}, \bar{t}') G^{(1)}(\bar{t}', t') w^{(2)}(\bar{t}'^+ - t') \\ &\quad - (i\hbar)^2 \int_{\mathcal{C}} d\bar{t} \int_{\mathcal{C}} d\bar{t}' G^{(1)}(t, t') w^{(2)}(t^+ - \bar{t}) w^{(2)}(t' - \bar{t}') G^{(1)}(\bar{t}, \bar{t}) G^{(1)}(\bar{t}, \bar{t}'^+). \quad (2.61)\end{aligned}$$



**Fig. 2.6** Diagrammatic representation of the second Born self-energy  $\Sigma^{(1),2B}(t, t')$  including terms of first and second order in  $w^{(2)}$ . The first two diagrams refer to the Hartree and the Fock (exchange) contribution, cf. Fig. 2.5

The many-body approximation (2.61) is known as the 2B approximation and is the simplest one that accounts for correlations. Diagrammatically, it is shown in Fig. 2.6. In the numerical results presented below, we will restrict ourselves to the 2B approximation. We note for completeness that other familiar, more advanced approximations for the one-particle self-energy such as the GW or T-matrix approximation (TM) include higher-order terms obtained in the subsequent iteration(s).

Concerning the derivation above, the question remains whether the obtained 2B self-energy leads to a conserving scheme, i.e., aside from the HF part which has already been discussed earlier. Interestingly, it turns out that 2B is indeed fully conserving. This is due to the fact that  $\Sigma^{(1),2B}$  can be derived from a generating thermodynamic potential  $\Phi$  [90]. In general, a conserving self-energy is obtained by removing propagator lines in all possible ways in the diagrammatic power series expansion of the Luttinger-Ward functional (LWF)  $\Phi = \ln\langle S_{\mathcal{L}} \rangle$ , i.e., calculating,

$$\Sigma^{(1)}(t, t') = \frac{\delta\Phi[G^{(1)}, w^{(2)}]}{\delta G^{(1)}(t', t)}. \quad (2.62)$$

Here, in the LWF,  $S_{\mathcal{L}}$  means the generalized S-matrix,

$$S_{\mathcal{L}} = \hat{T}_{\mathcal{L}} \exp \left[ -\frac{i}{2\hbar} \int_{\mathcal{L}} dt \int_{\mathcal{L}} dt' w^{(2)}(t - t') \hat{f}^{\dagger}(t) \hat{f}^{\dagger}(t') \hat{f}(t') \hat{f}(t) \right]. \quad (2.63)$$

An approximation derived from Eq. (2.62) is often called “ $\Phi$ -derivable” and fully satisfies the requirements of a conserving approximation given in Sect. 2.3.1. For details and examples on how to perform the diagrammatic expansion of the LWF under the relevant Feynman rules before evaluating  $\delta\Phi/\delta G^{(1)}$ , the reader is referred to Ref. [91]. An explicit formula for  $\Phi$  including prefactors and the topologically distinct diagrams can be found, e.g., in [92].

## 2.4 Quantum Kinetic Equations for Single-Time Quantities

In many practical situations, the presence of the over-time-expanding memory kernel (i.e., the retardation) in the KBEs inhibits a successful two-time propagation of the 1pNEGF or limits it to a certain maximum time. Only for “increasingly smooth”

kernels<sup>29</sup> efficient solvers exist that do not rely *a priori* on massive parallelization, e.g., Ref. [93]. On the other hand, much information about the considered quantum many-body system is already contained in the 1pRDM  $\rho_1(t)$ , which is a single-time quantity. Therefore, it is reasonable to ask the question of whether it is possible to derive quantum kinetic equations which are based solely on one time variable.

Mathematically, this poses the question of how to reconstruct two-time quantities in the KBEs from single-time (or time-diagonal) ones. In this section, we review such a reconstruction scheme based on the early works of Lipavský et al., Ref. [23]. It demonstrates that there indeed exists an exact relation between the two-time correlation functions and the 1pRDM (or phase-space distribution function). As a direct implication, the reconstruction theorem will lead over to the generalized Kadanoff-Baym ansatz (GKBA) which generates the time-diagonal limit of the KBEs though requiring further approximations. Conceptually, the GKBA paves the way for rigorously transforming the KBEs into familiar equations of motion for the Wigner distribution function such as the Boltzmann, Landau or Balescu-Lenard equations, e.g., Ref. [94]. These equations are accurate for slowly varying disturbances and “simple” transport processes. But non-Markovian extensions of these single-time quantum kinetic equations exist as well, see, e.g., [11, 95, 96], and can be derived applying the GKBA.

### 2.4.1 The Reconstruction Problem for the One-Particle Green's Function

The reconstruction scheme for  $G^{(1),\gtrless}(t, t')$  (at  $t \neq t'$ ) as introduced in the original publication (see Ref. [23]) is somewhat subtle, and also reviews of the same authors (see, e.g., Refs. [24–26]) include some nested elaborations. For this reason, we present a detailed derivation below which hopefully will be more clear to the reader. For simplicity, we again drop any indices that refer to spin or spatial degrees of freedom. Also, we focus on the lesser matrix component of the Green's function. The reconstruction of the greater component is carried out in the same manner.

First of all, we define two auxiliary functions,

$$\begin{aligned} G_R^{(1),<}(t, t') &= \theta_{\mathcal{C}}(t - t') G^{(1),<}(t, t'), \\ G_A^{(1),<}(t, t') &= -\theta_{\mathcal{C}}(t' - t) G^{(1),<}(t, t'), \end{aligned} \quad (2.64)$$

which must not be confused with the usual retarded and advanced Green's functions and allow us to recover the full lesser correlation function from  $G^{(1),<}(t, t') = G_R^{(1),<}(t, t') - G_A^{(1),<}(t, t')$ . In particular,  $[G_R^{(1),<}(t, t')]^\dagger = G_A^{(1),<}(t', t)$ . Second, we evaluate the time derivative,

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<sup>29</sup>Evoked by the time dependence of the 1pNEGF and (or) the 1pSE.

$$\begin{aligned}
i\hbar \frac{\partial}{\partial t} G_{\mathbf{R}}^{(1),<}(t, t') &= i\hbar \delta_{\mathcal{C}}(t - t') G^{(1),<}(t, t') \\
&\quad + i\hbar \theta_{\mathcal{C}}(t - t') \frac{\partial}{\partial t} G^{(1),<}(t, t').
\end{aligned} \tag{2.65}$$

Third, we summarize some important relations for the inverse of the retarded, advanced and non-interacting Green's functions (note that the short-hand notation  $AB|_{(t,t')}$  includes the contour integral  $\int_{\mathcal{C}} d\bar{t} A(t, \bar{t}) B(\bar{t}, t')$ ),

$$\begin{aligned}
[G^{(1),\mathbf{R/A}}]^{-1}(t, t') &= [G_0^{(1)}]^{-1}(t, t') - \Sigma^{(1),\mathbf{R/A}}(t, t'), \\
[G_0^{(1)}]^{-1} G_0^{(1),\geq}|_{(t,t')} &= G_0^{(1),\geq} [G_0^{(1)}]^{-1}|_{(t,t')} = 0, \\
[G^{(1),\mathbf{R}}]^{-1} G^{(1),\geq}|_{(t,t')} &= \Sigma^{(1),\geq} G^{(1),\mathbf{A}}|_{(t,t')}.
\end{aligned} \tag{2.66}$$

Our goal is now to express the two-time functions of Eq. (2.64) in terms of the density matrix. We treat both expressions separately (comments on notations and transformations made are given below Eq. (2.67) and Eq. (2.68)):

(i) For  $G_{\mathbf{R}}^{(1),<}$ , we consider,

$$\begin{aligned}
&[G^{(1),\mathbf{R}}]^{-1} G_{\mathbf{R}}^{(1),<}|_{(t,t')} \\
&= \{[G_0^{(1)}]^{-1} - \Sigma^{(1),\mathbf{R}}\} G_{\mathbf{R}}^{(1),<}|_{(t,t')} \\
&\stackrel{(a)}{=} i\hbar \delta_{\mathcal{C}}(t - t') G^{(1),<}(t, t') \\
&\quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(\bar{t} - t') [G_0^{(1)}]^{-1}(t, \bar{t}) G^{(1),<}(\bar{t}, t') \\
&\quad - \Sigma^{(1),\mathbf{R}} G_{\mathbf{R}}^{(1),<}|_{(t,t')} \\
&\stackrel{(b)}{=} i\hbar \delta_{\mathcal{C}}(t - t') G^{(1),<}(t, t') \\
&\quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(\bar{t} - t') [G^{(1),\mathbf{R}}]^{-1}(t, \bar{t}) G^{(1),<}(\bar{t}, t') \\
&\quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(\bar{t} - t') \Sigma^{(1),\mathbf{R}}(t, \bar{t}) G^{(1),<}(\bar{t}, t') \\
&\quad - \Sigma^{(1),\mathbf{R}} G_{\mathbf{R}}^{(1),<}|_{(t,t')} \\
&\stackrel{(c)}{=} i\hbar \delta_{\mathcal{C}}(t - t') G^{(1),<}(t, t') \\
&\quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \Sigma^{(1),<}(t, \bar{t}) G^{(1),\mathbf{A}}(\bar{t}, t') \\
&\quad - \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(t' - \bar{t}) [G^{(1),\mathbf{R}}]^{-1}(t, \bar{t}) G^{(1),<}(\bar{t}, t') \\
&\stackrel{(d)}{=} i\hbar \delta_{\mathcal{C}}(t - t') G^{(1),<}(t, t') \\
&\quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(t' - \bar{t}) \Sigma^{(1),<}(t, \bar{t}) G^{(1),\mathbf{A}}(\bar{t}, t') \\
&\quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(t' - \bar{t}) \Sigma^{(1),\mathbf{R}}(t, \bar{t}) G^{(1),<}(\bar{t}, t').
\end{aligned} \tag{2.67}$$

The transformations carried out in Eq. (2.67) are as follows:

- (a) This equality is obtained by using the definition of the inverse Green's function  $[G_0^{(1)}]^{-1}(t, t') = \delta_{\mathcal{C}}(t - t')\{i\hbar \frac{\partial}{\partial t'} - h^{(1)}(t')\}$  together with Eq. (2.65).
- (b) Here, we reinsert the expression for  $[G_0^{(1)}]^{-1}$  in terms of the retarded Green's function and the retarded self-energy (first line of Eq. (2.66)). By definition, the last two terms involving  $\Sigma^{(1),R}$  on the r.h.s. are equal and cancel.
- (c) Use the third identity in Eq. (2.66). The last term with negative sign corrects for the presence of the step function.
- (d) This is the result of again writing out the inverse  $[G^{(1),R}]^{-1}$  and noting that  $\int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(t' - \bar{t})[G_0^{(1)}]^{-1}(t, \bar{t})G^{(1),<}(\bar{t}, t')$  evaluates to zero (cf. Eq. (2.66)). The inclusion of the step function into the second line is consistent with the definition of the advanced Green's function, see Eq. (2.19).

(ii) For  $G_A^{(1),<}$ , we consider,

$$\begin{aligned}
 & G_A^{(1),<} [G^{(1),A}]^{-1} \Big|_{(t,t')} \\
 & \stackrel{(*)}{=} \{ [G_0^{(1)}]^{-1} - \Sigma^{(1),A} \}^\dagger [G_A^{(1),<}]^\dagger \Big|_{(t',t)} \\
 & \stackrel{(a)}{=} i\hbar \delta_{\mathcal{C}}(t' - t) G^{(1),<}(t, t') \\
 & \quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(\bar{t} - t) [G_0^{(1)}]^{-1}(t', \bar{t}) G^{(1),<}(\bar{t}, t) \Big|^\dagger \\
 & \quad - \Sigma^{(1),R} G_R^{(1),<} \Big|_{(t,t')}^\dagger \\
 & \stackrel{(b)}{=} i\hbar \delta_{\mathcal{C}}(t' - t) G^{(1),<}(t, t') \\
 & \quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(\bar{t} - t) [G^{(1),R}]^{-1}(t', \bar{t}) G^{(1),<}(\bar{t}, t) \Big|^\dagger \\
 & \quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(\bar{t} - t) \Sigma^{(1),R}(t', \bar{t}) G^{(1),<}(\bar{t}, t) \Big|^\dagger \\
 & \quad - \Sigma^{(1),R} G_R^{(1),<} \Big|_{(t,t')}^\dagger \\
 & \stackrel{(c)}{=} i\hbar \delta_{\mathcal{C}}(t' - t) G^{(1),<}(t, t') \\
 & \quad + \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \Sigma^{(1),<}(t', \bar{t}) G^{(1),A}(\bar{t}, t) \Big|^\dagger \\
 & \quad - \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(t - \bar{t}) [G^{(1),R}]^{-1}(t', \bar{t}) G^{(1),<}(\bar{t}, t) \Big|^\dagger \\
 & \stackrel{(d)}{=} i\hbar \delta_{\mathcal{C}}(t' - t) G^{(1),<}(t, t') \\
 & \quad - \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(t - \bar{t}) G^{(1),R}(t, \bar{t}) \Sigma^{(1),<}(\bar{t}, t') \\
 & \quad - \theta_{\mathcal{C}}(t - t') \int_{\mathcal{C}} d\bar{t} \theta_{\mathcal{C}}(t - \bar{t}) G^{(1),<}(t, \bar{t}) \Sigma^{(1),A}(\bar{t}, t'). \tag{2.68}
 \end{aligned}$$

Comments on the transformations:

- (\*) Here, the notation  $AB|_{(t',t)}$  is to be understood as  $\int_{\mathcal{C}} d\bar{t} A(\bar{t}, t') B(t, \bar{t})$ , and  $AB|_{(t',t)}^\dagger$  denotes  $\int_{\mathcal{C}} d\bar{t} B^\dagger(t', \bar{t}) A^\dagger(\bar{t}, t)$ .
- (a) We use that the adjoint of  $[G_0^{(1)}]^{-1}(t, t')$  is given by  $[G_0^{(1)}]^{-1}(t', t)$  and apply Eqs. (2.64) and (2.65). Note, that  $[\Sigma^{(1),A}(t, t')]^\dagger = \Sigma^{(1),R}(t', t)$ .
- (b) As in (i), we substitute the expression for the inverse of the non-interacting Green's function. Again, the last two terms on the r.h.s. cancel.
- (c), (d) These equalities follow in the same way as points (c) and (d) in Eq. (2.67).

Equations (2.67) and (2.68) almost complete the reconstruction. As the final step, we multiply Eq. (2.67) from the left by  $G^{(1),R}$  and Eq. (2.68) from the right by  $G^{(1),A}$ , integrate over another intermediate time coordinate and identify the 1pRDM  $\rho_1(t) = -i\hbar G^{(1),<}(t, t)$ . We finally obtain,

$$\begin{aligned}
 G^{(1),<}(t, t') &= -G^{(1),R}(t, t') \rho_1(t') \\
 &+ \int_{t'}^t d\bar{t} \int_{t_0}^{t'} d\bar{\bar{t}} G^{(1),R}(t, \bar{t}) \Sigma^{(1),<}(\bar{t}, \bar{\bar{t}}) G^{(1),A}(\bar{\bar{t}}, t') \\
 &+ \int_{t'}^t d\bar{t} \int_{t_0}^{t'} d\bar{\bar{t}} G^{(1),R}(t, \bar{t}) \Sigma^{(1),R}(\bar{t}, \bar{\bar{t}}) G^{(1),<}(\bar{\bar{t}}, t') \\
 &+ \rho_1(t) G^{(1),A}(t, t') \\
 &+ \int_{t'}^t d\bar{t} \int_{t_0}^{t'} d\bar{\bar{t}} G^{(1),R}(t, \bar{t}) \Sigma^{(1),<}(\bar{t}, \bar{\bar{t}}) G^{(1),A}(\bar{\bar{t}}, t') \\
 &+ \int_{t'}^t d\bar{t} \int_{t_0}^{t'} d\bar{\bar{t}} G^{(1),<}(t, \bar{t}) \Sigma^{(1),A}(\bar{t}, \bar{\bar{t}}) G^{(1),A}(\bar{\bar{t}}, t'). \quad (2.69)
 \end{aligned}$$

A very similar equation is valid for the greater component of the 1pNEGF. The only difference is that we cannot identify the 1pRDM in the non-integral terms (compare with Eq. (2.70)).

### 2.4.2 The Generalized Kadanoff-Baym Ansatz

The reconstruction (2.69) is exact as long as the exact advanced and retarded propagators are used. However, it has still the form of an integral equation the iterative solution of which is complicated. A simple approximation is to retain only the non-integral terms. This procedure is known as the generalized Kadanoff-Baym ansatz<sup>30</sup> (GKBA) [23]:

<sup>30</sup>Sometimes, it is also called Lipavský ansatz, e.g., [11].

$$\begin{aligned}
G^{(1),\gtrless}(t, t') &= -G^{(1),\text{R}}(t, t')\rho_1^{\gtrless}(t') + \rho_1^{\gtrless}(t)G^{(1),\text{A}}(t, t') \\
&= \frac{i}{\hbar} A(t, t') \{ \theta_{\mathcal{C}}(t - t') \rho^{\gtrless}(t') + \theta_{\mathcal{C}}(t' - t) \rho^{\gtrless}(t) \}, \quad (2.70)
\end{aligned}$$

where,

$$\rho_1^{\gtrless}(t) = -i\hbar G^{(1),\gtrless}(t, t), \quad (2.71)$$

and  $A(t, t')$  denotes the spectral function of Eq. (2.17) [69]. In the limit of equal times, the GKBA is an identity for the lesser and greater correlation function<sup>31</sup>, which automatically implies particle number conservation. For other times  $t$  and  $t'$ , the correlation functions explicitly depend on the retarded and advanced propagators. These have to be specified when making practical use of the ansatz as they are again functions of two time variables and, hence, cannot be treated on the same approximation level of MBPT.

In contrast to the common (or original) Kadanoff-Baym ansatz, e.g., [24], where one postulates,

$$G^{(1),<}(t, t') = f\left(\frac{t + t'}{2}\right) \{ G^{(1),\text{A}}(t, t') - G^{(1),\text{R}}(t, t') \}, \quad (2.72)$$

with  $f$  being the Wigner (distribution) function [28], Eq. (2.70) maintains a causal time structure. It is this causal structure of the GKBA which ensures the conservation of total energy, momentum and density whenever a conserving approximation is used for the self-energy and which allows for applications beyond the quasi-particle picture. Moreover, the GKBA is better suited for dealing with temporally and (or) spatially fast varying perturbations than Eq. (2.72). Details on the implementation of the GKBA, particularly when treating the retarded and advanced propagators on the HF level, are compiled in Sect. 4.2.3.

Applications of the GKBA to spatially homogeneous systems can be found in various fields and include the numerical treatment of ultrafast carrier relaxation in the dense electron gas and (laser) plasmas [63, 97, 98], the study of quantum transport phenomena [61, 99] and quantum diffusion [100]. In this respect, it is often used to connect different time scales studying the crossover from the transient regime to the long-time behavior [101]. Tests of the GKBA against full two-time calculations have been performed in Refs. [97, 102, 103]. In the presence of phonons and laser excitations, the GKBA has been applied to semiconductor electron-hole plasmas in Refs. [104, 105], and to dynamical screening effects of carrier-phonon and carrier-carrier interactions in [106]. For extensions to electrons in quantum dots and wells, see Refs. [107–110]. In addition, the GKBA is discussed in the context of (improved) non-Lorentzian spectral functions [69], and a gauge-invariant formulation of the GKBA can be found in [98] and is used in Refs. [111, 112] for dynamical screening and harmonics generation in dense laser plasmas. An extension of the GKBA to spatially inhomogeneous finite systems has been presented in Ref. [113] and will be discussed in more detail in Sect. 4.2.3.

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<sup>31</sup>This is easily verified as the integral in Eq. (2.69) vanishes in that case.



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