Chapter 7
Nonequilibrium Green Functions

The Nonequilibrium Green Function (NGF) method is the most promising approach to describe quantum transport at nanoscale. The current through a nanosystem (as well as other observables) can be expressed with the help of NGFs. Before going to the explicit formulation of the method for transport through nanosystems, we discuss in this chapter the general properties of nonequilibrium Green functions and formulate the main equations.

First, in Sect. 7.1 we give the definitions of retarded, advanced, lesser, and greater Green functions and consider some simple examples, in particular the noninteracting case. We introduce Green functions of three different types: for fermions (electrons), for bosons and the special type for vibrons.

Then we include interactions and introduce the *interaction representation* in Sect. 7.2—the first important step to the diagrammatic approach. In Sect. 7.3 we discuss an important concept of the *Schwinger-Keldysh closed-time contour*, define the so-called *contour Green functions* and establish the relations between these functions and the real-time Green functions.

The rest of the chapter is devoted to the equations for NGFs within two approaches: *Equation of Motion method* (EOM) in Sect. 7.4 and the *Kadanoff-Baym-Keldysh method* in Sect. 7.5. We derive the expressions of the diagrammatic technique and come to the self-consistent equations in the integral and differential form.

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7.1 Definition and Properties

7.1.1 Retarded (G^R) and Advanced (G^A) Functions

Definition

The retarded Green function for fermions is defined as[1]

$$G^R_{\alpha\beta}(t_1,t_2) = -i\theta(t_1-t_2)\left\langle\left[c_\alpha(t_1), c^\dagger_\beta(t_2)\right]_+\right\rangle, \tag{7.1}$$

where $c^\dagger_\alpha(t)$, $c_\alpha(t)$ are creation and annihilation time-dependent (Heisenberg) operators, $[c,d]_+ = cd + dc$ is the anti-commutator, and $\langle\ldots\rangle$ denotes averaging over the initial equilibrium state.

We use notations α, β, ... to denote single-particle quantum states, the other possible notation is more convenient for bulk systems

$$G^R(x_1,x_2) = -i\theta(t_1-t_2)\left\langle[c(x_1), c^\dagger(x_2)]_+\right\rangle, \tag{7.2}$$

where $x \equiv \boldsymbol{r}, t, \sigma, \ldots$ or $x \equiv \boldsymbol{k}, t, \sigma, \ldots$, etc. Some other types of notations can be found in the literature, they are equivalent.

The advanced function for fermions is defined as

$$G^A_{\alpha\beta}(t_1,t_2) = i\theta(t_2-t_1)\left\langle\left[c_\alpha(t_1), c^\dagger_\beta(t_2)\right]_+\right\rangle. \tag{7.3}$$

Finally, retarded and advanced functions for *bosons* can be defined as

$$B^R_{\alpha\beta}(t_1,t_2) = -i\theta(t_1-t_2)\left\langle\left[a_\alpha(t_1), a^\dagger_\beta(t_2)\right]_-\right\rangle, \tag{7.4}$$

$$B^A_{\alpha\beta}(t_1,t_2) = i\theta(t_2-t_1)\left\langle\left[a_\alpha(t_1), a^\dagger_\beta(t_2)\right]_-\right\rangle, \tag{7.5}$$

where $a^\dagger_\alpha(t)$, $a_\alpha(t)$ are creation and annihilation boson operators, $[a,b]_- = ab - ba$ is the commutator.

Averaging

The average value of any operator $\hat{O}$ can be written as $\langle\hat{O}\rangle = \langle t|\hat{O}^S|t\rangle$ in the Schrödinger representation or $\langle\hat{O}\rangle = \langle 0|\hat{O}^H(t)|0\rangle$ in the Heisenberg representation, where $|0\rangle$ is some initial state. This initial state is in principle arbitrary, but in

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[1] There are many equivalent notations used in the literature, some of them are $G_{\alpha\beta}(t_1,t_2)$, $G_{n\sigma,m\sigma'}(t_1,t_2)$, $G(x,t,x',t')$, $G(x_1,x_2)$, $G(1,2)$, $\boldsymbol{G}\ldots$ We use different notations depending on the representation.

many-particle problems it is convenient to take this state as an equilibrium state, consequently without time-dependent perturbations we obtain usual equilibrium Green functions.

In accordance with this definition the Heisenberg operators $c_\alpha(t)$, $c^\dagger_\beta(t)$, etc. are equal to the time-independent Schrödinger operators at some initial time t_0: $c_\alpha(t_0) = c_\alpha$, etc. Density matrix of the system is assumed to be equilibrium at this time $\hat{\rho}(t_0) = \hat{\rho}_{eq}$. Usually we can take $t_0 = 0$ for simplicity, but if we want to use $t_0 \neq 0$ the transformation to the Heisenberg operators should be written as

$$\hat{f}^H(t) = e^{i\hat{H}(t-t_0)}\hat{f}^S e^{-i\hat{H}(t-t_0)}. \tag{7.6}$$

In fact, the initial conditions are not important because of dissipation (the memory about the initial state is completely lost after the relaxation time). However, in some pathological cases, for example for free noninteracting particles, the initial state determines the state at all times. Note also, that the initial conditions can be more conveniently formulated for Green functions itself, instead of corresponding initial conditions for operators or wave functions.

Nevertheless, thermal averaging is widely used and we define it here explicitly. If we introduce the basis of exact time-independent many-particle states $|n\rangle$ with energies E_n, the averaging over equilibrium states can be written as

$$\langle \hat{O} \rangle = \frac{1}{Z}\sum_n e^{-E_n/T}\left\langle n \left| \hat{O}^H(t) \right| n \right\rangle, \quad Z = \sum_n e^{-E_n/T}. \tag{7.7}$$

In the following when we use notations like $\left\langle \hat{O} \right\rangle$ or $\left\langle \Psi \left| \hat{O}(t) \right| \Psi \right\rangle$, we assume the averaging with the density matrix (density operator) $\hat{\rho}$

$$\left\langle \hat{O} \right\rangle = Sp\left(\hat{\rho}\hat{O}\right), \tag{7.8}$$

for equilibrium density matrix and Heisenberg operators it is equivalent to (7.7).

Time-Independent Case and Mixed Representation

Nonequilibrium Green functions are originally defined as the two-time functions $G(t_1, t_2)$. This complication is the price we pay for a possibility to consider time-dependent and moreover time-nonlocal phenomena with retarded interactions, memory, etc. In the stationary case without time-dependent external fields the Green functions depend only on time differences $G(t_1 - t_2) = G(\tau)$. In this case it is convenient to introduce the Fourier transform $G(\epsilon)$. We define it in the same way as before by the expression (3.19) for the retarded function:

$$G^R(\epsilon) = \lim_{\eta\to 0^+}\int_{-\infty}^{\infty} G^R(\tau)e^{i(\epsilon+i\eta)\tau/\hbar}d\tau, \tag{7.9}$$

and for the advanced one:

$$G^A(\epsilon) = \lim_{\eta \to 0^+} \int_{-\infty}^{\infty} G^A(\tau) e^{i(\epsilon - i\eta)\tau/\hbar} d\tau. \tag{7.10}$$

More generally, transformation (7.9) can be considered as the Laplace transformation with complex argument $z = \epsilon + i\eta$.

For slowly varying time processes the mixed representation (also called Wigner) $G(t, \epsilon)$ can be used with the same Fourier transform in time difference and the time $t = (t_1 + t_2)/2$.

Spectral Function

Finally, we introduce the important combination of retarded and advanced functions known as *spectral* or *spectral weight* function[2]

$$A_{\alpha\beta}(\epsilon) = i \left(G^R_{\alpha\beta}(\epsilon) - G^A_{\alpha\beta}(\epsilon) \right), \tag{7.11}$$

in equilibrium case the Fourie-transformed retarded and advanced functions are complex conjugate $G^A(\epsilon) = \left(G^R(\epsilon)\right)^*$, and $A_{\alpha\beta}(\epsilon) = -2\text{Im}G^R_{\alpha\beta}(\epsilon)$.

For free fermions the spectral function is[3]

$$A_{\alpha\beta}(\epsilon) = -2\text{Im}\left(\frac{\delta_{\alpha\beta}}{\epsilon - \epsilon_\alpha + i\eta} \right) = 2\pi\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}. \tag{7.12}$$

The result is transparent—the function $A_{\alpha\beta}(\epsilon)$ is nonzero only at particle eigenenergies, such that

$$\rho(\epsilon) = \frac{1}{2\pi}\text{Sp}A_{\alpha\beta}(\epsilon) = \frac{1}{2\pi}\sum_\alpha A_{\alpha\alpha}(\epsilon) = \sum_\alpha \delta(\epsilon - \epsilon_\alpha) \tag{7.13}$$

is the usual energy density of states. Note that the imaginary part $i\eta$ is necessary to obtain this result, thus it is not only a mathematical trick, but reflects the physical sense of the retarded Green function.

If we introduce the finite relaxation time τ, the Green function of free particles becomes

$$G^R_{\alpha\beta}(\tau) = -i\theta(\tau)e^{-i\epsilon_\alpha\tau - \gamma\tau}\delta_{\alpha\beta}, \tag{7.14}$$

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[2] We already introduced the spectral function in Chap. 3, as well as some other functions, but repeat it here to keep consistency.

[3] We derive it later, see the Green function (7.52) for free fermions.

then the spectral function has the familiar Lorentzian form

$$A_{\alpha\beta}(\epsilon) = \frac{2\gamma\delta_{\alpha\beta}}{(\epsilon - \epsilon_\alpha)^2 + \gamma^2}. \tag{7.15}$$

Finally, spectral function has a special property, so-called *sum rule*, namely

$$\int_{-\infty}^{\infty} A_{\alpha\beta}(\epsilon)\frac{d\epsilon}{2\pi} = \delta_{\alpha\beta}. \tag{7.16}$$

7.1.2 Lesser ($G^<$) and Greater ($G^>$) Functions

Definition

Retarded and advanced functions, described before, determine the single-particle properties of the system, such as quasiparticle energy, broadening of the levels (lifetime), and density of states. These functions can be modified in nonequilibrium state, but most important *kinetic* properties, such as distribution function, charge, and current, are determined by the lesser Green function

$$G^<_{\alpha\beta}(t_1, t_2) = i\left\langle c^\dagger_\beta(t_2)c_\alpha(t_1)\right\rangle. \tag{7.17}$$

Indeed, the density matrix is the same as the equal-time lesser function

$$\rho_{\alpha\beta}(t) = \left\langle c^\dagger_\beta(t)c_\alpha(t)\right\rangle = -iG^<_{\alpha\beta}(t,t). \tag{7.18}$$

The number of particles in state $|\alpha\rangle$ (distribution function) is

$$n_\alpha(t) = \left\langle c^\dagger_\alpha(t)c_\alpha(t)\right\rangle = -iG^<_{\alpha\alpha}(t,t), \tag{7.19}$$

the tunneling current is

$$\begin{aligned} J(t) &= \frac{ie}{\hbar}\sum_{kq}\left[V_{qk}\left\langle c^\dagger_q(t)c_k(t)\right\rangle - V^*_{qk}\left\langle c^\dagger_k(t)c_q(t)\right\rangle\right] \\ &= \frac{2e}{\hbar}\mathrm{Re}\left(\sum_{kq} V_{qk}G^<_{kq}(t,t)\right). \end{aligned} \tag{7.20}$$

In addition to the lesser, the other (greater) function is used

$$G^>_{\alpha\beta}(t_1, t_2) = -i\left\langle c_\alpha(t_1)c^\dagger_\beta(t_2)\right\rangle. \tag{7.21}$$

For bosons, the lesser and greater functions are defined as

$$B^{<}_{\alpha\beta}(t_1, t_2) = -i\left\langle a^{\dagger}_{\beta}(t_2)a_{\alpha}(t_1)\right\rangle, \tag{7.22}$$

$$B^{>}_{\alpha\beta}(t_1, t_2) = -i\left\langle a_{\alpha}(t_1)a^{\dagger}_{\beta}(t_2)\right\rangle. \tag{7.23}$$

The name "lesser" originates from the time-ordered Green function, the main function in equilibrium theory, which can be calculated by the diagrammatic technique

$$G_{\alpha\beta}(t_1, t_2) = -i\left\langle T\left(c_{\alpha}(t_1)c^{\dagger}_{\beta}(t_2)\right)\right\rangle, \tag{7.24}$$

$$G_{\alpha\beta}(t_1, t_2) = \begin{cases} -i\left\langle c_{\alpha}(t_1)c^{\dagger}_{\beta}(t_2)\right\rangle \text{ if } t_1 > t_2 \Rightarrow & G_{\alpha\beta} \equiv G^{>}_{\alpha\beta}, \\ i\left\langle c^{\dagger}_{\beta}(t_2)c_{\alpha}(t_1)\right\rangle \quad \text{ if } t_1 < t_2 \Rightarrow & G_{\alpha\beta} \equiv G^{<}_{\alpha\beta}, \end{cases} \tag{7.25}$$

here the additional sing minus appears for interchanging of fermionic creation-annihilation operators. Lesser means that $t_1 < t_2$.

7.1.3 Some Useful Relations

From the definitions it is clear that the retarded and advanced functions can be combined from lesser and greater functions

$$G^{R}_{\alpha\beta}(t_1, t_2) = \theta(t_1 - t_2)\left[G^{>}_{\alpha\beta}(t_1, t_2) - G^{<}_{\alpha\beta}(t_1, t_2)\right], \tag{7.26}$$

$$G^{A}_{\alpha\beta}(t_1, t_2) = \theta(t_2 - t_1)\left[G^{<}_{\alpha\beta}(t_1, t_2) - G^{>}_{\alpha\beta}(t_1, t_2)\right]. \tag{7.27}$$

The other useful relation is

$$G^{R}_{\alpha\beta}(t_1, t_2) - G^{A}_{\alpha\beta}(t_1, t_2) = G^{>}_{\alpha\beta}(t_1, t_2) - G^{<}_{\alpha\beta}(t_1, t_2), \tag{7.28}$$

and the symmetry relations

$$G^{<}_{\alpha\beta}(t_1, t_2) = -\left[G^{<}_{\beta\alpha}(t_2, t_1)\right]^{*}, \tag{7.29}$$

$$G^{>}_{\alpha\beta}(t_1, t_2) = -\left[G^{>}_{\beta\alpha}(t_2, t_1)\right]^{*}, \tag{7.30}$$

$$G^{A}_{\alpha\beta}(t_1, t_2) = \left[G^{R}_{\beta\alpha}(t_2, t_1)\right]^{*}. \tag{7.31}$$

The same relations hold in the mixed (Wigner) representation

$$G^<_{\alpha\beta}(t,\epsilon) = -\left[G^<_{\beta\alpha}(t,\epsilon)\right]^*, \tag{7.32}$$

$$G^>_{\alpha\beta}(t,\epsilon) = -\left[G^>_{\beta\alpha}(t,\epsilon)\right]^*, \tag{7.33}$$

$$G^A_{\alpha\beta}(t,\epsilon) = \left[G^R_{\beta\alpha}(t,\epsilon)\right]^*. \tag{7.34}$$

It can be written in the matrix representation using Hermitian conjugation †

$$\mathbf{G}^<(t,\epsilon) = -\mathbf{G}^{<\dagger}(t,\epsilon), \tag{7.35}$$

$$\mathbf{G}^>(t,\epsilon) = -\mathbf{G}^{>\dagger}(t,\epsilon), \tag{7.36}$$

$$\mathbf{G}^A(t,\epsilon) = \mathbf{G}^{R\dagger}(t,\epsilon). \tag{7.37}$$

Obviously, these relations are true also in the time-independent case.

7.1.4 Equilibrium Case. Fluctuation-Dissipation Theorem

Now we want to consider some general properties of interacting systems. In equilibrium the lesser function is not independent and is simply related to the spectral function by the relation

$$G^<_{\alpha\beta}(\epsilon) = iA_{\alpha\beta}(\epsilon)f^0(\epsilon). \tag{7.38}$$

This relation is important because it establishes an equilibrium initial condition for the nonequilibrium lesser function, and proposes a useful Ansatz if the equilibrium distribution function $f^0(\epsilon)$ is replaced by some unknown nonequilibrium function.

Here we prove this relation using the *Lehmann representation*—quite useful method in the theory of Green functions. The idea of the method is to use the exact many-particle eigenstates $|n\rangle$, even if they are not explicitly known.

Consider first the greater function. Using states $|n\rangle$ we represent this function as

$$\begin{aligned} G^>_{\alpha\beta}(t_1,t_2) &= -i\left\langle c_\alpha(t_1)c^\dagger_\beta(t_2)\right\rangle = -\frac{i}{Z}\sum_n\left\langle n\left|e^{-\hat{H}/T}c_\alpha(t_1)c^\dagger_\beta(t_2)\right|n\right\rangle \\ &= -\frac{i}{Z}\sum_{nm}e^{-E_n/T}\langle n|c_\alpha|m\rangle\langle m|c^\dagger_\beta|n\rangle e^{i(E_n-E_m)(t_1-t_2)}. \end{aligned} \tag{7.39}$$

In Fourier representation

$$G^>_{\alpha\beta}(\epsilon) = -\frac{2\pi i}{Z}\sum_{nm}e^{-E_n/T}\langle n|c_\alpha|m\rangle\langle m|c^\dagger_\beta|n\rangle\delta(E_n-E_m+\epsilon). \tag{7.40}$$

Similarly, for the lesser function we find

$$G^{<}_{\alpha\beta}(\epsilon) = \frac{2\pi i}{Z}\sum_{nm} e^{-E_m/T}\langle n|c^{\dagger}_{\beta}|m\rangle\langle m|c_{\alpha}|n\rangle\delta(E_m - E_n + \epsilon). \tag{7.41}$$

Now we can use these expressions to obtain some general properties of Green functions without explicit calculation of the matrix elements. By exchanging indices n and m in the expression (7.41) and taking into account that $E_m = E_n - \epsilon$ because of the delta-function, we see that

$$G^{>}_{\alpha\beta}(\epsilon) = -e^{-\epsilon/T}G^{<}_{\alpha\beta}(\epsilon). \tag{7.42}$$

From this expression and relation (7.26), which can be written as

$$A_{\alpha\beta}(\epsilon) = i\left[G^{>}_{\alpha\beta}(\epsilon) - G^{<}_{\alpha\beta}(\epsilon)\right] \tag{7.43}$$

we derive (7.38).

7.1.5 Free Fermions

Free-Particle Retarded Function for Fermions

Now consider the simplest possible example—the retarded Green function for free particles (fermions).

The free-particle Hamiltonian has an equivalent form if one uses Schrödinger or Heisenberg operators

$$\hat{H} = \sum_{\alpha}\epsilon_{\alpha}c^{\dagger}_{\alpha}c_{\alpha} = \sum_{\alpha}\epsilon_{\alpha}c^{\dagger}_{\alpha}(t)c_{\alpha}(t), \tag{7.44}$$

because (here we assume $t_0 = 0$)

$$c^{\dagger}_{\alpha}(t)c_{\alpha}(t) = e^{i\hat{H}t}c^{\dagger}_{\alpha}e^{-i\hat{H}t}e^{i\hat{H}t}c_{\alpha}e^{-i\hat{H}t} = e^{i\hat{H}t}c^{\dagger}_{\alpha}c_{\alpha}e^{-i\hat{H}t} = c^{\dagger}_{\alpha}c_{\alpha}, \tag{7.45}$$

where we used that $c^{\dagger}_{\alpha}c_{\alpha}$ is commutative with the Hamiltonian $\hat{H} = \sum_{\alpha}\epsilon_{\alpha}c^{\dagger}_{\alpha}c_{\alpha}$.

From the definitions (7.1) and (7.7) it follows that:

$$\begin{aligned}
&\left\langle\left[c_{\alpha}(t_1), c^{\dagger}_{\beta}(t_2)\right]_{+}\right\rangle = \left\langle c_{\alpha}(t_1)c^{\dagger}_{\beta}(t_2) + c^{\dagger}_{\beta}(t_2)c_{\alpha}(t_1)\right\rangle \\
&= \left\langle e^{i\hat{H}t_1}c_{\alpha}(t_1)e^{-i\hat{H}t_1}e^{i\hat{H}t_2}c^{\dagger}_{\beta}(t_2)e^{-i\hat{H}t_2} + e^{i\hat{H}t_2}c^{\dagger}_{\beta}(t_2)e^{-i\hat{H}t_2}e^{i\hat{H}t_1}c_{\alpha}(t_1)e^{-i\hat{H}t_1}\right\rangle \\
&= e^{i\epsilon_{\beta}t_2 - i\epsilon_{\alpha}t_1}\left\langle c_{\alpha}c^{\dagger}_{\beta} + c^{\dagger}_{\beta}c_{\alpha}\right\rangle = e^{-i\epsilon_{\alpha}(t_1-t_2)}\delta_{\alpha\beta},
\end{aligned} \tag{7.46}$$

$$\begin{aligned} G^R_{\alpha\beta}(t_1,t_2) &= -i\theta(t_1-t_2)\left\langle\left[c_\alpha(t_1), c^\dagger_\beta(t_2)\right]_+\right\rangle \\ &= -i\theta(t_1-t_2)e^{-i\epsilon_\alpha(t_1-t_2)}\delta_{\alpha\beta}, \end{aligned} \tag{7.47}$$

where we used some obvious properties of the creation and annihilation operators and commutation relations.

We consider also the other method, based on the equations of motion for operators. From the Liouville–von Neuman equation we find (all c-operators are Heisenberg operators in the formula below, the time dependence (t) is omitted for shortness)

$$\begin{aligned} i\frac{dc_\alpha(t)}{dt} &= [c_\alpha(t), H]_- = \sum_\beta \epsilon_\beta\left[c_\alpha, c^\dagger_\beta c_\beta\right]_- \\ &= \sum_\beta \epsilon_\beta\left(c_\alpha c^\dagger_\beta c_\beta - c^\dagger_\beta c_\beta c_\alpha\right) = \sum_\beta \epsilon_\beta\left(c_\alpha c^\dagger_\beta c_\beta + c^\dagger_\beta c_\alpha c_\beta\right) \\ &= \sum_\beta \epsilon_\beta\left(c_\alpha c^\dagger_\beta + c^\dagger_\beta c_\alpha\right)c_\beta = \sum_\beta \epsilon_\beta\delta_{\alpha\beta}c_\beta = \epsilon_\alpha c_\alpha(t), \end{aligned} \tag{7.48}$$

so that Heisenberg operators for free fermions are

$$c_\alpha(t) = e^{-i\epsilon_\alpha t}c_\alpha(0), \quad c^\dagger_\alpha(t) = e^{i\epsilon_\alpha t}c^\dagger_\alpha(0). \tag{7.49}$$

Substituting these expressions into (7.1) we obtain again (7.47). Note also that if we take $t_0 \neq 0$, the Heisenberg operators for free fermions are

$$c_\alpha(t) = e^{-i\epsilon_\alpha(t-t_0)}c_\alpha(t_0), \quad c^\dagger_\alpha(t) = e^{i\epsilon_\alpha(t-t_0)}c^\dagger_\alpha(t_0), \tag{7.50}$$

but the result for the Green functions is just the same, because

$$\begin{aligned} \left\langle\left[c_\alpha(t_1), c^\dagger_\beta(t_2)\right]_+\right\rangle &= -\left\langle c_\alpha(t_1)c^\dagger_\beta(t_2) + c^\dagger_\beta(t_2)c_\alpha(t_1)\right\rangle \\ &= e^{i\epsilon_\beta(t_2-t_0)-i\epsilon_\alpha(t_1-t_0)}\left\langle c_\alpha c^\dagger_\beta + c^\dagger_\beta c_\alpha\right\rangle = e^{-i\epsilon_\alpha(t_1-t_2)}\delta_{\alpha\beta}. \end{aligned} \tag{7.51}$$

It is interesting to make Fourier-transform of this function. In equilibrium the two-time function $G^R_{\alpha\beta}(t_1,t_2)$ is a function of the time difference only, so that we apply the transform (7.9). Adding an infinitely small positive complex part to ϵ is required to make this integral well defined in the upper limit (this is necessary for free particles without dissipation because function (7.47) oscillates at large times $\tau = t_1 - t_2$ and the integral (7.9) can not be calculated without $i\eta$ term). Then we obtain

$$G^R_{\alpha\beta}(\epsilon) = \frac{\delta_{\alpha\beta}}{\epsilon - \epsilon_\alpha + i\eta}. \tag{7.52}$$

This Green function looks exactly the same as the retarded matrix function (3.105) introduced in Chap. 3. It is not surprising, that the retarded Green functions of the NGF formalism for noninteracting systems are exactly the same as the single-particle retarded Green functions which we used before.

Free-Particle Lesser Function for Fermions

Now let us consider again free fermions. Heisenberg operators for free fermions are ($t_0 = 0$)

$$c_\alpha(t) = e^{-i\epsilon_\alpha t} c_\alpha(0), \quad c_\alpha^\dagger(t) = e^{i\epsilon_\alpha t} c_\alpha^\dagger(0). \tag{7.53}$$

Lesser function is

$$\begin{aligned} G^<_{\alpha\beta}(t_1,t_2) =& i\left\langle c_\beta^\dagger(t_2) c_\alpha(t_1)\right\rangle = i e^{i\epsilon_\beta t_2 - i\epsilon_\alpha t_1}\left\langle c_\beta^\dagger c_\alpha\right\rangle \\ &= i e^{-i\epsilon_\alpha(t_1-t_2)} f^0(\epsilon_\alpha)\delta_{\alpha\beta}, \end{aligned} \tag{7.54}$$

one sees that contrary to the retarded function, the lesser function is proportional to the distribution function, in equilibrium this is the Fermi distribution function

$$f^0(\epsilon) = \frac{1}{e^{\frac{\epsilon-\mu}{T}} + 1}. \tag{7.55}$$

It is interesting to compare this answer with the result for *nonthermal* initial conditions. Assume that the initial state is described by the density matrix $\rho^0_{\alpha\beta} = \left\langle c_\beta^\dagger c_\alpha\right\rangle$, now with nonzero off-diagonal elements. The time dependence of the density matrix is given by

$$\rho_{\alpha\beta}(t) = e^{i(\epsilon_\beta - \epsilon_\alpha)t}\rho^0_{\alpha\beta}. \tag{7.56}$$

We obtain the well known result that off-diagonal elements oscillate in time.

Now define the Fourier-transform for the lesser function ($\tau = t_1 - t_2$)

$$G^<(\epsilon) = \int_{-\infty}^{\infty} G^<(\tau) e^{i\left[\epsilon + i\eta \mathrm{sign}(\tau)\right]\tau} d\tau, \tag{7.57}$$

note that here we use Fourie-transform with complicated term $i\eta\mathrm{sign}(\tau)$, which makes this transformation consistent with previously introduced transformations (7.9) for retarded ($\tau > 0$) and (7.10) advanced ($\tau < 0$) functions.

Applying this transformation to (7.54) we obtain

$$\begin{aligned} G^<_{\alpha\beta}(\epsilon) =& i f^0(\epsilon_\alpha)\delta_{\alpha\beta}\int_{-\infty}^{\infty} e^{+i\left[\epsilon - \epsilon_\alpha + i\eta\mathrm{sign}(\tau)\right]\tau} d\tau \\ &= 2\pi i f^0(\epsilon_\alpha)\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}. \end{aligned} \tag{7.58}$$

For free fermions, the greater function is given by

$$G^{>}_{\alpha\beta}(t_1, t_2) = -ie^{-i\epsilon_\alpha(t_1-t_2)}(1 - f^0(\epsilon_\alpha))\delta_{\alpha\beta}, \tag{7.59}$$

$$G^{>}_{\alpha\beta}(\epsilon) = -2\pi i(1 - f^0(\epsilon_\alpha))\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}. \tag{7.60}$$

7.1.6 Free Bosons

For free bosons the retarded and advanced functions are exactly the same and the lesser and the greater functions are similar, of course the distribution function now is the Bose function instead of Fermi-Dirac. We give here only the results of calculations:

$$B^{R}_{\alpha\beta}(t_1, t_2) = -i\theta(t_1 - t_2)e^{-i\epsilon_\alpha(t_1-t_2)}\delta_{\alpha\beta}, \tag{7.61}$$

$$B^{A}_{\alpha\beta}(t_1, t_2) = i\theta(t_2 - t_1)e^{-i\epsilon_\alpha(t_1-t_2)}\delta_{\alpha\beta}, \tag{7.62}$$

$$B^{R}_{\alpha\beta}(\epsilon) = \frac{\delta_{\alpha\beta}}{\epsilon - \epsilon_\alpha + i0}, \quad B^{A}_{\alpha\beta}(\epsilon) = \frac{\delta_{\alpha\beta}}{\epsilon - \epsilon_\alpha - i0}, \tag{7.63}$$

$$B^{<}_{\alpha\beta}(t_1, t_2) = -ie^{-i\epsilon_\alpha(t_1-t_2)}f^0_B(\epsilon_\alpha)\delta_{\alpha\beta}, \tag{7.64}$$

$$B^{>}_{\alpha\beta}(t_1, t_2) = -ie^{-i\epsilon_\alpha(t_1-t_2)}(1 + f^0_B(\epsilon_\alpha))\delta_{\alpha\beta}, \tag{7.65}$$

$$B^{<}_{\alpha\beta}(\epsilon) = -2\pi i f^0_B(\epsilon_\alpha)\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}, \tag{7.66}$$

$$B^{>}_{\alpha\beta}(\epsilon) = -2\pi i(1 + f^0_B(\epsilon_\alpha))\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}, \tag{7.67}$$

$$f^0_B(\epsilon) = \frac{1}{e^{\frac{\epsilon}{T}} - 1}. \tag{7.68}$$

7.1.7 Green Functions for Vibrons

As one can see from the Hamiltonian of the electron-vibron interaction (6.13), the relevant operator to describe vibrons is not an individual boson operator, but the density fluctuation operator $A_\alpha = a_\alpha + a^\dagger_\alpha$. Because of that all expressions for vibron functions are different from both fermion and usual boson functions discussed previously.

Definition

Using the Heisenberg density fluctuation operators $A_\alpha(t) = a_\alpha(t) + a_\alpha^\dagger(t)$, we define retarded, advanced, lesser, greater and Keldysh (explained later) Green functions for vibrons:

$$D^R_{\alpha\beta}(t_1, t_2) = -i\theta(t_1 - t_2)\left\langle \left[A_\alpha(t_1), A_\beta(t_2)\right]_- \right\rangle, \tag{7.69}$$

$$D^A_{\alpha\beta}(t_1, t_2) = i\theta(t_2 - t_1)\left\langle \left[A_\alpha(t_1), A_\beta(t_2)\right]_- \right\rangle, \tag{7.70}$$

$$D^<_{\alpha\beta}(t_1, t_2) = -i\left\langle A_\beta(t_2) A_\alpha(t_1) \right\rangle, \tag{7.71}$$

$$D^>_{\alpha\beta}(t_1, t_2) = D^<_{\beta\alpha}(t_2, t_1) = -i\left\langle A_\alpha(t_1) A_\beta(t_2) \right\rangle, \tag{7.72}$$

$$D^R_{\alpha\beta}(t_1, t_2) = \theta(t_1 - t_2)\left[D^>_{\alpha\beta}(t_1, t_2) - D^<_{\alpha\beta}(t_1, t_2)\right], \tag{7.73}$$

$$D^A_{\alpha\beta}(t_1, t_2) = \theta(t_2 - t_1)\left[D^<_{\alpha\beta}(t_1, t_2) - D^>_{\alpha\beta}(t_1, t_2)\right], \tag{7.74}$$

$$D^K_{\alpha\beta}(t_1, t_2) = D^<_{\alpha\beta}(t_1, t_2) + D^>_{\alpha\beta}(t_1, t_2). \tag{7.75}$$

Symmetry Relations

The symmetry relations are essentially different because of using commutators in the definition. The most important peculiarities are the special symmetries due to inversion of $\epsilon \Rightarrow -\epsilon$:

$$D^<_{\alpha\beta}(t_1, t_2) = -\left[D^<_{\beta\alpha}(t_2, t_1)\right]^*, \quad D^>_{\alpha\beta}(t_1, t_2) = -\left[D^>_{\beta\alpha}(t_2, t_1)\right]^*, \tag{7.76}$$

$$D^>_{\alpha\beta}(t_1, t_2) = D^<_{\beta\alpha}(t_2, t_1), \tag{7.77}$$

$$D^A_{\alpha\beta}(t_1, t_2) = \left[D^A_{\alpha\beta}(t_1, t_2)\right]^* = D^R{}_{\beta\alpha}(t_2, t_1) = \left[D^R_{\beta\alpha}(t_2, t_1)\right]^*. \tag{7.78}$$

In the mixed (Wigner) representation

$$D^<_{\alpha\beta}(t, \epsilon) = -\left[D^<_{\beta\alpha}(t, \epsilon)\right]^*, \quad D^>_{\alpha\beta}(t, \epsilon) = -\left[D^>_{\beta\alpha}(t, \epsilon)\right]^*, \tag{7.79}$$

$$D^>_{\alpha\beta}(t, \epsilon) = D^<_{\beta\alpha}(t, -\epsilon), \tag{7.80}$$

$$D^A_{\alpha\beta}(t, \epsilon) = \left[D^A_{\alpha\beta}(t, -\epsilon)\right]^* = D^R_{\beta\alpha}(t, -\epsilon) = \left[D^R_{\beta\alpha}(t, \epsilon)\right]^*. \tag{7.81}$$

In the matrix representation using Hermitian conjugation †

$$\mathbf{D}^<(t, \epsilon) = -\mathbf{D}^{<\dagger}(t, \epsilon), \quad \mathbf{D}^>(t, \epsilon) = -\mathbf{D}^{>\dagger}(t, \epsilon), \tag{7.82}$$

$$\mathbf{D}^>(t, \epsilon) = \mathbf{D}^{<\mathbf{T}}(t, -\epsilon), \tag{7.83}$$

$$\mathbf{D}^A(t, \epsilon) = \mathbf{D}^{A*}(t, -\epsilon) = \mathbf{D}^{R\mathbf{T}}(t, -\epsilon) = \mathbf{D}^{R\dagger}(t, \epsilon). \tag{7.84}$$

Free-Particle Functions

Free-particle functions also look significantly different:

$$D^R_{\alpha\beta}(t_1,t_2) = -i\theta(t_1-t_2)\left[e^{-i\epsilon_\alpha(t_1-t_2)} - e^{i\epsilon_\alpha(t_1-t_2)}\right]\delta_{\alpha\beta}, \tag{7.85}$$

$$D^A_{\alpha\beta}(t_1,t_2) = i\theta(t_2-t_1)\left[e^{-i\epsilon_\alpha(t_1-t_2)} - e^{i\epsilon_\alpha(t_1-t_2)}\right]\delta_{\alpha\beta}, \tag{7.86}$$

$$D^R_{\alpha\beta}(\epsilon) = \frac{\delta_{\alpha\beta}}{\epsilon-\epsilon_\alpha+i\eta} - \frac{\delta_{\alpha\beta}}{\epsilon+\epsilon_\alpha+i\eta}, \quad D^A_{\alpha\beta}(\epsilon) = \frac{\delta_{\alpha\beta}}{\epsilon-\epsilon_\alpha-i\eta} - \frac{\delta_{\alpha\beta}}{\epsilon+\epsilon_\alpha-i\eta}, \tag{7.87}$$

$$D^<_{\alpha\beta}(t_1,t_2) = -i\left[e^{-i\epsilon_\alpha(t_1-t_2)} f^0_B(\epsilon_\alpha) + e^{i\epsilon_\alpha(t_1-t_2)}(1+f^0_B(\epsilon_\alpha))\right]\delta_{\alpha\beta}, \tag{7.88}$$

$$D^<_{\alpha\beta}(\epsilon) = -2\pi i\left[f^0_B(\epsilon_\alpha)\delta(\epsilon-\epsilon_\alpha) + (1+f^0_B(\epsilon_\alpha))\delta(\epsilon+\epsilon_\alpha)\right]\delta_{\alpha\beta}, \tag{7.89}$$

$$D^>_{\alpha\beta}(\epsilon) = -2\pi i\left[f^0_B(\epsilon_\alpha)\delta(\epsilon+\epsilon_\alpha) + (1+f^0_B(\epsilon_\alpha))\delta(\epsilon-\epsilon_\alpha)\right]\delta_{\alpha\beta}, \tag{7.90}$$

$$f^0_B(\epsilon) = \frac{1}{e^{\epsilon/T}-1}, \tag{7.91}$$

$$f^0_B(-\epsilon) = -(1+f^0_B(\epsilon)). \tag{7.92}$$

We do not present the details of calculations here, they are exactly the same as we made for fermions. The differences originates from other definition of Green functions and other commutation relations for boson operators.

Finally the definition for the spectral function is the same:

$$A^D_{\alpha\beta}(\epsilon) = i\left(D^R_{\alpha\beta}(\epsilon) - D^A_{\alpha\beta}(\epsilon)\right). \tag{7.93}$$

For free vibrons the spectral function is

$$A^D_{\alpha\beta}(\epsilon) = 2\pi\left[\delta(\epsilon-\epsilon_\alpha)\delta_{\alpha\beta} - \delta(\epsilon+\epsilon_\alpha)\right]\delta_{\alpha\beta}. \tag{7.94}$$

The sum rule is

$$\int_{-\infty}^{\infty} A^D_{\alpha\beta}(\epsilon)\frac{d\epsilon}{2\pi} = 0. \tag{7.95}$$

It is obvious for free particles, and true for all spectral function because the spectral function is asymmetric in ϵ.

In equilibrium we have the following relations:

$$D^{<}_{\alpha\beta}(\epsilon) = -iA^{D}_{\alpha\beta}(\epsilon)f^{0}_{B}(\epsilon), \tag{7.96}$$

$$D^{>}_{\alpha\beta}(\epsilon) = -iA^{D}_{\alpha\beta}(\epsilon)(1 + f^{0}_{B}(\epsilon)), \tag{7.97}$$

$$D^{>}_{\alpha\beta}(\epsilon) = e^{\epsilon/T}D^{<}_{\alpha\beta}(\epsilon). \tag{7.98}$$

7.2 Interaction Representation

Previously we found that nonequilibrium Green functions can be quite easily calculated for free particles, and equations of motion for one-particle Green functions (the functions which are the averages of two creation-annihilation operators) can be formulated if we add interactions and time-dependent perturbations, but these equations include high-order Green functions (the averages of three, four, and larger number of operators). The equations can be truncated and formulated in terms of one-particle Green functions in some simple approximations. However, a systematic approach is needed to proceed with perturbation expansion and self-consistent methods (all together is known as *diagrammatic approach*). The main idea of the diagrammatic approach is to start from some "simple" Hamiltonian (usually for free particles), treating interactions and external fields as a perturbation, formulate perturbation expansion, and summarize all most important terms (diagrams) *in all orders of perturbation theory*. The result of such a procedure gives, in principle, a *non-perturbative* description (ordinary mean-field theory is the simplest example). The starting point of the method is the so-called *interaction representation*.

Let us consider the full Hamiltonian $\hat{H}$ as the sum of a *free-particle* time-independent part $\hat{H}_0$ and (possibly time-dependent) perturbation $\hat{V}(t)$ (note that this "perturbation" should not be necessarily small)

$$\hat{H} = \hat{H}_0 + \hat{V}(t). \tag{7.99}$$

We define new operators in *interaction representation* by

$$\hat{f}^{I}(t) = e^{i\hat{H}_0 t}\hat{f}^{S}e^{-i\hat{H}_0 t}, \tag{7.100}$$

where $\hat{f}^{S}$ is the time-independent Schrödinger operator. This is equivalent to the time-dependent Heisenberg operator, defined by the part $\hat{H}_0$ of the Hamiltonian. For a free-particle Hamiltonian $\hat{H}_0$ the operators $\hat{f}^{I}(t)$ can be calculated exactly.

A new wave function corresponding to (7.100) is

$$\Psi^{I}(t) = e^{i\hat{H}_0 t}\Psi^{S}(t). \tag{7.101}$$

It is easy to see that transformation (7.100), (7.101) is a unitary transformation and conserves the average value of any operator

$$\langle \Psi^S | \hat{f}^S | \Psi^S \rangle = \langle \Psi^I | \hat{f}^I | \Psi^I \rangle. \tag{7.102}$$

Substituting (7.101) into the ordinary Schrödinger equation, we derive the equation

$$i \frac{\partial \Psi^I}{\partial t} = \hat{V}^I(t) \Psi^I, \tag{7.103}$$

where $\hat{V}^I(t) = e^{i\hat{H}_0 t} \hat{V}^S(t) e^{-i\hat{H}_0 t}$ is in the interaction representation.

Equation (7.103) seems to be quite simple, however the operator nature of $\hat{V}$ makes this problem nontrivial. Indeed, consider a small time-step Δt. Then

$$\Psi(t + \Delta t) = \left[1 - i\hat{V}^S(t)\Delta t\right] \Psi(t) = \exp^{-i\hat{V}^S(t)\Delta t} \Psi(t), \tag{7.104}$$

linear in Δt term can be transformed into the exponent if we understand the exponential function of the operator in the usual way

$$\exp^{\hat{A}} = 1 + \hat{A} + \frac{1}{2!}\hat{A}^2 + \cdots + \frac{1}{n!}\hat{A}^n + \cdots , \tag{7.105}$$

and assume that only linear terms should be taken at $\Delta t \to 0$.

If we now repeat this procedure at times t_i with step Δt, we obtain finally

$$\Psi^I(t) = \hat{S}(t, t_0) \Psi^I(t_0), \tag{7.106}$$

with

$$\hat{S}(t, t_0) = \prod_{t_i = t_0}^{t} \exp\left(-i\hat{V}^I(t_i)\Delta t\right). \tag{7.107}$$

This product, however, is not simply $\exp\left(-i\int_{t_0}^{t} \hat{V}^I(t')dt'\right)$ in the limit $\Delta t \to 0$, because operators $\hat{V}^I(t')$ are not commutative at different times, and for two non-commutative operators $\hat{A}$ and $\hat{B}$ it holds that $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}}$.

In the product (7.107) operators at earlier times should be applied first, before operators at later times. In the limit $\Delta t \to 0$ we obtain

$$\hat{S}(t, t_0) = T \exp\left(-i\int_{t_0}^{t} \hat{V}^I(t')dt'\right), \tag{7.108}$$

where T is the time-ordering operator ("-" for fermionic operators)

$$T\left(\hat{A}(t_1)\hat{B}(t_2)\right) = \begin{cases} \hat{A}(t_1)\hat{B}(t_2) & \text{if } t_1 > t_2, \\ \pm\hat{B}(t_2)\hat{A}(t_1) & \text{if } t_1 < t_2. \end{cases} \tag{7.109}$$

Of course, expression (7.108) is defined only in the sense of expansion (7.105). Consider for example the second-order term in the time-ordered expansion.

$$\begin{aligned} T\left[\int_{t_0}^{t} \hat{V}^I(t')dt'\right]^2 &= T\left[\int_{t_0}^{t} \hat{V}^I(t')dt' \int_{t_0}^{t} \hat{V}^I(t'')dt''\right] \\ &= \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}^I(t')\hat{V}^I(t'') + \int_{t_0}^{t} dt'' \int_{t_0}^{t''} dt' \hat{V}^I(t'')\hat{V}^I(t'). \end{aligned} \tag{7.110}$$

If we exchange t' and t'' in the second integral, we see finally that

$$T\left[\int_{t_0}^{t} \hat{V}^I(t')dt'\right]^2 = 2\int_{t_0}^{t} dt' \int_{t_0}^{t'} dt'' \hat{V}^I(t')\hat{V}^I(t''). \tag{7.111}$$

Properties of $\hat{S}(t, t_0)$

$\hat{S}$ is the unitary operator and

$$\hat{S}^{-1}(t, t_0) = \hat{S}^{\dagger}(t, t_0) = \tilde{T} \exp\left(i\int_{t_0}^{t} \hat{V}^I(t')dt'\right), \tag{7.112}$$

where $\tilde{T}$ is time-anti-ordering operator. Some other important properties are

$$\hat{S}^{-1}(t, t_0) = \hat{S}(t_0, t), \tag{7.113}$$

$$\hat{S}(t_3, t_2)\hat{S}(t_2, t_1) = \hat{S}(t_3, t_1), \tag{7.114}$$

$$\hat{S}^{-1}(t_2, t_1)\hat{S}^{-1}(t_3, t_2) = \hat{S}^{-1}(t_3, t_1). \tag{7.115}$$

Finally, we need the expression of a Heisenberg operator, defined by the full Hamiltonian $\hat{H} = \hat{H}_0 + \hat{V}(t)$, through an operator in the interaction representation. The transformation, corresponding to (7.106), is given by

$$\hat{f}^H(t) = e^{-i\hat{H}_0 t_0}\hat{S}^{-1}(t, t_0)\hat{f}^I(t)\hat{S}(t, t_0)e^{i\hat{H}_0 t_0}, \tag{7.116}$$

and the state $\Psi^I(t_0)$ is related to the Heisenberg time-independent wave function by

$$\Psi^I(t_0) \equiv e^{i\hat{H}_0 t_0}\Psi^S(t_0) = e^{i\hat{H}_0 t_0}\Psi^H, \tag{7.117}$$

in accordance with our previous discussion of averaging we assume that at time $t = t_0$ Heisenberg operators coincide with time-independent Schrödinger operators $\hat{f}^H(t_0) = \hat{f}^S$, and Schrödinger wave function coincides at the same time with Heisenberg time-independent wave function $\Psi^S(t_0) = \Psi^H$. To avoid these additional exponents in (7.116) we can redefine the transformation to the interaction representation as

$$\hat{f}^I(t) = e^{i\hat{H}_0(t-t_0)}\hat{f}^S e^{-i\hat{H}_0(t-t_0)}, \tag{7.118}$$

in accordance with the transformation (7.6) for the time-independent Hamiltonian. Previously we showed that free-particle Green functions are not dependent on t_0 for equilibrium initial condition, if we want to consider some nontrivial initial conditions, it is easier to formulate these conditions directly for Green functions. Thus below we shall use relations

$$\hat{f}^H(t) = \hat{S}^{-1}(t, t_0)\hat{f}^I(t)\hat{S}(t, t_0), \tag{7.119}$$

and

$$\Psi^I(t_0) \equiv \Psi^S(t_0) = \Psi^H. \tag{7.120}$$

Green Functions in the Interaction Representation

Consider, for example, the lesser function

$$G^<_{\alpha\beta}(t_1, t_2) = i\left\langle c^\dagger_\beta(t_2)c_\alpha(t_1)\right\rangle = i\left\langle \Psi^H\left|c^\dagger_\beta(t_2)c_\alpha(t_1)\right|\Psi^H\right\rangle, \tag{7.121}$$

c-operators here are Heisenberg operators and they should be replaced by operators $c^I(t) \equiv \tilde{c}(t)$ in the interaction representation:

$$G^<_{\alpha\beta}(t_1, t_2) = i\left\langle \Psi^H\left|\hat{S}^{-1}(t_2, t_0)\tilde{c}^\dagger_\beta(t_2)\hat{S}(t_2, t_0)\hat{S}^{-1}(t_1, t_0)\tilde{c}_\alpha(t_1)\hat{S}(t_1, t_0)\right|\Psi^H\right\rangle. \tag{7.122}$$

Using properties of $\hat{S}$ operators, we rewrite this expression as

$$G^<_{\alpha\beta}(t_1, t_2) = i\left\langle \hat{S}(t_0, t_2)\tilde{c}^\dagger_\beta(t_2)\hat{S}(t_2, t_1)\tilde{c}_\alpha(t_1)\hat{S}(t_1, t_0)\right\rangle. \tag{7.123}$$

7.3 Schwinger-Keldysh Time Contour

7.3.1 Closed Time-Path Integration

Now let us introduce one useful trick, the so-called *closed time-path contour of integration*. First, note that the expression of the type

$$\hat{f}^H(t) = \hat{S}^{-1}(t, t_0)\hat{f}^I(t)\hat{S}(t, t_0) = \tilde{T}e^{i\int_{t_0}^{t}\hat{V}^I(t')dt'}\hat{f}^I(t)Te^{-i\int_{t_0}^{t}\hat{V}^I(t')dt'}, \tag{7.124}$$

can be written as

$$\hat{f}^H(t) = T_{C_t}\exp\left(-i\int_{C_t}\hat{V}^I(t')dt'\right)\hat{f}^I(t), \tag{7.125}$$

where the integral is taken along closed time contour from t_0 to t and then back from t to t_0

$$\int_{C_t} dt' = \int_{t_0}^{t} dt' + \int_{t}^{t_0} dt'. \tag{7.126}$$

The contour time-ordering operator T_{C_t} works along the contour C_t, it means that for times $t^{\rightarrow}$ it is usual time-ordering operator T, and for times $t^{\leftarrow}$ it is anti-time-ordering operator $\tilde{T}$. Symbolically

$$T_{C_t}\int_{C_t} dt' = T\int_{\rightarrow} dt' + \tilde{T}\int_{\leftarrow} dt'. \tag{7.127}$$

Consider now the application of this closed time-path contour to calculation of Green functions. It is convenient to start from the time-ordered function at $t_2 > t_1$

$$\left\langle T\left(\hat{B}(t_2)\hat{A}(t_1)\right)\right\rangle = \left\langle\hat{S}(t_0, t_2)\tilde{B}(t_2)\hat{S}(t_2, t_1)\tilde{A}(t_1)\hat{S}(t_1, t_0)\right\rangle, \tag{7.128}$$

here $\hat{A}(t)$ and $\hat{B}(t)$ are Heisenberg operators, $\tilde{A}(t)$ and $\tilde{B}(t)$ are operators in the interaction representation, and in the case of fermionic operators the additional minus should be added for any permutation of two operators.

Using the properties of the $\hat{S}$-operator, we transform this expression as

$$\begin{aligned}\left\langle\hat{S}(t_0, t_2)\tilde{B}(t_2)\hat{S}(t_2, t_1)\tilde{A}(t_1)\hat{S}(t_1, t_0)\right\rangle &= \left\langle\hat{S}^{-1}(t_2, t_0)\tilde{B}(t_2)\hat{S}(t_2, t_1)\tilde{A}(t_1)\hat{S}(t_1, t_0)\right\rangle\\ = \left\langle\hat{S}^{-1}(\infty, t_0)\hat{S}(\infty, t_2)\tilde{B}(t_2)\hat{S}(t_2, t_1)\tilde{A}(t_1)\hat{S}(t_1, t_0)\right\rangle &= \left\langle\hat{S}^{-1}T\left(\tilde{B}(t_2)\tilde{A}(t_1)\hat{S}\right)\right\rangle,\end{aligned} \tag{7.129}$$

where we defined operator

$$\hat{S} = \hat{S}(\infty, t_0). \tag{7.130}$$

Using contour integration, it can be written as

$$\left\langle T\left(\hat{B}(t_2)\hat{A}(t_1)\right)\right\rangle = \left\langle T_C\left(\hat{S}_C\tilde{B}(t_2^{\rightarrow})\tilde{A}(t_1^{\rightarrow})\right)\right\rangle, \tag{7.131}$$

$$\hat{S}_C = T_C\exp\left(-i\int_C\hat{V}^I(t')dt'\right), \tag{7.132}$$

where the contour C goes from t_0 through t_1 and t_2, and back to t_0. If $t_2 > t_1$ it is obvious that contour ordering along $C^{\rightarrow}$ gives the terms from $\hat{S}(t_1, t_0)$ to $\hat{B}(t_2)$ in (7.128). The integral over the back path $C^{\leftarrow}$ gives

$$T_C \exp\left(-i \int_{\leftarrow} \hat{V}^I(t')dt'\right) = \tilde{T} \exp\left(-i \int_{t_2}^{t_0} \hat{V}^I(t')dt'\right)$$
$$= \tilde{T} \exp\left(i \int_{t_0}^{t_2} \hat{V}^I(t')dt'\right) = \hat{S}^{-1}(t_2, t_0) = \hat{S}(t_0, t_2). \tag{7.133}$$

For $t_2 < t_1$ the operators in (7.128) are reordered by T-operator and we again obtain (7.131).

The lesser and greater functions are not time-ordered and arguments of the operators are not affected by time-ordering operator. Nevertheless we can write such functions in the same form (7.131). The trick is to use one time argument from the forward contour and the other from the backward contour, for example

$$\left\langle \hat{B}(t_2)\hat{A}(t_1)\right\rangle = \left\langle T_C\left(\hat{S}_C \tilde{B}(t_2^{\leftarrow})\tilde{A}(t_1^{\rightarrow})\right)\right\rangle, \tag{7.134}$$

here the time t_1 is always before t_2.

7.3.2 Contour (Contour-Ordered) Green Function

Now we are able to define *contour* or *contour-ordered* Green function—the useful tool of Keldysh diagrammatic technique. The definition is similar to the previous one

$$G^C_{\alpha\beta}(\tau_1, \tau_2) = -i\left\langle T_C\left(c_\alpha(\tau_1)c^\dagger_\beta(\tau_2)\right)\right\rangle, \tag{7.135}$$

where, however, τ_1 and τ_2 are contour times. This function includes all nonequilibrium Green functions introduced before. Indeed, depending on contour position of times we obtain lesser, greater, or time-ordered functions (below we give different notations used in the literature)

$$G^C_{\alpha\beta}(\tau_1, \tau_2) = \begin{cases} \tau_1, \tau_2 \in C^{\rightarrow}: & -i\left\langle T c_\alpha(t_1)c^\dagger_\beta(t_2)\right\rangle \Longrightarrow\ G^{--}\ or\ G^T(t_1, t_2), \\ \tau_1 \in C^{\leftarrow}, \tau_2 \in C^{\rightarrow}: & -i\left\langle c_\alpha(t_1)c^\dagger_\beta(t_2)\right\rangle \Longrightarrow\ G^{+-}\ or\ G^>(t_1, t_2), \\ \tau_1 \in C^{\rightarrow}, \tau_2 \in C^{\leftarrow}: & i\left\langle c^\dagger_\beta(t_2)c_\alpha(t_1)\right\rangle \Longrightarrow\ G^{-+}\ or\ G^<(t_1, t_2), \\ \tau_1, \tau_2 \in C^{\leftarrow}: & -i\left\langle \tilde{T} c_\alpha(t_1)c^\dagger_\beta(t_2)\right\rangle \Longrightarrow\ G^{++}\ or\ G^{\tilde{T}}(t_1, t_2). \end{cases} \tag{7.136}$$

These four functions are not independent, from definitions it follows that

$$G^{<} + G^{>} = G^{T} + G^{\tilde{T}}, \tag{7.137}$$

and anti-Hermitian relations hold:

$$G^{T}_{\alpha\beta}(t_1, t_2) = -G^{T*}_{\beta\alpha}(t_2, t_1), \tag{7.138}$$

$$G^{<}_{\alpha\beta}(t_1, t_2) = -G^{<*}_{\beta\alpha}(t_2, t_1), \tag{7.139}$$

$$G^{>}_{\alpha\beta}(t_1, t_2) = -G^{>*}_{\beta\alpha}(t_2, t_1). \tag{7.140}$$

It is more convenient to use retarded and advanced functions instead of time-ordered functions. There is a number of ways to express G^R and G^A through above defined functions

$$G^{R} = \theta(t_1 - t_2)\left[G^{>} - G^{<}\right] = G^{T} - G^{<} = G^{>} - G^{\tilde{T}}, \tag{7.141}$$

$$G^{A} = \theta(t_2 - t_1)\left[G^{<} - G^{>}\right] = G^{T} - G^{>} = G^{<} - G^{\tilde{T}}. \tag{7.142}$$

This technique at real-time axes can be formulated for matrix functions

$$\breve{G} = \begin{pmatrix} G^{++} & G^{+-} \\ G^{-+} & G^{--} \end{pmatrix}. \tag{7.143}$$

It is, however, more convenient to use the linear dependence of four functions and after the rotation in "Keldysh space" we get

$$\breve{G} = \begin{pmatrix} G^{R} & G^{K} \\ 0 & G^{A} \end{pmatrix}, \tag{7.144}$$

where we obtain retarded ans advanced functions at the matrix diagonal and introduced new *Keldysh function* G^K

$$G^{K} = G^{>} + G^{<} = -i\langle [c_\alpha(t_1), c^{+}_{\beta}(t_2)]_{-}\rangle, \tag{7.145}$$

$$G^{<} = \tfrac{1}{2}G^{K} + \tfrac{i}{2}A. \tag{7.146}$$

7.3.3 Contour Green Function in the Interaction Representation

In the interaction representation one should repeat the calculations performed before and given the expressions (7.123), (7.128), and then replace usual times by contour times τ, so we obtain

$$\left\langle T_C\left(c_\alpha(\tau_1)c_\beta^\dagger(\tau_2)\right)\right\rangle \quad = \left\langle T_C\left(\hat{S}(\tau_0,\tau_2)\tilde{c}_\beta^\dagger(\tau_2)\hat{S}(\tau_2,\tau_1)\tilde{c}_\alpha(\tau_1)\hat{S}(\tau_1,\tau_0)\right)\right\rangle. \tag{7.147}$$

Using contour integration, it can be written as

$$G^C_{\alpha\beta}(\tau_1,\tau_2) = -i\left\langle T_C\left(c_\alpha(\tau_1)c_\beta^\dagger(\tau_2)\right)\right\rangle = -i\left\langle T_C\left(\hat{S}_C\tilde{c}_\alpha(\tau_1)\tilde{c}_\beta^\dagger(\tau_2)\right)\right\rangle, \tag{7.148}$$

$$\hat{S}_C = T_C\exp\left(-i\int_C \hat{V}^I(t')dt'\right). \tag{7.149}$$

7.4 Nonequilibrium Equation of Motion Method

Now we start to consider the case of interacting nanosystems. Although it is possible to derive the *exact* expression for the current through an interacting central region (we consider it in Chap. 8), the problem to find the Green functions of the central region is sometimes highly nontrivial. At the present time there are several techniques developed to solve this problem.

The nonequilibrium equation of motion (NEOM) method is the simplest approximate approach. In spite of its simplicity, it is very useful in many cases, and is very convenient for numerical implementation. In this section we consider only a general formulation, some particular examples are considered further.

We start from the general definition of a Green function as the average of two Heisenberg operators $\hat{A}(t)$ and $\hat{B}(t)$, denoted as

$$\langle\langle\hat{A}(t_1),\hat{B}(t_2)\rangle\rangle^{R,A,<}.$$

The particular definitions of the averages for spectral and kinetic functions are

$$\left\langle\left\langle\hat{A}(t_1),\hat{B}(t_2)\right\rangle\right\rangle^R = -i\theta(t_1-t_2)\left\langle\left[\hat{A}(t_1),\hat{B}(t_2)\right]_\mp\right\rangle, \tag{7.150}$$

where upper sign here and below is for boson functions, lower sign for fermions,

$$\left\langle\left\langle\hat{A}(t_1),\hat{B}(t_2)\right\rangle\right\rangle^< = -i\left\langle\hat{A}(t_1),\hat{B}(t_2)\right\rangle. \tag{7.151}$$

The equations of motion for NGF are obtained from the Heisenberg equation of motion for operators

$$i\frac{\partial\hat{A}}{\partial t} = \left[\hat{A},\hat{H}\right]_- = \hat{A}\hat{H}-\hat{H}\hat{A}, \tag{7.152}$$

for any Heisenberg operator $\hat{A}(t)$. Here and below all Hamiltonians are *time-independent*. We consider the *stationary problem*.

7.4.1 Spectral (Retarded and Advanced) Functions

Let us start from a retarded function

$$\left\langle\!\left\langle \hat{A}(t_1), \hat{B}(t_2) \right\rangle\!\right\rangle^R = -i\theta(t_1 - t_2)\left\langle \left[\hat{A}(t_1), \hat{B}(t_2) \right]_{\mp} \right\rangle. \tag{7.153}$$

Taking the time derivative we obtain

$$i\frac{\partial}{\partial t_1}\left\langle\!\left\langle \hat{A}(t_1), \hat{B}(t_2) \right\rangle\!\right\rangle^R = \delta(t_1 - t_2)\left\langle \left[\hat{A}(t_1), \hat{B}(t_1) \right]_{\mp} \right\rangle + \left\langle\!\left\langle \left[\hat{A}(t_1), \hat{H} \right]_{-}, \hat{B}(t_2) \right\rangle\!\right\rangle^R, \tag{7.154}$$

where the first term originates from the time-derivative of the θ-function, and the (7.152) is used in the second term.

In the stationary case the Fourier transform can be used

$$(\epsilon + i\eta)\left\langle\!\left\langle \hat{A}, \hat{B} \right\rangle\!\right\rangle^R_{\epsilon} = \left\langle \left[\hat{A}, \hat{B} \right]_{\mp} \right\rangle + \left\langle\!\left\langle \left[\hat{A}, \hat{H} \right]_{-}, \hat{B} \right\rangle\!\right\rangle^R_{\epsilon}. \tag{7.155}$$

Now let us assume that the Hamiltonian can be divided into "free particle" and "interaction" parts $\hat{H} = \hat{H}_0 + \hat{H}_1$, and $[\hat{A}, \hat{H}_0]_- = \hat{\epsilon}_0\hat{A}$. (The simple example. For the free particle Hamiltonian $\hat{H}_0 = \sum_\beta \epsilon_\beta d^\dagger_\beta d_\beta$ and the operator $\hat{A} = d^\dagger_\alpha$ one has $[\hat{A}, \hat{H}_0]_- = \sum_\beta \epsilon_\beta [d^\dagger_\alpha, d^\dagger_\beta d_\beta]_- = \epsilon_\alpha d^\dagger_\alpha$, $\hat{\epsilon}_0 = \epsilon_\alpha$ is simply a number. In general, $\hat{\epsilon}_0$ is some time-independent operator). So that

$$(\epsilon + i\eta - \hat{\epsilon}_0)\left\langle\!\left\langle \hat{A}, \hat{B} \right\rangle\!\right\rangle^R_{\epsilon} = \left\langle \left[\hat{A}, \hat{B} \right]_{\mp} \right\rangle + \left\langle\!\left\langle \left[\hat{A}, \hat{H}_1 \right]_{-}, \hat{B} \right\rangle\!\right\rangle^R_{\epsilon}, \tag{7.156}$$

the second term includes interaction and can not be easy simplified.

It is convenient now to introduce the "free particle" function $\hat{g}^R_\epsilon$ as a solution of the equation

$$(\epsilon + i\eta - \hat{\epsilon}_0)\hat{g}^R_\epsilon = 1. \tag{7.157}$$

Now we multiply the right and left parts of (7.156) by $\hat{g}^R_\epsilon$. Using the function $\hat{g}^R(t) = \int \hat{g}^R_\epsilon e^{-i\epsilon t}\frac{d\epsilon}{2\pi}$ we can write the time-dependent solution of (7.154) as

$$\begin{aligned}\left\langle\!\left\langle \hat{A}(t_1), \hat{B}(t_2) \right\rangle\!\right\rangle^R &= \hat{g}^R(t_1 - t_2)\left\langle \left[\hat{A}(t_1), \hat{B}(t_1) \right]_{\mp} \right\rangle \\ &\quad + \int \hat{g}^R(t_1 - t')\left\langle\!\left\langle \left[\hat{A}(t'), \hat{H}_1 \right]_{-}, \hat{B}(t_2) \right\rangle\!\right\rangle^R dt'. \end{aligned} \tag{7.158}$$

7.4.2 EOM at the Schwinger-Keldysh Contour

The calculation of the lesser functions by the EOM technique requires some care. To demonstrate it let us compare the EOM for retarded and lesser functions of free particles.

The equation for $g^R_{\alpha\beta}$ is (assuming the diagonal matrix $\tilde{\epsilon}_{\alpha\beta}$)

$$(\epsilon + i\eta - \tilde{\epsilon}_\alpha)\, g^R_{\alpha\beta} = \delta_{\alpha\beta}, \tag{7.159}$$

from which the free-particle Green function is easily obtained.

At the same time for the lesser function we have the equation

$$(\epsilon - \tilde{\epsilon}_\alpha)\, g^<_{\alpha\beta} = 0, \tag{7.160}$$

from which, however, the free-particle lesser function $g^<_{\alpha\beta} = 2\pi f_0(\epsilon)\delta(\epsilon - \epsilon_\alpha)\delta_{\alpha\beta}$ can not be obtained.

The problem can be generally resolved by using the EOM on the Schwinger-Keldysh time contour. The contour-ordered Green function is defined as

$$\left\langle\!\left\langle \hat{A}(\tau_1), \hat{B}(\tau_2) \right\rangle\!\right\rangle^C = -i\left\langle T_C\left(\hat{A}(\tau_1), \hat{B}(\tau_2)\right)\right\rangle, \tag{7.161}$$

where $\hat{A}(\tau_1)$ and $\hat{B}(\tau_2)$ are two Heisenberg operators, defined along the contour.

Taking the time derivative we obtain the equation

$$i\frac{\partial}{\partial\tau_1}\left\langle\!\left\langle \hat{A}(\tau_1), \hat{B}(\tau_2) \right\rangle\!\right\rangle^C = \delta^c(\tau_1 - \tau_2)\left\langle\left[\hat{A}(\tau_1), \hat{B}(\tau_1)\right]_\mp\right\rangle + \left\langle\!\left\langle \left[\hat{A}(\tau_1), \hat{H}\right]_-, \hat{B}(\tau_2) \right\rangle\!\right\rangle^C, \tag{7.162}$$

in the stationary case this equation can be formally solved if one applies the Fourier transform along the contour, or perturbation expansion in the interaction representation (Niu et al. 1999). Using the free particle solution $\hat{g}^C(\tau_1 - \tau_2)$ we can write the time-dependent solution as

$$\begin{aligned}\left\langle\!\left\langle \hat{A}(\tau_1), \hat{B}(\tau_2) \right\rangle\!\right\rangle^C =& \hat{g}^C(\tau_1 - \tau_2)\left\langle\left[\hat{A}(\tau_1), \hat{B}(\tau_1)\right]_\mp\right\rangle \\ &+ \int \hat{g}^C(\tau_1 - \tau')\left\langle\!\left\langle \left[\hat{A}(\tau'), \hat{H}_1\right]_-, \hat{B}(\tau_2) \right\rangle\!\right\rangle^C d\tau'.\end{aligned} \tag{7.163}$$

7.4.3 Kinetic (Lesser) Function

Applying now the Langreth rules (see the next section for details), which shows, that from

$$C(\tau_1, \tau_2) = \int_C A(\tau_1, \tau_3) B(\tau_3, \tau_2) d\tau_3 \tag{7.164}$$

it follows

$$C^R(t_1, t_2) = \int A^R(t_1, t_3) B^R(t_3, t_2) dt_3, \tag{7.165}$$

$$C^<(t_1, t_2) = \int \left(A^R(t_1, t_3) B^R(t_3, t_2) + A^<(t_1, t_3) B^A(t_3, t_2) \right) dt_3, \tag{7.166}$$

we get (7.158) for the retarded function, and

$$\begin{aligned} \left\langle\!\left\langle \hat{A}(t_1), \hat{B}(t_2) \right\rangle\!\right\rangle^< &= \hat{g}^<(t_1 - t_2) \left\langle \left[\hat{A}(t_1), \hat{B}(t_1) \right]_\mp \right\rangle \\ &+ \int \hat{g}^R(t_1 - t') \left\langle\!\left\langle \left[\hat{A}(t'), \hat{H}_1 \right]_-, \hat{B}(t_2) \right\rangle\!\right\rangle^< dt' \\ &+ \int \hat{g}^<(t_1 - t') \left\langle\!\left\langle \left[\hat{A}(t'), \hat{H}_1 \right]_-, \hat{B}(t_2) \right\rangle\!\right\rangle^A dt' \end{aligned} \tag{7.167}$$

for the lesser function. And the Fourier transform is

$$\left\langle\!\left\langle \hat{A}, \hat{B} \right\rangle\!\right\rangle_\epsilon^< = \hat{g}_\epsilon^< \left\langle \left[\hat{A}, \hat{B} \right]_\mp \right\rangle + \hat{g}_\epsilon^R \left\langle\!\left\langle \left[\hat{A}, \hat{H}_1 \right]_-, \hat{B} \right\rangle\!\right\rangle_\epsilon^< + \hat{g}_\epsilon^< \left\langle\!\left\langle \left[\hat{A}, \hat{H}_1 \right]_-, \hat{B} \right\rangle\!\right\rangle_\epsilon^A . \tag{7.168}$$

7.5 Kadanoff-Baym-Keldysh Method

Now we review briefly the other approach. The Kadanoff-Baym-Keldysh method systematically extends the equilibrium many-body theory to the nonequilibrium case. Potentially, it is the most powerful approach. Below we give a simple introduction into the method, which is currently actively developed.

7.5.1 *Perturbation Expansion and Diagrammatic Rules for Contour Functions*

We found that Green functions can be written in the interaction representation with a help of the $\hat{S}$-operator. For example, the time-ordered fermionic Green function is

$$G^T_{\alpha\beta}(t_1, t_2) = -i \left\langle T \left(c_\alpha(t_1) c^\dagger_\beta(t_2) \right) \right\rangle = -i \left\langle \hat{S}^{-1} T \left(\tilde{c}_\alpha(t_1) \tilde{c}^\dagger_\beta(t_2) \hat{S} \right) \right\rangle, \tag{7.169}$$

using "usual" $\hat{S}$-operator

$$\hat{S} = \hat{S}(\infty, t_0) = T \exp\left(-i \int_{t_0}^{\infty} \hat{V}^I(t')dt'\right), \tag{7.170}$$

or

$$G^T_{\alpha\beta}(t_1, t_2) = -i\left\langle T_C \left(\tilde{c}_\alpha(t_1^{\rightarrow})\tilde{c}^\dagger_\beta(t_2^{\rightarrow})\hat{S}_C\right)\right\rangle, \tag{7.171}$$

using "contour" $\hat{S}_C$-operator

$$\hat{S}_C = T_C \exp\left(-i \int_C \hat{V}^I(t')dt'\right). \tag{7.172}$$

We first consider the zero temperature case, when one can set $t_0 = -\infty$,

$$\hat{S} = \hat{S}(\infty, -\infty) = T \exp\left(-i \int_{-\infty}^{\infty} \hat{V}^I(t')dt'\right), \tag{7.173}$$

and assume that interaction is switched on and switched off at $t \rightarrow +\infty$ *adiabatically*. This condition is necessary to prevent excitation of the system from its ground state. The other necessary condition is that the perturbation is time-independent in the Schrödinger representation. In this case if the initial state $|\Psi(t = -\infty)\rangle = |\Psi_0\rangle$ is the ground state (of free particles), then the final state $|\Psi(t = +\infty)\rangle = \hat{S}|\Psi^0\rangle = e^{i\theta}|\Psi^0\rangle$ is also the ground state, only the phase can be changed. Now, using the average value of the $\hat{S}$-operator

$$\langle\hat{S}\rangle = \langle\Psi^0|\hat{S}|\Psi^0\rangle = e^{i\theta}\langle\Psi^0|\Psi^0\rangle = e^{i\theta}, \tag{7.174}$$

we obtain

$$\hat{S}|\Psi^0\rangle = \langle\hat{S}\rangle|\Psi^0\rangle, \tag{7.175}$$

and

$$\langle\Psi^0|\hat{S}^{-1} = \frac{\langle\Psi^0|}{\langle\hat{S}\rangle}. \tag{7.176}$$

So that (7.169) can be written as

$$G^T_{\alpha\beta}(t_1, t_2) = -i\frac{\left\langle T\left(\tilde{c}_\alpha(t_1)\tilde{c}^\dagger_\beta(t_2)\hat{S}\right)\right\rangle}{\langle\hat{S}\rangle}. \tag{7.177}$$

Now we can expand the exponent (note that S-operator is defined only in the sense of this expansion)

$$\begin{aligned}\hat{S} &= T\exp\left(-i\int_{-\infty}^{\infty}\hat{V}^I(t')dt'\right)\\ &= T\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1'\ldots\int_{-\infty}^{\infty}dt_n'\;\hat{V}^I(t_1')\ldots\hat{V}^I(t_n'),\end{aligned} \tag{7.178}$$

and numerator and denominator of the expression (7.177) are

$$\begin{aligned}&\left\langle T\left(\tilde{c}_\alpha(t_1)\tilde{c}_\beta^\dagger(t_2)\hat{S}\right)\right\rangle\\ &\quad=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1'\ldots\int_{-\infty}^{\infty}dt_n'\left\langle T\tilde{c}_\alpha(t_1)\tilde{c}_\beta^\dagger(t_2)\hat{V}^I(t_1')\ldots\hat{V}^I(t_n')\right\rangle,\end{aligned} \tag{7.179}$$

$$\langle\hat{S}\rangle=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_{-\infty}^{\infty}dt_1'\ldots\int_{-\infty}^{\infty}dt_n'\left\langle T\hat{V}^I(t_1')\ldots\hat{V}^I(t_n')\right\rangle. \tag{7.180}$$

These expressions are used to produce the perturbation series.

The main quantity to be calculated is the contour Green function

$$G(1,2)\equiv G_{\alpha\beta}^C(\tau_1,\tau_2)=-i\left\langle T_C\left(c_\alpha(\tau_1)c_\beta^\dagger(\tau_2)\right)\right\rangle, \tag{7.181}$$

where τ_1 and τ_2 are contour times. Here $1_c\equiv\alpha,\tau_1$.

The general diagrammatic rules for contour Green functions are exactly the same as in the usual zero-temperature technique (we call it standard rules). The correspondence between diagrams and analytical expressions is established in the following way:

1. Open bare electron line is $iG_0(1,2)$.
2. Closed bare electron line is $n_0(1)\equiv n_\alpha^{(0)}(\tau_1)$.
3. Bare interaction line is $-iv(1,2)$.
4. Self-energy is $-i\Sigma(1,2)$.
5. Integration over internal vertices, and other standard rules.

7.5.2 Langreth Rules

Although the basic equations and diagrammatic rules are formulated for contour Green functions, the solution of these equations and final results are much more transparent when represented by real-time spectral and kinetic functions.

As in the ordinary diagrammatic technique, the important role is played by the integration (summation) over space and contour-time arguments of Green functions, which is denoted as

$$\int d1_c \equiv \sum_\alpha \int_C d\tau_1. \tag{7.182}$$

After application of the Langreth rules [1], for real-time functions these integrals become

$$\int d1 \equiv \sum_\alpha \int_{-\infty}^{\infty} dt_1. \tag{7.183}$$

The Langreth rules show, for example, that from

$$C(\tau_1, \tau_2) = \int_C A(\tau_1, \tau_3) B(\tau_3, \tau_2) d\tau_3 \tag{7.184}$$

it follows

$$C^R(t_1, t_2) = \int A^R(t_1, t_3) B^R(t_3, t_2) dt_3, \tag{7.185}$$

$$C^<(t_1, t_2) = \int \big(A^R(t_1, t_3) B^<(t_3, t_2) + A^<(t_1, t_3) B^A(t_3, t_2)\big) dt_3. \tag{7.186}$$

The other important rules are: from

$$C(\tau_1, \tau_2) = A(\tau_1, \tau_2) B(\tau_1, \tau_2) \tag{7.187}$$

it follows

$$C^R(t_1, t_2) = A^R(t_1, t_2) B^R(t_1, t_2) + A^R(t_1, t_2) B^<(t_1, t_2) + A^<(t_1, t_2) B^R(t_1, t_2), \tag{7.188}$$

$$C^<(t_1, t_2) = A^<(t_1, t_2) B^<(t_1, t_2), \tag{7.189}$$

and from

$$C(\tau_1, \tau_2) = A(\tau_1, \tau_2) B(\tau_2, \tau_1) \tag{7.190}$$

it follows

$$C^R(t_1, t_2) = A^R(t_1, t_2) B^<(t_2, t_1) + A^<(t_1, t_2) B^A(t_2, t_1), \tag{7.191}$$

$$C^<(t_1, t_2) = A^<(t_1, t_2) B^>(t_2, t_1). \tag{7.192}$$

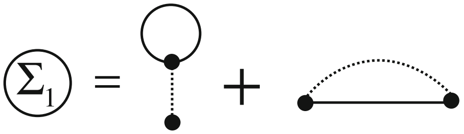

Fig. 7.1 Diagrammatic representation of the first-order self-energy

7.5.3 First-Order Self-Energy and Polarization Operator

Consider, as an example, the first order expression for the self-energy, shown in Fig. 7.1. Following the diagrammatic rules, we find

$$\Sigma_1(1,2) = \delta(1-2)\int v(1,3)n_0(3)d3 + iv(1,2)G_0(1,2), \tag{7.193}$$

where the first term is the Hartree contribution, which can be included into the unperturbed Green function $G_0(1,2)$. This expression is actually symbolic, and translation from contour (Keldysh-time) to real-time functions is necessary. Using the Langreth rules, one obtains

$$\begin{aligned}\Sigma_1^R(1,2) =&\delta(1^+-2)\int v^R(1,3)n_0(3,3)d3 + iv^R(1,2)G_0^R(1,2)\\ &+ iv^<(1,2)G_0^R(1,2) + iv^R(1,2)G_0^<(1,2),\end{aligned} \tag{7.194}$$

$$\Sigma_1^<(1,2) = iv^<(1,2)G_0^<(1,2). \tag{7.195}$$

There is no Hartree term for lesser function, because the times τ_1 and τ_2 are always at the different branches of the Keldysh contour, and the δ-function $\delta(\tau_1-\tau_2)$ is zero.

In the stationary case and using explicit matrix indices, we have, finally (here $\tau = t_1 - t_2$, not to mix with the Keldysh time)

$$\begin{aligned}\Sigma_{\alpha\beta}^{R(1)}(\tau) = \delta(\tau^+)\delta_{\alpha\beta}\textstyle\sum_\gamma \tilde{v}_{\alpha\gamma}^R(0)n_\gamma^{(0)} + iv_{\alpha\beta}^R(\tau)G_{\alpha\beta}^{R(0)}\tau)&\\ +iv_{\alpha\beta}^<(\tau)G_{\alpha\beta}^{R(0)}(\tau) + iv_{\alpha\beta}^R(\tau)G_{\alpha\beta}^{<(0)}(\tau),&\end{aligned} \tag{7.196}$$

$$\Sigma_{\alpha\beta}^{<(1)}(\tau) = iv_{\alpha\beta}^<(\tau)G_{\alpha\beta}^{<(0)}(\tau), \tag{7.197}$$

and we define the Fourier transform of the bare interaction

$$\tilde{v}_{\alpha\gamma}^R(0) = \int v_{\alpha\gamma}^R(\tau)d\tau. \tag{7.198}$$

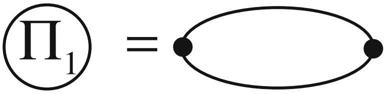

Fig. 7.2 Diagrammatic representation of the first-order polarization operator

Finally, the Fourier transforms are

$$\Sigma^{R(1)}_{\alpha\beta}(\epsilon) = \delta_{\alpha\beta}\sum_{\gamma}\tilde{v}^R_{\alpha\gamma}(0)n^{(0)}_{\gamma}$$
$$+ i\int\frac{d\epsilon'}{2\pi}\left[v^R_{\alpha\beta}(\epsilon')G^{R(0)}_{\alpha\beta}(\epsilon-\epsilon') + v^<_{\alpha\beta}(\epsilon')G^{R(0)}_{\alpha\beta}(\epsilon-\epsilon') + v^R_{\alpha\beta}(\epsilon')G^{<(0)}_{\alpha\beta}(\epsilon-\epsilon')\right], \tag{7.199}$$

$$\Sigma^{<(1)}_{\alpha\beta}(\epsilon) = i\int\frac{d\epsilon'}{2\pi}v^<_{\alpha\beta}(\epsilon')G^{<(0)}_{\alpha\beta}(\epsilon-\epsilon'). \tag{7.200}$$

The second important function is the polarization operator (“self-energy for interaction”), shown in Fig. 7.2. Following the diagrammatic rules, we find

$$\Pi_1(1,2) = -iG_0(1,2)G_0(2,1), \tag{7.201}$$

note the order of times in this expression.

Using the Langreth rules,

$$\Pi^R_1(1,2) = iG^R_0(1,2)G^<_0(2,1) + iG^<_0(1,2)G^A_0(2,1), \tag{7.202}$$

$$\Pi^<_1(1,2) = iG^<_0(1,2)G^>_0(2,1). \tag{7.203}$$

And in the stationary case, restoring the matrix indices

$$\Pi^{R(1)}_{\alpha\beta}(\tau) = -i\left[G^{R(0)}_{\alpha\beta}(\tau)G^{<(0)}_{\beta\alpha}(-\tau) + G^{<(0)}_{\alpha\beta}(\tau)G^{A(0)}_{\beta\alpha}(-\tau)\right], \tag{7.204}$$

$$\Pi^{<(1)}_{\alpha\beta}(\tau) = -iG^{<(0)}_{\alpha\beta}(\tau)G^{>(0)}_{\beta\alpha}(-\tau). \tag{7.205}$$

In the Fourier representation

$$\Pi^{R(1)}_{\alpha\beta}(\epsilon) = -i\int\frac{d\epsilon'}{2\pi}\left[G^{R(0)}_{\alpha\beta}(\epsilon')G^{<(0)}_{\beta\alpha}(\epsilon'-\epsilon) + G^{<(0)}_{\alpha\beta}(\epsilon')G^{A(0)}_{\beta\alpha}(\epsilon'-\epsilon)\right], \tag{7.206}$$

$$\Pi^{<(1)}_{\alpha\beta}(\epsilon) = -i\int\frac{d\epsilon'}{2\pi}G^{<(0)}_{\alpha\beta}(\epsilon')G^{>(0)}_{\beta\alpha}(\epsilon'-\epsilon). \tag{7.207}$$

These expressions are quite general and can be used for both electron-electron and electron-vibron interaction.

For Coulomb interaction the bare interaction is is $v(1,2) \equiv U_{\alpha\beta}\delta(\tau_1^+ - \tau_2)$, so that

$$v^R(1,2) \equiv U_{\alpha\beta}\delta(t_1^+ - t_2), \tag{7.208}$$

$$v^<(1,2) = 0. \tag{7.209}$$

7.5.4 Self-consistent Equations

Hedin's Equations at Keldysh Contour

The diagrams can be partially summed in all orders of perturbation theory. The resulting equations are known as Dyson equations for the dressed Green function $G(1,2)$ and the effective interaction $W(1,2)$ (Fig. 7.3). Analytically these equations are written as (in general nonequilibrium case the functions are contour functions and integration is over Keldysh contour)

$$G(1,2) = G_0(1,2) + \iint G_0(1,3)\Sigma(3,4)G(4,2)d3d4, \tag{7.210}$$

$$W(1,2) = v(1,2) + \iint v(1,3)\Pi(3,4)W(4,2)d3d4. \tag{7.211}$$

In the perturbative approach the first order (or higher order) expressions for the self-energy and the polarization operator are used. The other possibility is to summarize further the diagrams and obtain the self-consistent approximations (Figs. 7.4 and 7.5), which include, however, a new unknown function, called vertex function. We shall write these expressions analytically, including the Hartree-Fock part in the unperturbed Green function $G_0(1,2)$.

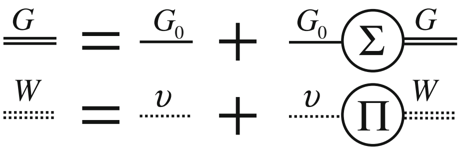

Fig. 7.3 Diagrammatic representation of the Dyson equations

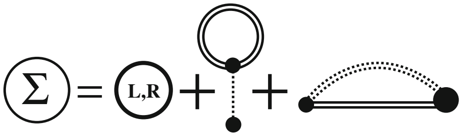

Fig. 7.4 Diagrammatic representation of the full self-energy

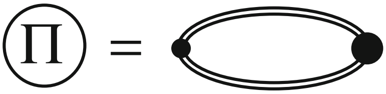

Fig. 7.5 Diagrammatic representation of the full polarization operator

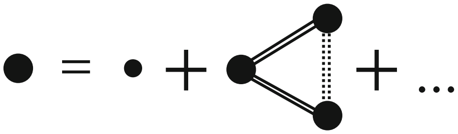

Fig. 7.6 Diagrammatic representation of the vertex function

$$\Sigma'(1,2) = i\iint W(1,3)G(1,4)\Gamma(3;4,2)d3d4, \tag{7.212}$$

$$\Pi(1,2) = -i\iint G(1,3)G(4,1)\Gamma(2;3,4)d3d4. \tag{7.213}$$

Here we introduce the vertex function $\Gamma(1;2,3)$ which depends on three coordinates and connects two electron lines and one interaction line. The equation for the vertex function can not be closed diagrammatically (Fig. 7.6). Nevertheless, it is possible to write a closed set of equations (*Hedin's equations* [2]), which are exact equations for full Green functions written through a functional derivative. Hedin's equations are (7.210)–(7.213) and the equation for the vertex function

$$\Gamma(1;2,3) = \delta(1,2)\delta(1,3) + \iiiint G(4,6)G(7,5)\Gamma(1;6,7)\frac{\delta\Sigma(2,3)}{\delta G(4,5)}d4d5d6d7. \tag{7.214}$$

Real-Time Equations

There are several ways to get real-time equations from Hedin's equations for contour functions. One is to use the Langreth rules. The other, equivalent, method was suggested by Keldysh [3]. Retarded G^R, advanced G^A and Keldysh G^K (or lesser $G^<$) functions can be considered as the components of matrices

$$\breve{G} = \begin{pmatrix} G^R & G^K(G^<) \\ 0 & G^A \end{pmatrix}, \qquad \breve{\Sigma} = \begin{pmatrix} \Sigma^R & \Sigma^K(\Sigma^<) \\ 0 & \Sigma^A \end{pmatrix}. \tag{7.215}$$

Below, the symbol $\breve{..}$ denotes the matrix in Keldysh space, and the spin-matrix structure of Green functions $G^{(R,A,K)}$ and $\Sigma^{(R,A,K)}$ is assumed if necessary. In the spin-degenerate case $G^{(R,A,K)}_{\alpha\beta} = G^{(R,A,K)}\delta_{\alpha\beta}$, in general $\breve{G}$ and $\breve{\Sigma}$ are matrices in Keldysh and spin spaces. It was shown that diagrammatic expansions for the matrix functions $\breve{G}$ and $\breve{\Sigma}$ are similar to corresponding expansions for equilibrium Green functions (see [4] and references there). If $\breve{\Sigma}$ is the known functional of $\breve{G}$, then the functions $G^{(R,A,K)}$ can be determined from the Dyson-Keldysh equation in differential form

$$\left[i\frac{\partial}{\partial t_1} - \breve{H}(t_1)\right]\breve{G} - \left\{\breve{\Sigma}\breve{G}\right\} = \breve{\delta}, \tag{7.216}$$

or in integral form

$$\breve{G} = \breve{G}_0 + \{\breve{G}_0\breve{\Sigma}\breve{G}\}, \tag{7.217}$$

where $\breve{\delta} = \breve{I}\delta_{\eta\eta'}\delta(t_1 - t_2)$, $\breve{I}$ is the unity matrix in Keldysh space,

$$\{AB\}_{\eta\eta'}(t_1, t_2) = \sum_{\gamma}\int dt_3 A_{\eta\gamma}(t_1, t_3)B_{\gamma\eta'}(t_3, t_2),$$

and $\breve{H}(t)$ is the single-particle Hamiltonian which determines the bare Green function $\breve{G}_0$. The self-energy $\breve{\Sigma}$ describes interactions. These equations are mathematically equivalent to the contour equation (7.210). Take now the components of this matrix equations.

The equations for the retarded (advanced) functions are:

$$\left[i\frac{\partial}{\partial t_1} - H\right]G^{R(A)} - \left\{\Sigma^{R(A)}G^{R(A)}\right\} = \delta(x_1 - x_2). \tag{7.218}$$

Or in integral form

$$G^{R(A)} = G_0^{R(A)} + \left\{G_0^{R(A)}\Sigma^{R(A)}G^{R(A)}\right\}. \tag{7.219}$$

And the equation for the Keldysh function is

$$\left[i\frac{\partial}{\partial t_1} - H\right]G^K - \left\{\Sigma^R G^K + \Sigma^K G^A\right\} = 0, \tag{7.220}$$

it is the same as the *Kadanoff-Baym equation* for the lesser function $G^<$. Or in integral form

$$G^K = \left\{G^R\Sigma^K G^A\right\}, \tag{7.221}$$

this equation is known as *Keldysh equation*. The time-independent equations are obtained then in usual way.

Self-consistent *GW* Approximation

One of the popular approximations is GW approximation, neglecting the vertex part. Here we present this equations already in explicit matrix notation.

For the self-energy shown in Fig. 7.4 we obtain

$$\Sigma^R_{\alpha\beta}(\epsilon) = i\int \frac{e^{i\eta\epsilon'}d\epsilon'}{2\pi}\Big[W^R_{\alpha\beta}(\epsilon')G^<_{\alpha\beta}(\epsilon-\epsilon') + W^<_{\alpha\beta}(\epsilon')G^R_{\alpha\beta}(\epsilon-\epsilon') + W^R_{\alpha\beta}(\epsilon')G^R_{\alpha\beta}(\epsilon-\epsilon') - \sum_\gamma v^R_{\alpha\gamma}G^<_{\gamma\gamma}(\epsilon')\delta_{\alpha\beta}\Big], \tag{7.222}$$

$$\Sigma^<_{\alpha\beta}(\epsilon) = i\int \frac{d\epsilon'}{2\pi} W^<_{\alpha\beta}(\epsilon')G^<_{\alpha\beta}(\epsilon-\epsilon'). \tag{7.223}$$

The usual self-consistent Hartree-Fock approximation is obtained from this self-energy if one neglects renormalization of the effective interaction $W_{\alpha\beta}$, and uses unperturbed values $v^R_{\alpha\beta}(\epsilon) = v^A_{\alpha\beta}(\epsilon) = U_{\alpha\beta}$, $v^<_{\alpha\beta}(\epsilon) = 0$.

For the polarization operator one gets

$$\Pi^R_{\alpha\beta}(\epsilon) = -i\int \frac{d\epsilon'}{2\pi}\left[G^<_{\alpha\beta}(\epsilon')G^A_{\beta\alpha}(\epsilon'-\epsilon) + G^R_{\alpha\beta}(\epsilon')G^<_{\beta\alpha}(\epsilon'-\epsilon)\right], \tag{7.224}$$

$$\Pi^<_{\alpha\beta}(\epsilon) = -i\int \frac{d\epsilon'}{2\pi} G^<_{\alpha\beta}(\epsilon')G^>_{\beta\alpha}(\epsilon'-\epsilon). \tag{7.225}$$

References

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