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Electron systems out of equilibrium: Nonequilibrium Green's function approach*

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This review deals with the state of the art and perspectives of description of nonequilibrium many-body systems using the nonequilibrium Green's function (NGF) method. The basic aim is to describe time evolution of the many-body system from its initial state over its transient dynamics to its long time asymptotic evolution. First, we discuss basic aims of transport theories to motivate the introduction of the NGF techniques. Second, this article summarizes the present view on construction of the electron transport equations formulated within the NGF approach to nonequilibrium. We discuss incorporation of complex initial conditions to the NGF formalism, and the NGF reconstruction theorem, which serves as a tool to derive simplified kinetic equations. Three stages of evolution of the nonequilibrium, the first described by the full NGF description, the second by a non-Markovian generalized master equation and the third by a Markovian master equation will be related to each other.

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1. Introduction

The aim of this article is to show, how to describe time evolution of one particle observables of many-body electron systems out of equilibrium within the nonequilibrium Green's function (NGF) approach. This article will be orientated on the nonequilibrium quantum field theory on the real time Schwinger–Keldysh contour. We will demonstrate that NGF provides useful tools, how to deal with

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several open questions of nonequilibrium statistical physics and enables to formulate the consistent quantum field theory of description of nonequilibrium quantum systems.

Recently developed experimental techniques enable us to observe details of time evolution of various electron systems far from equilibrium and to perform many interesting measurements on various natural or artificially prepared structures including mesoscopic (nanoscopic) systems,[1–3] where quantum processes, like quantum coherences, play decisive role. The growing area of nonequilibrium mesoscopic systems is naturally pervaded by open questions. Some of the problem open up newly during the research, some others have been resolved already, but in a provisional or an incomplete fashion. In general, the possibilities of the description of nonequilibrium many-body systems, not only mesoscopic ones, is far from being satisfactory due to the complexity of problems involved.

To understand complex behavior of many-body systems out of equilibrium, and to interpret results of various recent experiments on mesoscopic systems, it is necessary to combine and to further improve methods of quantum field theory,[4–7] many-body physics,[8–14] statistical physics,[15–40] and quantum transport theory.[38–58] Before going to details of the NGF approach, which uses knowledge of all these fields, we will mention problems, which every candidate on a successful theory of nonequilibrium systems has to tackle.

There are several key problems of nonequilibrium statistical physics to be understood on the way to adequate methods of the description of many-body systems out of equilibrium. Here we will mention some of them.

1.1. *Challenges, open questions, techniques*

- Proper description of many-body character of systems, which represents a real challenge already in equilibrium. In addition there is a problem with consistency of used approximations: to ensure this consistency we have to check conservation laws, which is often not an easy task;
- Formulation and incorporation of nontrivial initial conditions into the formalism;
- Understanding of different nonequilibrium regimes and their description from short to long times evolution;
- Influence of external fields on time evolution;
- Time evolution of open systems: formulation, what is the system and its surrounding representing reservoirs and proper treatment of interactions between these two parts, loss of quantum coherences and dissipation processes.

These problems are still far from their complete solutions. Due to complexity of problems and technical difficulties involved, several complementary approaches have been developed, which are dealing with various aspects of the above problems in more or less details. These are the following techniques: time dependent density functional theory (TDDFT),[59–69] time dependent dynamical mean-field theory (TDMFT)[70–74] and various versions of density matrix renormalization group

(DMRG) techniques.[75–80] We will not follow these "competitive" techniques to solve above mentioned key problems of nonequilibrium dynamics here.

1.2. *Nonequilibrium Green's functions*

In this review we will address problems of nonequilibrium statistical physics via NGFs techniques.[81–131]

As we will see later on this approach is based on methods of quantum field theory, and is able to deal with many important problems of statistical physics[17–27] and generalization of equilibrium many-body techniques[8–14] to nonequilibrium systems.

This approach has been used for such diverse nonequilibrium systems as particles in plasmas,[119,120] electrons, spins and phonons in various condensed matter systems like metals, semiconductors, superconductors and mesoscopic systems[132–175] or nuclei[106,128,176–181] as it is well documented also in the special volume dedicated to workshops and conferences about the NGF techniques.[111–115] It enables to describe nonequilibrium extended systems as well as mesoscopic (nanoscopic) systems, which have to be treated like open systems. The time evolution of observables can be calculated in various nonequilibrium regimes. In particular, the NGF formalism can also be conveniently used for the description of various steady state and equilibrium situations. NGF have been used not only for calculations of nonequilibrium occupation numbers, currents, current densities, but they have been also generalized to provide noise characteristics.[182–186] They have been able to describe such different processes like decay of initial correlations, dynamics of formation of correlations or quasiparticles, various transient and transport regimes, fast electron and spin dynamics, quantum coherence and decoherence processes, thermalization, physics of nonequilibrium cold atoms, e.g., dynamics of bosonic and fermionic systems in traps. Nowadays computers enable to solve complicated NGF equations for simplified, but often quite realistic models. Over the recent years many numerical calculations of the NGF equations have been performed.[111–115,120,129,187–192]

1.2.1. *Note on the NGF history*

The text of the article will not follow the historical developments of the NGF techniques. It is, however, useful to mention several key figures and lines of early developments of the NGF technique. The beginning of the NGF technique is related to Julian Schwinger at the end of the forties followed by works of his school represented e.g., by Martin, Kadanoff, Baym, Korenman, Craig, Horing. Later on two streams of developments have been related to the influential articles and the book written by Kadanoff and Baym[85] on the one side and Keldysh[89] and his followers on the other side.

The reader can find many interesting details about early developments of the NGF techniques in the following references.[81–101]

1.3. *Topics*

We may now formulate more precisely the subjects of this review: to overview the possibilities of the NGF techniques to describe nonequilibrium behavior of many-body systems either of bulk (very large) or small sizes for the whole time evolution of the system: from short to long times.

The general problems of nonequilibrium statistical physics mentioned above are mirrored in the following topics, which will be discussed in this article within the NGF frame.

1.3.1. *Formulation of transport theory and NGF*

The first topic of this paper is to formulate demands on transport theory to motivate the NGF approach to nonequilibrium systems, see Sec. 2.

We will introduce NGF in more detail in the following Sec. 3. An important aspect of the theory are controlled approximations. We will briefly mention related conservation laws like particle number and energy conservation, Ward identities and their generalization for nonequilibrium situations at the end of the section.

1.3.2. *Initial conditions*

The second topic deals with the task how to incorporate a nontrivial initial condition to the NGF formalism and implementation of the NGF techniques in the case of a fast transient process starting at a finite initial time and induced by a nonstationary initial condition and/or by an external field turned on at the initial time. The ways of incorporating complex initial conditions in the NGF methods are already known in several variants.[92,102,110,118,125,129,131,154,167,168,171,193–210]

We will discuss various approaches to initial conditions in Sec. 4.

1.3.3. *Transport in open systems*

There is still another aspect especially concerning electronic systems. Originally, the NGF based transport theory has been formulated for extended systems. The attention is presently shifting more and more toward the nano-structures and nano-devices. We will not deal with this aspect separately, but the presentation will be broad enough to encompass these systems.

The important point is that, in addition to the internal nonequilibrium dynamics of electrons driven perhaps by external fields, there may be expected important effects of a *changing* environment. Consider a suddenly opened thermal link between the system and a phonon bath. This will have an immediate influence on the electron Green's function, which must adapt to the new decay channels which will cause a loss of coherence of the propagation, reduce the relaxation time, etc. This process of adaptation will be gradual, having the character of a transient.

It turns out that there is a possibility of a uniform treatment of transient processes induced by external fields and by changes in the environment of the system.

This is achieved by reformulating the complex initial conditions for the many-particle state in terms of the history of its single-particle Green's function, and a consistently constructed description of the subsequent transient evolution.

To achieve this task we will introduce the time-partitioning formalism[168] which is suited for description of such process: the preparation stage is without the thermal contact and it defines the initial state for the follow-up, the process of relaxation of the electron sub-system induced by the suddenly attached thermal bath. We have thus at our disposal a Green's function formalism parallel to the Nakajima–Zwanzig projection method or to the path integral formulation, both developed within the density matrix technique.

1.3.4. *Reconstruction theorems*

The fourth topic of the review, see Sec. 5, is a general scheme, based on the so-called reconstruction theorem, which provides a scheme how to calculate NGF and in the same time reduction of the complete NGF machinery to kinetic equations, which will be discussed in more detail in the following Sec. 6.

1.3.5. *NGF and kinetic equations*

The last topic of this review, see Sec. 6, will close the circle: we will return to the formulation of the transport theory and derivation of quantum kinetic equations based on NGF techniques.

The initial period of a transient process is characterized by a complicated evolution known under the name of decay of initial correlations. If the external conditions are not very irregular, the system tends to a kinetic stage as the intermediate and late periods of the process. The evolution during the kinetic stage is characterized by availability of simplified dynamic equations, quantum kinetic equations, generally speaking. This is the contents of the famous Bogolyubov conjecture.[38–40]

This conjecture brings us to the question of a meaning of the simplified description of dynamics with the help of kinetic equations. Nowadays, due to powerful computers, it is already possible to solve directly equations for NGF in many cases. In the same time, however, it is important to have simplified description for studies of more complicated systems. As we will see the NGF method enables us to construct quantum kinetic equations in a well controlled way. These equations are easier to solve than the full NGF equations. This approach and its applications has been a flourishing and successful research field over the past 30 years. There are at least three reasons why to address the current state of this problem.

First, we have to ask, which advantages are offered by this approach as compared with the direct use of NGF — at the time of an important breakthrough in the area of NGF solvers and the increasing power of contemporary computers.

Second, this theme is not really new: the basic concept of an "Ansatz", an approximate truncation reducing the NGF equations to transport equations for a quantum distribution, has been introduced by Kadanoff and Baym more than

50 years ago.[85,109] Yet the procedure is still not quite routine, as witnessed by the continuing research activity, and the question Why? is fully justified.

A standard tool for this task has been one type of approximate decoupling of the particle correlation function going by name of Kadanoff–Baym Ansatz (KBA).[85,109] This Ansatz has been modified to a class of the so-called causal Ansatzes including a particularly successful generalized Kadanoff–Baym Ansatz.[109,116,118,125,129,211–217] We will describe an improved version we call Quasi-Particle Kadanoff–Baym Ansatz (QKBA).[125] It is based on the notion of nonequilibrium quasi-particle.[218]

The third reason is specific for electrons in atomic systems (we will have in mind the electrons as a specific example) (... solids). Just as it happened before for systems in equilibrium and the Kohn–Sham density functional theory, the systematic quantum field treatment of many-body systems out of equilibrium seems to face emerging competitors in the TDDFT, Time dependent dynamical mean-field theory (TDMFT) and various versions of density matrix renormalization group (DMRG) techniques.

1.4. *Advantages of NGF*

Problems indicated above are very often formulated within various reduced density matrix approaches.[219–239] It now makes sense to indicate the space open for the use of the largely complementary approach based on NGF.

First, they are congruous with tasks of finding one-particle observables, like currents and current densities, occupation numbers, spin densities.

Second, they accentuate a "holistic" look on the system, permitting any strength of the coupling between the system and the environment and easily providing the true observable quantities, like the currents within the leads, for example.

Third, they capture, thanks to their two-time nature, the coherence and decoherence in the system in a natural way. As a consequence, NGF appear to permit a controlled transition to simplified theories suitable for moderately fast transient processes and describing the time evolution by a quantum transport equation, in this case having the form of a generalized master equation (GME, a master equation with memory). Conditions for a further reduction to a plain master equation are also at hand.

It should be stated that the problems discussed in this review are posed on a general level. All results are equally valid for both, extended and small (mesoscopic) systems. Even if we have in mind mainly electrons out of equilibrium, these techniques can be easily adapted also to other fermions, and are widely used not only to describe fermions, but also to describe dynamics of bosons.

2. Transport Theory: Prototype Description of Nonequilibrium Systems

To define the "transport theory", we may start from the more general nonequilibrium quantum dynamics of a system described by the many-body statistical

operator (density matrix) $\mathcal{P}(t)$. The dynamics is driven by the full Hamiltonian $\mathcal{H}$ which can contain also an additive external time dependent disturbance $\mathcal{U}(t)$.

An initial state $\mathcal{P}_I$ at $t = t_I$ has also to be specified, and it may be an arbitrary equilibrium or out-of-equilibrium state. For any observable $\mathcal{X}$, the average value is $\langle\mathcal{X}\rangle_t = \mathrm{Tr}\mathcal{X}\mathcal{P}(t)$. A transport theory can be derived, if the observables are restricted to those, which are relevant to the observed sub-system and additive. This permits a description in terms of reduced quantities, namely the single-particle distributions. There are two possibilities.

Generalizing the Landau theory of Fermi liquids,[8–14] one makes use of the quasi-particle distribution $f(\mathbf{r}, \mathbf{k}, t)$. To obtain a closed theory, generalizing famous Boltzmann approach for classical systems, a time-local quantum Boltzmann equation is usually constructed.

The other possibility is to work with the single-particle density matrix $\rho(t)$ defined by the correspondence

$$\begin{aligned} \langle\mathcal{X}\rangle_t = \mathrm{Tr}\mathcal{X}\mathcal{P}(t) &\xrightarrow{\text{additive}\mathcal{X}} \langle\mathcal{X}\rangle_t \equiv \bar{X}(t) = \mathrm{Tr}X\rho(t), \\ \mathcal{P}(t) &\xrightarrow{\text{reduction}} \rho(t)\,. \end{aligned} \tag{2.1}$$

In other words, the average values are, for all additive (single-particle) observables A, given by the single particle reduced density matrix:

$$A_{\mathsf{Av}}(t) = \mathrm{Tr}(\rho(t)A)\,, \tag{2.2}$$

$$\rho(x, y, t) = \mathrm{Tr}(\mathcal{P}(t)\psi^\dagger(y)\psi(x))\,, \tag{2.3}$$

Here $\mathcal{P}$ is the full many-body statistical operator, and $\psi^\dagger$ and ψ are field operators for particles (often electrons in this article).

In particular, the local particle density n of electrons is given by

$$n(x, t) = \rho(x, x, t)\,. \tag{2.4}$$

For a single band $\epsilon(k)$, the local current density j equals

$$j(x, t) = \frac{1}{2m}\left(\frac{\partial\epsilon}{\partial k}(i\nabla_x) + \frac{\partial\epsilon}{\partial k}(-i\nabla_y)\right)\rho(x, y, t)|_{y=x}\,. \tag{2.5}$$

We will now discuss these two approaches starting from the Boltzmann equation.

2.1. *Prototype transport equation: Boltzmann equation*

A prototype of all kinetic equations, the Boltzmann equation (BE) of classical physics[15,16] reads

$$\frac{\partial f}{\partial t} - \mathsf{drift}[f(t)] = I_{\mathrm{in}}[f(t)] - I_{\mathrm{out}}[f(t)]\,, \tag{2.6}$$

where the drift term is the classical Poisson bracket

$$\mathsf{drift}[f(t)] = \frac{\partial\varepsilon}{\partial k}\frac{\partial f}{\partial r} - \frac{\partial\varepsilon}{\partial r}\frac{\partial f}{\partial k}\,. \tag{2.7}$$

This is, in principle, an equation for a single particle distribution function $f(k,r,t)$ in phase space, representing balance between the drift of particles (with energy $\varepsilon = \epsilon_k + U(r,t)$ and velocity $(\partial/\partial k)\varepsilon = (\partial/\partial k)\epsilon_k$ in the external force field $-(\partial/\partial r)\varepsilon = -(\partial/\partial r)U$), as given by the left-hand side of the BE, and the irreversible evolution due to collisions described by the scattering integrals $I_{\rm in}$ and $I_{\rm out}$ on the right-hand side.

2.2. *Transport theory: Physical concepts*

To understand physics beyond the Boltzmann equation, it will be important to recall several fundamental ideas, which run through the development of the transport theory. As will be seen, the physical principles of the contemporary NGF approach are not different from those which were in the minds of the founders of nonequilibrium statistical physics. The issues remain, the understanding and attitudes change. We pick up just the following topics.

I. The central idea of the transport theory has always been a **reduced description** of the system. The relevant information about a gas of particles was contained in the one-particle distribution function $f(x,p,t)$. The essential step was to search for a closed equation governing this function, that is for the transport equation. This was only possible, if, say, the description of binary collisions in the gas was given in terms of the function f. As a systematic program, this seems to appear first in the work of Chapman and Enskog[15,16] but the principle dates back to Boltzmann himself with his Stosszahlansatz for the binary distribution f_{12} expressed as $f_{12} \sim f_1 \times f_2$. This type of factorization, or, more generally, decoupling of higher correlation functions was systematically developed in the BBGKY technique. We have to say more about Bogolyubov, to whom we owe the postulate[38–40] that *in a chaotized many-body system all higher particle correlation functions become a functional of the distribution function.*

Thus

$$f_{12} \xrightarrow{\text{chaot.}} \Phi[f_1, f_2]\,. \tag{2.8}$$

The functional has yet to be specified, but this is of secondary importance. As will be described later, the KB Ansatz also singles out the one-particle distribution as the determining characteristic of the nonequilibrium system. This brings us to the **reconstruction problem**: under which conditions the full description of the many-body interacting system can be built up from the knowledge of single-particle characteristics? This seemingly outrageous question was seriously treated in several contexts. We will discuss later two of them: the TDDFT and the Generalized Kadanoff–Baym Ansatz related techniques.

II. The second crucial notion is the **hierarchy of characteristic times**. There are three intrinsic times related to a many-particle interacting system. In a reminiscence of a non-dilute gas, they are often identified as the *collision duration time* $\tau_c = a/\bar{v}$, the *collision time* $\tau_r = \ell/\bar{v}$ and the *hydrodynamic time* $\tau_h = L/\bar{v}$. Here,

$\bar{v}$ is the average thermal velocity for a classical gas, the Fermi velocity v_F for a degenerate Fermi gas. The characteristic lengths are: a is the interaction potential range (particle size), ℓ is the mean free path (mean inter-particle distance), L is the characteristic length of spatial inhomogeneities in the system. In the modern interpretation, the three times are: $\tau_c \cdots$ the chaotization time characterizing the decay of correlations, $\tau_r \cdots$ the relaxation time characterizing the thermalization of the system (local relaxation) and, finally, $\tau_h \cdots$ characterizes the process of relaxation of spatial inhomogeneities. In "normal" situations, the three times obey the inequality

$$\tau_c \ll \tau_r \ll \tau_h \,, \tag{2.9}$$

separating the chaotization stage, the kinetic stage, and the hydrodynamic stage. This structuring of the spontaneous return to equilibrium was also introduced by Bogolyubov; he postulated Eq. (2.8) only for times later than the chaotization time τ_c. The Boltzmann equation proper corresponds to the limit

$$0 \leftarrow \tau_c \lll \tau_r \lll \tau_h \to \infty \,. \tag{2.10}$$

We will be mostly concerned with the opposite, more realistic case, when the distinction between τ_c and τ_r will be less sharp. Further, the time range of interest will be specified by the external fields. For example, an optical pulse is characterized by its duration, the ground period of the signal and its Rabi period measuring the pulse strength. These times should be compared with the intrinsic times of the system. This will, at last, specify the situation and the necessary version of transport theory used.

III. The last basic concept is that of the **quasi-particles**.[8–14] With that, we, as a matter of fact, move over to the quantum realm. There are several streams merging into the generalized notion of a quasi-particle. Firstly, the polaron, an electron dragging along a cloud of lattice polarization. In the quantum field language, the electron is dressed by virtual phonons. This compound object has some features characteristic of a particle, like a dispersion law (renormalized by the self-energy), which has an operational meaning in experiments. The self-energy is typically complex, and this leads to the finite life-time τ of the quasi-particles, closely related to the transport relaxation time τ_r. Secondly, and even more to the point, in a non-dilute system of interacting particles, their individuality is suppressed by mutual correlations and the use of a transport equation seems to be hopeless. However, the weakly excited states may appear to mimic a gas of weakly interacting quasi-particles. This was at the bottom of the Landau theory of the Fermi liquid, whose part was a proper adaptation of the Boltzmann equation. This approximate, but highly precise description of the Fermion systems had, of course, a number of predecessors, like the Sommerfeld electrons in simple metals, and parallels, like the quasi-particles in nuclei, where the self-energy has been originally introduced under the name of the optical potential. It might seem that the quantum transport equations for strongly interacting systems will all deal with the quasi-particles. This

is, to some extent, true. However, the quasi-particles are vulnerable and elusive objects and cease to exist under some harsher conditions, like beyond the quasi-classical regime, for strong and/or transient disturbances, or if the system itself is not favoring their existence. This can sometime be judged by the Landau–Peierls criterion. Take the gas of quasi-particles with energies around the Fermi level E_F and a lifetime τ due to impurity scattering. The criterion reads: if $\tau \simeq \hbar/E_F$, the BE-like transport theory is not applicable. Now $\hbar/E_F$ can be interpreted as the "quasi-particle formation time" τ_Q. If $\tau \simeq \tau_Q$, the quasi-particle decays before having formed. On the other hand, τ is closely related to τ_r, whereas τ_Q appears to play the role of τ_c. The Landau–Peierls criterion thus says that if the quasi-particles do not form, then τ_r becomes comparable to τ_c and the condition (2.10) is not obeyed.

2.3. *Boltzmann equation for quantum systems*

After overviewing the basic concepts beyond the Boltzmann equation and the transport theory in general we can return to the properties of the Boltzmann equations to discuss possibilities how to generalize it toward quantum systems.

First of all we note that in the scattering integrals of the Boltzmann equation, collisions are approximated as instant randomizing events, so that the BE is Markovian. This is in agreement with the first inequality in (2.10). The other inequality demands all inhomogeneities in the system, including external fields, to be smooth enough to allow a sufficient time for local equilibration.

The BE has been used for many classical systems and it was extended very early also to the transport by quantized particles, in particular by electrons in metals. The quantum effects were incorporated mainly in the scattering integrals where the collision rates were calculated by the Fermi Golden Rule and the exclusion principle was taken into account by means of the Pauli blocking factors.

The average values of additive observables were calculated from formulas taken over from classical kinetic theory of gases. Thus, the particle density and the particle current density were

$$n(r,t) = \int \frac{dk}{(2\pi)^3} f(k,r,t)\,, \tag{2.11}$$

$$j(r,t) = \int \frac{dk}{(2\pi)^3} \frac{\partial \epsilon}{\partial k} f(k,r,t)\,. \tag{2.12}$$

Now, we depart from the BE in the direction toward quantum dynamic equations far from equilibrium. There are several extensions of the BE we will first explore separately:

(1) From particles to quasi-particles. The interaction energy will no longer be negligible, but will be renormalized in the quasi-particle transformation.
(2) From near-equilibrium to "arbitrary" nonequilibrium. This will be reflected in the memory of the system and taken into account by the non-Markovian GME.

2.3.1. *Quasi-particles and transport*

In dense systems, the particle interactions cannot be reduced to rare collisions randomizing the motion of otherwise free particles. Quantum statistics for such systems at near-equilibrium is often well described by the Landau theory of quasi-particles. In this theory, weakly excited states of the interacting particles are described as a gas of quasi-particles with energy

$$\varepsilon(k, r, t) = \epsilon_k + U_{\text{eff}}(r, t) + \sigma(\varepsilon, k, r, t)\,, \tag{2.13}$$

where U_{eff} may include the mean-field part of the interaction and the self-energy σ describes the mass renormalization. The quasi-particles are coupled by a weak residual interaction.

2.3.2. *Quantum kinetic equation for quasi-particles*

These quasi-particle features have consequences for transport properties, which are described by the Landau kinetic equation. It has exactly the structure of the BE (2.6). However, the energy entering the drift term is now the quasi-particle energy ε. Scattering integrals I_{in} and I_{out} contain scattering rates calculated again by the Fermi Golden Rule, but with the residual interactions reflecting that they are reduced by the many-particle wavefunction renormalization. Finally, the function $f(k, r, t)$ is the *quasi-particle distribution function.*

Because of its intuitive character, the "Boltzmann" equation for quasi-particles provided many insights into the behavior of nonequilibrium many-particle systems. In particular, it offered a retrospective explanation of the over-successful Sommerfeld model of metals with noninteracting electrons responding to external fields. While various modifications of the BE-like approach have been applied successfully to many systems and situations, there are also many physical cases, in which it is bound to fail. The limitations of the Boltzmann equation include: (1) The BE well describes quantum systems if the quasi-particle picture is justified. This may no longer be valid in highly nonequilibrium quantum systems. (2) It is based on the intuitive idea of instant collisions between quasi-particles, which requires the collision duration time to be very short. (3) At the same time, the BE will not be well suited to describe systems with abrupt changes in space, including small structures, where quantum effects are essential and the quasi-classical approach hidden behind the BE is far from being sufficient.

2.3.3. *Observables and quantum distribution function*

Relations between the quasi-particle distribution function and the expectation values of observables are more complicated than (2.11), (2.12). For example, the expression for current density must incorporate the back-flow accompanying the motion of quasi-particles. Rules for evaluating observables have been from the outset an integral part of the Landau equilibrium theory. A natural question emerges: which is

the relation between the quasi-particle distribution function f and the expectation values out of equilibrium?

Our task is then to find a functional relation

$$\{f,\, A\} \mapsto A_{\mathsf{Av}} = \mathrm{Tr}(\rho A)\,,$$

which is equivalent to finding a functional $\rho[f]$ associating the single-particle density matrix with any given quasi-particle distribution. To relate the reduced density matrix ρ with the distribution function $f(k,r,t)$ it is convenient to express ρ in the (k,r) representation. This can be done in different ways, but we choose the so-called Wigner representation

$$\tilde{\rho}(k,r,t) = \int dx \mathrm{e}^{-ikx} \rho\left(r + \frac{x}{2}, r - \frac{x}{2}, t\right). \tag{2.14}$$

The reduced density $\tilde{\rho}(k,r,t)$ in the Wigner representation is commonly known under the name of Wigner distribution. It can be viewed as a distribution of electrons in the phase space and the expectation values

$$n(r,t) = \int \frac{dk}{(2\pi)^3} \tilde{\rho}(k,r,t)\,, \tag{2.15}$$

$$j(r,t) = \int \frac{dk}{(2\pi)^3} \frac{\partial \epsilon}{\partial k} \tilde{\rho}(k,r,t)\,, \tag{2.16}$$

have the same form as in the Boltzmann theory.

2.3.4. *Wigner and quasi-particle distributions*

These suggestive properties of the Wigner distribution should not lead us to the conclusion that this function is the "right" quantum generalization of the classical distribution function and that the proper quantum generalization of the Boltzmann equation will be a kinetic equation of the Boltzmann form (2.6) for the Wigner distribution function. We can see that this is not the case from the following argument given already by Landau.

Consider a homogeneous system. In equilibrium, the BE-like kinetic equation for electrons is solved by the Fermi–Dirac function regardless of the interactions in the system. Thus, at zero temperature, the distribution f jumps from 1 to 0 at the Fermi level. In contrast, the Wigner distribution describes the occupation numbers of true particles and it differs from the Fermi–Dirac function by depletion of the momentum states below the Fermi level. These missing states emerge as states above the Fermi level, where they form the so-called high-momenta tails of the Wigner function. The step of the distribution $\tilde{\rho}$ is accordingly reduced to $1-2z$, where z is the renormalization constant for quasi-particles at the Fermi level.

We may summarize that the quasi-particle kinetic theory consists of two steps. First, the quantum kinetic equation is solved for the quasi-particle distribution. Second, the true quantum particle distribution is constructed by means of the functional $\rho[f]$ and the expectation values of the observables are calculated.

2.4. *Generalized master equations: beyond the quantum kinetic equations*

In this section, we will not follow the Boltzmann like direction, which is the description using the concept of a quasiparticle distribution function and is suited for "slow" processes, like a stationary transport. Instead of this approach, we will now discuss the second possibility how to develop a quantum transport theory: we will deal with description based on the single particle density matrix ρ. So, the aim will be to introduce (and later on to derive from the full set of the NGF equations) a general master equation (GME) which governs ρ.

A closed quantum transport equation for ρ has the general form

$$\frac{\partial \rho}{\partial t} - \text{drift} = \Phi_t[\rho(\tau); \tau < t]\,, \tag{2.17}$$

where "drift" means the bare one-particle dynamics and the effect of all interactions is contained in the generalized collision term on the right-hand side. The functional Φ_t has a form parametrically dependent on time and is functionally dependent on the full history of the distribution function itself. Thus, the equation is a one-particle version of the so-called generalized master equation. This is very formal. We should now address several questions, whose answers will depend on the physical nature of the system under consideration:

- ◇ Proof of the existence of the quantum transport equation.
- ◇ Explicit construction of the generalized collision term Φ_t.
- ◇ Introduction of the initial conditions at t_0, both explicitly and also through the form of Φ_t.

We intend to analyze these points from the angle of the Green's functions. It will be seen, however, that physical principles of the contemporary NGF approach are very close to those which were formulated by the founders of nonequilibrium statistical physics.

As already mentioned, quantum kinetic equations of the Boltzmann type have a restricted range of validity and these limits can be transgressed only by resorting to a more general framework, permitting, at least in principle, to start from a fully quantum description and work directly with an equation for the reduced density matrix (or the equivalent Wigner function), the so-called quantum generalized master equation (GME). There are several approaches and approximations leading to the GME. Its general form (2.17) can be rewritten as

$$\begin{aligned} \frac{\partial \rho}{\partial t} - \mathsf{drift}[\rho(t)] &= \text{interaction term}\,, \\ \frac{\partial \rho}{\partial t} + i[\underbrace{T + U_{\text{eff}}(t)}_{H_0}, \rho(t)]_- &= \int_{-\infty}^{t} d\bar{t} F[\rho(\bar{t})]\,. \end{aligned} \tag{2.18}$$

This equation is shown in an entirely symbolic form on the first line, and it is not really explicit on the second one either. We will discuss the detailed structure of this

type of equation below. Here, we only touch its most salient features. The GME is a closed equation for ρ. It is non-Markovian, because the interaction term is nonlocal in time.

At the end of Sec. 2.3.2, we pointed out three important limiting factors for the use of the quantum kinetic equations. These factors will now be discussed from the point of view of the GME.

2.4.1. *GME is an equation for ρ*

Equation (2.18) is a dynamical equation for the distribution of particles instead of quasi-particles as was the case of the BE. Therefore, it does not hinge on the use of quasi-particles, and it is free of the physical limitations necessary for introducing the gas of quasi-particles. In particular, the system may evolve under conditions which do not permit the quasi-particle states to consolidate. This does not preclude using some of the quasi-particle features where applicable. Thus, the left-hand side of the equation describes bare particles drifting under the influence of the effective field. All other features involving interactions are included in the right-hand side. It may be possible to transfer parts of the right-hand side to the drift term and achieve evolution in re-normalized bands.

2.4.2. *Interaction term*

We prefer to call the right-hand side of (2.18) interaction term rather than scattering integrals. In principle, the GME is exact, so that the interaction term must incorporate all of the sub-dynamics of ρ reflecting not only particle collisions, but also the short time dynamics, off-shell propagation and coherence between the collisions and with the external fields, multiparticle correlations, gradual saturation of the scattering rates after the onset of a nonequilibrium process, etc.

It is remarkable that all this rich physics can be absorbed in an interaction term depending only on the one-particle density matrix. This is made possible by the subtle memory effect reflected in the time integration over the full depth of the past in (2.18). Clearly, this form of the interaction term agrees with the Bogolyubov postulate quoted above in Sec. 2.2, at least for times beyond τ_c after the onset of the process. We will return to the related reconstruction theorems later on.

2.4.3. *Quasi-classical expansion*

In the GME (2.18), neither the drift term, nor the interaction integral, are restricted to smooth variation of the fields and distributions in space. The drift term is given by the quantum Poisson bracket rather than by the classical one appearing in (2.7). For smooth functions, it can be quasiclassically expanded; the formal expansion parameter is $\hbar^2$. For the Wigner distribution $\tilde{\rho}$ defined in Eq. (2.14), we obtain,

writing, by exception, the Planck constant explicitly:

$$\begin{aligned}&\mathsf{drift}[\rho(t)] = (i\hbar)^{-1}[T + U_{\mathrm{eff}}(t), \rho(t)]_- \to \\ &\mathsf{drift}[\tilde{\rho}(t)] = \frac{\partial \epsilon}{\partial p}\frac{\partial \tilde{\rho}}{\partial r} - \frac{\partial U_{\mathrm{eff}}}{\partial r}\frac{\partial \tilde{\rho}}{\partial p} - \frac{\hbar^2}{3!}\left(\frac{\partial^3 \epsilon}{\partial p^3}\frac{\partial^3 \tilde{\rho}}{\partial r^3} - \frac{\partial^3 U_{\mathrm{eff}}}{\partial r^3}\frac{\partial^3 \tilde{\rho}}{\partial p^3}\right) + \cdots .\end{aligned} \tag{2.19}$$

This expansion, suited for comparison of the GME in the quasiclassical limit with the corresponding kinetic equation is, in fact, a Fourier transformed expansion around the space diagonal $x_1 = x_2$.

3. NGF Approach to Nonequilibrium Systems: Basic Concepts

This section is the first of the central parts of the paper, in which we introduce and formally elaborate on the NGF.[102–131] Later on we will discuss the NGF method from two points of view:

(1) To describe properly the dynamics of nonequilibrium systems by directly solving full set of equations for the NGF;
(2) To derive and analyze the simplified nonequilibrium dynamic equations of either the BE or the GME type as we discussed them in previous sections of this article.

3.1. *Definition of the system*

The NGF theory is formulated for closed systems, which have a well defined Hamiltonian and undergo a strictly unitary evolution. This does not preclude irreversible evolution, if at least some parts of the whole system are extended and possess a continuous spectrum. In fact, a finite isolated system possessing bound states would be a difficult case for the present approach. The system as a whole has to incorporate both the "relevant" sub-system and all other components, like thermal baths an particle reservoirs. The relevant sub-system then appears as open and its evolution has the signatures of irreversibility. The baths are typically taken as ideal, that is inert, not participating in the dynamics, but acting to impose temperature and/or chemical potential. The state of the system is then specified by the density matrix of the relevant sub-system and the parameters of its environment, its dynamics is governed by the corresponding Hamiltonian.

We have already given practical reasons, why the systems we will specifically consider will be electrons under various external conditions and driven by classical external fields. They will be interacting by instantaneous pair forces, typically of Coulomb origin.

The Hamiltonian of the system will be denoted $\mathcal{H}(t)$. Calligraphic letters relate to many-body quantities. The Hamiltonian has several parts of different nature:

$$\mathcal{H} = \mathcal{H}_0(t) + \mathcal{W}\,, \quad \mathcal{H}_0(t) = \mathcal{T} + \mathcal{V} + \mathcal{H}'_{\mathrm{e}}(t)\,. \tag{3.1}$$

$\mathcal{H}_0(t)$ is the one-particle part of the Hamiltonian. For a quiescent spatially homogeneous system, this would be just the kinetic energy operator $\mathcal{T}$. In general, it also incorporates $\mathcal{V}$ which accounts for static internal fields specifying the geometry, atomic composition and other characteristics. $\mathcal{V}$ thus uniquely defines the system under consideration. The departure from the equilibrium state is driven by $\mathcal{H}'_{\rm e}(t)$ which for simplicity is assumed to include only scalar local external fields. Finally, $\mathcal{W}$ is the pair interaction term, as characterized above.

In a second-quantized form written for fermions, we have

$$\begin{aligned}\mathcal{H}_0(t) &= \int dx\psi^\dagger(x)\left(-\frac{1}{2m}\Delta + V(x)\right)\psi(x) + \int dx\psi^\dagger(x)V_{\rm e}(x,t)\psi(x)\,,\\ &= \int dx\psi^\dagger(x)h_0(t)\psi(x)\,, \qquad (3.2)\end{aligned}$$

$$\mathcal{W} = \frac{1}{2}\iint dxdy\psi^\dagger(x)\psi^\dagger(y)w(x,y)\psi(y)\psi(x)\,, \qquad (3.3)$$

$$x = \{\mathbf{r},\sigma\}\,, \quad \int dx = \int d\mathbf{r}\sum_\sigma\,,$$

$$\begin{aligned}[\psi(x),\psi^\dagger(x')]_+ &= \delta(x-x') \equiv \delta(\mathbf{r}-\mathbf{r}')\delta_{\sigma\sigma'}\,,\\ [\psi(x),\psi(x')]_+ &= 0\,, \quad [\psi^\dagger(x),\psi^\dagger(x')]_+ = 0\,.\end{aligned} \qquad (3.4)$$

3.2. *Evolution operator*

In the nonequilibrium physics, the Hamiltonian determines primarily the time evolution of the system from given initial conditions. For example, for an initial state given by a (many-body) wavefunction $|\Psi\rangle_{t=t_i} = |\Psi_i\rangle$ at an initial time $t_{\rm I}$, we have to solve the Schrödinger equation

$$i\frac{\partial}{\partial t}|\Psi\rangle_t = \mathcal{H}(t)|\Psi\rangle_t\,. \qquad (3.5)$$

This solution can be formally written in a form universal for all initial conditions employing the evolution operator $\mathcal{S}$:

$$|\Psi\rangle_t = \mathcal{S}(t,t_{\rm I})|\Psi_{\rm I}\rangle\,. \qquad (3.6)$$

The evolution operator will serve as a universal tool in this paper and we shall discuss some of its properties now.

3.2.1. *Properties of the evolution operator*

Given the Hamiltonian, its evolution operator $\mathcal{S}(t,t')$ is a function of two time arguments. It is determined by the Schrödinger equation and the initial condition at equal time arguments, consistently with Eq. (3.6):

$$i\frac{\partial}{\partial t}\mathcal{S}(t,t') = \mathcal{H}(t)\mathcal{S}(t,t')\,, \quad \mathcal{S}(t',t') = \mathbf{1}\,. \qquad (3.7)$$

Equivalently, it is given by an analogous initial value problem for the other time variable:

$$i\frac{\partial}{\partial t'}\mathcal{S}(t,t') = -\mathcal{S}(t,t')\mathcal{H}(t')\,, \quad \mathcal{S}(t,t) = \mathbf{1}\,. \tag{3.8}$$

The evolution operator obeys two basic rules, it is unitary and has the group property:

$$\mathcal{S}(t,t')\mathcal{S}^\dagger(t,t') = \mathcal{S}^\dagger(t,t')\mathcal{S}(t,t') = \mathbf{1}\,, \tag{3.9}$$

$$\mathcal{S}(t,t') = \mathcal{S}(t,t'')\mathcal{S}(t'',t')\,. \tag{3.10}$$

The so-called group property expresses a composition rule for two subsequent time segments of evolution. Because the evolution is unitary, there is no restriction on the values of the times involved, the intermediate time may in fact precede both terminal times, etc. As a consequence, the following identities are obtained in particular:

$$\mathcal{S}^\dagger(t,t') = \mathcal{S}^{-1}(t,t') = \mathcal{S}(t',t)\,. \tag{3.11}$$

3.2.2. *Schrödinger and Heisenberg pictures*

In the customary representation of quantum dynamics, the Schrödinger picture, the quantum states evolve in time. For pure states, this evolution is described by Eq. (3.6). Similarly, the evolution operator allows to express the evolution of a general state of the many-body system by its state operator $\mathcal{P}$ (many-body density matrix) from an initial time t_I to the time t as

$$\mathcal{P}_\mathrm{S}(t) = \mathcal{S}(t,t_\mathrm{I})\mathcal{P}(t_\mathrm{I})\mathcal{S}^\dagger(t,t_\mathrm{I})\,. \tag{3.12}$$

The calligraphic capital $\mathcal{P}$ is used to denote capital Greek Rho rather than Roman P. The label indicates the Schrödinger picture.

In Green's function theory, it is preferable to work in the Heisenberg picture, in which the state operator is time independent and the time evolution is transferred to the operators of observables such that the resulting average values are the same in both pictures:

$$\begin{aligned}\langle\mathcal{X}\rangle_t = \mathrm{Tr}(\mathcal{P}_\mathrm{S}(t)\mathcal{X}) &= \mathrm{Tr}(\mathcal{S}(t,t_\mathrm{I})\mathcal{P}(t_\mathrm{I})\mathcal{S}^\dagger(t,t_\mathrm{I})\mathcal{X}(t)) \\ &= \mathrm{Tr}(\mathcal{P}(t_\mathrm{I})\underbrace{\mathcal{S}^\dagger(t,t_\mathrm{I})\mathcal{X}(t)\mathcal{S}(t,t_\mathrm{I})}_{\mathcal{X}_\mathrm{H}(t)})\,.\end{aligned} \tag{3.13}$$

Clearly, the Heisenberg operator may combine two distinct time dependences, the explicit one, and the other one reflecting the evolution of the system. We get the following equation of motion for the Heisenberg operator of any observable and the associated initial value problem:

$$i\frac{\partial\mathcal{X}_H(t)}{\partial t} = [\mathcal{X}_H(t),\mathcal{H}_H(t)]_- + i\left(\frac{\partial}{\partial t}\mathcal{X}_S(t)\right)_H\,, \quad \mathcal{X}_H(t_\mathrm{I}) = \mathcal{X}_S(t_\mathrm{I})\,. \tag{3.14}$$

The operators in the Heisenberg picture can be written in the form derived in (3.13), or in its modification employing (3.11):

$$\mathcal{X}_{\mathrm{H}}(t) = \mathcal{S}^{\dagger}(t,t_{\mathrm{I}})\mathcal{X}(t)\mathcal{S}(t,t_{\mathrm{I}}) = \mathcal{S}(t_{\mathrm{I}},t)\mathcal{X}(t)\mathcal{S}(t,t_{\mathrm{I}})\,. \tag{3.15}$$

The second form is suggestive of evolution from t_{I} to t and back. This idea is at the heart of the Schwinger–Keldysh NGF formalism, as will become clear soon.

The Heisenberg picture may be seen to offer two important advantages. First, the averaging at all times is performed over the same time-independent many-body state. Second, in this manner, it is possible to obtain averages of any number of observables detected at their individual times and in this way to study space–time correlations of an arbitrary order.

3.2.3. *Explicit expressions for the evolution operator*

Finding the evolution operator is an immensely difficult task, except for simple special cases. One problem is an admitted time dependence of the Hamiltonian. If the Hamiltonian is time-independent, Eq. (3.7) is easily solved by

$$\mathcal{S}(t,t') = e^{-i\mathcal{H}\cdot(t-t')}\,. \tag{3.16}$$

For a time-dependent Hamiltonian, Eq. (3.16) is easily generalized in the rather exceptional case that $\mathcal{H}(t)$ can be diagonalized for all times in the same basis:

$$\mathcal{S}(t,t') = e^{-i\int_{t'}^{t} d\tau \mathcal{H}(\tau)}\,, \quad [\mathcal{H}(t_1),\mathcal{H}(t_2)]_- = 0\,, \tag{3.17}$$

In the general case, a solution extending the last expression can be given with the use of the time-ordering (chronological) operator T:

$$\mathcal{S}(t,t') = \mathsf{T}e^{-i\int_{t'}^{t} d\tau\, \mathcal{H}(\tau)}\,, \quad [\mathcal{H}(t_1),\mathcal{H}(t_2)]_- \neq 0\,, \quad t > t'\,. \tag{3.18}$$

To understand the structure of this deceivingly simple formula, we have to expand the exponential into the power series. The T "operator" acts on operators. It is linear and in a product of several operators, it rearranges them in the order of their time arguments, the latest time coming first on the left. For two operators this means

$$\mathsf{T}\{A(t)B(t')\} = A(t)B(t') \quad t > t'\,, \tag{3.19}$$

$$\mathsf{T}\{A(t)B(t')\} = B(t')A(t) \quad t' > t\,. \tag{3.20}$$

The expression (3.18) for $\mathcal{S}$ becomes

$$\mathcal{S}(t,t') = \sum_n \frac{1}{n!}(-i)^n \int_{t'}^{t}\cdots\int_{t'}^{t} dt_1\cdots dt_n\, \mathsf{T}\{\mathcal{H}(t_1)\cdots\mathcal{H}(t_n)\}\,, \tag{3.21}$$

Consider now the nth order term of the series. The time-ordering operator permutes the n factors in all possible manners and yields a nonzero result when the permuted

times have their values ordered. Thus the integral splits into $n!$ contributions mutually equal because of the symmetric structure of the integral and it is enough to keep just one multiplied by $n!$. With the notation for permutations

$$P:\ \{1,\dots,n\}\ \to\ \{1_P,\dots,n_P\}\,,$$

we have

$$\begin{aligned}\mathcal{S}(t,t') &= \sum_n \frac{1}{n!}(-i)^n \sum_P \int_{t'}^{t} dt_{1_P}\cdots\int_{t'}^{t_{(n-1)_P}} dt_{n_P}\mathcal{H}(t_{1_P})\cdots\mathcal{H}(t_{n_P})\\ &= \sum_n (-i)^n \int_{t'}^{t} dt_1\cdots\int_{t'}^{t_{(n-1)}} dt_n\mathcal{H}(t_1)\cdots\mathcal{H}(t_n)\,. \end{aligned} \tag{3.22}$$

The last series is the well-known iterative solution of the initial value problem (3.7) which is conveniently recast into a Volterra integral equation for that purpose:

$$\mathcal{S}(t,t') = \mathbf{1} - i\int_{t'}^{t} dt_1\mathcal{H}(t_1)\mathcal{S}(t_1,t')\,. \tag{3.23}$$

In a similar fashion, (3.8) has the integral form

$$\mathcal{S}(t,t') = \mathbf{1} + i\int_{t}^{t'} dt_1\mathcal{S}(t,t_1)\mathcal{H}(t_1) \tag{3.24}$$

and its solution for $t' > t$ is given by

$$\mathcal{S}(t,t') = \tilde{\mathsf{T}}e^{+i\int_t^{t'} d\tau\,\mathcal{H}(\tau)}\,,\quad t' > t\,. \tag{3.25}$$

This is of the same structure as Eq. (3.18), but involving the anti-chronological time-ordering operator $\tilde{\mathsf{T}}$ which orders the operators in the order of time arguments increasing from the right to the left.

3.2.4. *Dirac picture*

For an actual work, often neither of the two pictures, Schrödinger or Heisenberg, is suited, and an intermediate Dirac picture, encompassing both as limiting cases, has to be introduced. The general scheme of the Dirac picture starts from decomposing the Hamiltonian in question into two parts,

$$\mathcal{H} = \mathcal{H}_{\mathsf{F}} + \mathcal{H}_{\mathsf{P}}\,. \tag{3.26}$$

Although it is not indicated explicitly, all components of the Hamiltonian may depend on time explicitly. The F ("free") component of the Hamiltonian is considered as a reference, while the P ("perturbation") component has to be included as an additional perturbation. This division is, of course, possible in different ways. For example, the pair interaction is taken as the perturbation, and the Dirac picture then serves to develop the many-body perturbation expansion. Alternatively, the external field enters as the perturbation, and the Dirac picture leads to the general nonlinear response theory.

The average values of observables should not depend on the picture used, and this will lead us directly to the Dirac picture definition by extending the procedure outlined in Eq. (3.13). The idea is to let the observable $\mathcal{X}$ undergo the "free" evolution and the state $\mathcal{P}$ to compensate for the difference between the free and the full evolution. Starting again from the Schrödinger picture, we get

$$\begin{aligned}\langle\mathcal{X}\rangle_t &= \mathrm{Tr}(\mathcal{P}_{\mathrm{S}}(t)\mathcal{X}) = \mathrm{Tr}(\mathcal{S}(t,t_{\mathrm{I}})\mathcal{P}(t_{\mathrm{I}})\mathcal{S}^{\dagger}(t,t_{\mathrm{I}})\mathcal{X})\\ &= \mathrm{Tr}(\mathcal{S}(t,t_{\mathrm{I}})\mathcal{P}(t_{\mathrm{I}})\mathcal{S}^{\dagger}(t,t_{\mathrm{I}})\mathcal{S}_{\mathsf{F}}(t,t_{\mathrm{I}})\underbrace{\mathcal{S}_{\mathsf{F}}^{\dagger}(t,t_{\mathrm{I}})\mathcal{X}\mathcal{S}_{\mathsf{F}}(t,t_{\mathrm{I}})}_{\mathcal{X}_D(t)}\mathcal{S}_{\mathsf{F}}^{\dagger}(t,t_{\mathrm{I}}))\\ &= \mathrm{Tr}(\overbrace{\mathcal{S}_{\mathsf{F}}^{\dagger}(t,t_{\mathrm{I}})\mathcal{S}(t,t_{\mathrm{I}})}^{\mathcal{S}_D(t,t_{\mathrm{I}})}\underbrace{\mathcal{P}(t_{\mathrm{I}})\overbrace{\mathcal{S}^{\dagger}(t,t_{\mathrm{I}})\mathcal{S}_{\mathsf{F}}(t,t_{\mathrm{I}})}^{\mathcal{S}_D^{\dagger}(t,t_{\mathrm{I}})}}_{\mathcal{P}_{\mathrm{D}}(t)}\underbrace{\mathcal{S}_{\mathsf{F}}^{\dagger}(t,t_{\mathrm{I}})\mathcal{X}\mathcal{S}_{\mathsf{F}}(t,t_{\mathrm{I}})}_{\mathcal{X}_{\mathrm{D}}(t)})\end{aligned}$$

$$\langle\mathcal{X}\rangle_t = \mathrm{Tr}(\mathcal{P}_{\mathrm{D}}(t)\mathcal{X}_{\mathrm{D}}(t))\,. \tag{3.27}$$

With the evolution operator in the Dirac picture thus defined, pure states evolve in time according to

$$\begin{aligned}|\Psi_{\mathrm{D}}\rangle(t) &= \mathcal{S}_D(t,t_{\mathrm{I}})|\Psi_{\mathrm{D}}\rangle(t_{\mathrm{I}})\,,\\ |\Psi_{\mathrm{D}}\rangle(t) &= |\Psi_{\mathrm{D}}\rangle(t_{\mathrm{I}})\mathcal{S}_D^{\dagger}(t,t_{\mathrm{I}}) = |\Psi_{\mathrm{D}}\rangle(t_{\mathrm{I}})\mathcal{S}_D(t_{\mathrm{I}},t)\,.\end{aligned} \tag{3.28}$$

The extension of the Dirac evolution operator as defined in (3.27) to an arbitrary pair of times is

$$\mathcal{S}_D(t,t') = \mathcal{S}_{\mathsf{F}}^{\dagger}(t,t_{\mathrm{I}})\mathcal{S}(t,t')\mathcal{S}_{\mathsf{F}}(t,t_{\mathrm{I}})\,. \tag{3.29}$$

It has the properties generalizing Eqs. (3.9), (3.10) and (3.11)

$$\mathcal{S}_D(t,t')\mathcal{S}_D^{\dagger}(t,t') = \mathcal{S}_D^{\dagger}(t,t')\mathcal{S}_D(t,t') = \mathbf{1}\,, \tag{3.30}$$

$$\mathcal{S}_D(t,t') = \mathcal{S}_D(t,t'')\mathcal{S}_D(t'',t')\,. \tag{3.31}$$

$$\mathcal{S}_D^{\dagger}(t,t') = \mathcal{S}_D^{-1}(t,t') = \mathcal{S}_D(t',t)\,. \tag{3.32}$$

The equation of motion for the evolution operator in the Dirac picture is

$$i\frac{\partial}{\partial t}\mathcal{S}_D(t,t') = \mathcal{H}_D(t)\mathcal{S}_D(t,t')\,,\quad \mathcal{S}_D(t',t') = \mathbf{1}\,. \tag{3.33}$$

The Hamiltonian in the Dirac picture has the form

$$\mathcal{H}_D(t) = \mathcal{S}_{\mathsf{F}}^{\dagger}(t,t_{\mathrm{I}})\mathcal{H}_{\mathsf{P}}\mathcal{S}_{\mathsf{F}}(t,t_{\mathrm{I}})\,. \tag{3.34}$$

Now it is straightforward to repeat the procedure of Sec. 3.2.3. The integral form of the equation of motion for $\mathcal{S}_D$ is

$$\mathcal{S}_D(t,t') = \mathbf{1} - i\int_{t'}^{t} dt_1\mathcal{H}_D(t_1)\mathcal{S}_D(t_1,t')\,. \tag{3.35}$$

Its solution results as

$$\mathcal{S}_D(t,t') = \mathcal{T} e^{-i\int_{t'}^{t} d\tau\, \mathcal{H}_D(\tau)}\,, \quad t > t'\,. \tag{3.36}$$

Similarly, for $t' > t$, $\mathcal{S}_D$ is given by

$$\mathcal{S}_D(t,t') = \tilde{\mathcal{T}} e^{+i\int_{t}^{t'} d\tau \mathcal{H}_D(\tau)}\,, \quad t' > t\,. \tag{3.37}$$

The last two relations find numerous applications in many-body theory.

3.3. *Motivation for introducing NGF*

It has been said that the Green's or correlation functions play a central role in quantum statistical physics, because they provide a link between experimentally relevant quantities and easily calculable quantities.[104,105,109,110,129,131] In this paragraph we look first at the physical relevance of NGF.

3.3.1. *Particle and hole correlation functions*

There are two guiding principles here: to use reduced quantities, as exemplified by the whole transport theory, but to avoid an excessive loss of physical content and flexibility in the process. This may be shown for the single particle density matrix ρ introduced in (2.2). In Heisenberg picture,

$$\begin{aligned} \mathcal{X}(t) &= \int dx_1 dx_2 \psi^\dagger(x_2,t) X(x_1,x_2) \psi(x_1,t)\,, \\ \langle \mathcal{X} \rangle_t &= \mathrm{Tr}(\mathcal{P}_\mathrm{I} \mathcal{X}(t)) \equiv \mathrm{Tr}(\rho(t) X)\,, \\ \rho(x_1,x_2;t) &= \mathrm{Tr}(\mathcal{P}_\mathrm{I} \psi^\dagger(x_2,t)\psi(x_1,t)) \\ &\equiv \langle \psi^\dagger(x_2,t)\psi(x_1,t)\rangle\,. \end{aligned} \tag{3.38}$$

Here $\mathcal{P}_\mathrm{I}$ is the full many-body statistical operator and $\psi^\dagger$ and ψ are the Heisenberg field operators. To find the density matrix ρ we have to solve the corresponding equation of motion,

$$\frac{\partial \rho}{\partial t} = \mathrm{Tr}\mathcal{P}_\mathrm{I} \left(\frac{\partial \psi^\dagger(x_2,t)}{\partial t} \psi(x_1,t) + \psi^\dagger(x_2,t) \frac{\partial \psi(x_1,t)}{\partial t} \right). \tag{3.39}$$

In view of Eqs. (3.2) and (3.3), the right-hand side time derivatives lead to expressions involving four field operators, and this appears as the beginning of a BBGKY-like hierarchy of equations. It is rather difficult to formulate well-defined approximations terminating or self-consistently closing this hierarchy. The difficulty is two-fold: *both* field operators have the same time argument, and, as a consequence, they are differentiated with respect to this single time argument simultaneously.

This is conveniently overcome by introducing a two time generalization of ρ, the so-called particle correlation function $g^<$, defined as

$$\begin{aligned} g^<(1,2) &= \mathrm{Tr}(\mathcal{P}_\mathrm{I} \psi^\dagger(2)\psi(1)) \\ &\equiv \langle \psi^\dagger(2)\psi(1)\rangle\,. \end{aligned} \tag{3.40}$$

Following convention, we introduce cumulative variables $1 \equiv x_1, t_1$, etc., denoted by numbers, instead of x, t.

The single particle density matrix is the time diagonal part of $g^<$:

$$\rho(x_1, x_2; t) = g^<(1,2)|_{t_{1,2}=t}\,. \tag{3.41}$$

The technical advantage of $g^<$ is that it depends on two time arguments, so that the dynamical behavior of each of the field operators can be treated independently, as will be shown in detail is Sec. 3.4. The two time structure of $g^<$ is also rich in physical content. It describes quantum coherences in a natural way as the time off-diagonal elements, and captures the related memory effects. A simple interpretation of $g^<$ refers to the general notion of a "survival amplitude". Let $t_1 < t_2$ (notice the $<$ sign in $g^<$). Then the meaning of $g^<$ is roughly as follows: an electron is extracted from the system at the worldpoint $1 \equiv x_1, t_1$, the resulting one-particle (in fact, a hole) excitation propagates, until an electron is injected back at $2 \equiv x_2, t_2$. The correlation function measures the amplitude of such an elementary process. Clearly, this amplitude depends on the dynamical behavior of the system, but also on the particle distribution: an electron can be extracted only from occupied places.

To probe in a similar fashion the unoccupied states, a complementary correlation function $g^>$ is introduced in an obvious manner:

$$\begin{aligned} g^>(1,2) &= \mathrm{Tr}(\mathcal{P}\psi(1)\psi^\dagger(2)) \\ &\equiv \langle \psi(1)\psi^\dagger(2)\rangle\,. \end{aligned} \tag{3.42}$$

Its interpretation seems even more intuitive, this time for $t_1 > t_2$. An electron is injected at t_2 and later, at t_1, extracted again.

An important step further is to define the spectral density operator,

$$a(1,2) = g^>(1,2) + g^<(1,2)\,. \tag{3.43}$$

By the anticommutation relation (3.4), the time diagonal part of the spectral density is an unit operator in the space of single-particle functions:

$$a(x_1, t, x_2, t) = \delta(x_1 - x_2)\,, \tag{3.44}$$

$$= g^>(x_1, t, x_2, t) + g^<(x_1, t, x_2, t)\,, \tag{3.45}$$

$$\equiv \rho_h(x_1, x_2; t) + \rho(x_1, x_2; t)\,, \tag{3.46}$$

$$\rho_h = 1 - \rho\,. \tag{3.47}$$

This appears in the first line. On the second line, the unit operator is decomposed into the time diagonal parts of the two correlation functions. As shown on the third line, one is the single-particle density matrix. In analogy, a single hole density matrix is introduced. The last line shows, in an operator form, that the two density matrices complement each other to the unit operator.

3.3.2. *Equilibrium as a special case. Fluctuation-dissipation theorem*

The state of the system in thermal equilibrium has some very particular properties. We will explore them for their own sake and also to shed some light back at the nonequilibrium.

First, in equilibrium, as in any stationary state, the system is homogeneous in time, so that the correlation functions depend only on the difference of both times:

$$g^<(1,2) = g^<(x_1,t_1,x_2,t_2) = g^<(x_1,t_1-t_2,x_2,0) \equiv g^<(x_1,x_2;t=t_1-t_2)\,. \tag{3.48}$$

This permits to go over to the spectral representation:

$$g^<(x_1,x_2;E) = \int dt \exp(iEt) g^<(x_1,x_2;t)\,. \tag{3.49}$$

These relations are written for $g^<$ for definiteness, but the same holds for the other two correlation functions $g^>$ and a.

The equilibrium state of the many-body system may be conveniently taken as the grand-canonical density matrix,

$$\mathcal{P}_{\rm eq} = Z^{-1} e^{-\beta(\mathcal{H}-\mu\mathcal{N})}\,, \quad Z = \mathrm{Tr}\, e^{-\beta(\mathcal{H}-\mu\mathcal{N})}\,. \tag{3.50}$$

Similarly, the evolution operator is simply

$$\mathcal{S}_{\rm eq}(t_1,t_2) = e^{-i\mathcal{H}\cdot(t_1-t_2)}\,. \tag{3.51}$$

These two operators mutually commute. This, together with the anticommutation relations (3.4), permits to derive the relation

$$g^<(x_1,x_2;E) = e^{-\beta(E-\mu)} g^>(x_1,x_2;E)\,. \tag{3.52}$$

With the above interpretation of the correlation functions as transition amplitudes, this relation may be said to reflect the principle of detailed balancing. An even more striking result is obtained, if the spectral density is introduced into the last equation:

$$g^<(x_1,x_2;E) = f_{\rm FD}(E) a(x_1,x_2;E)\,, \tag{3.53}$$

$$g^>(x_1,x_2;E) = (1-f_{\rm FD}(E)) a(x_1,x_2;E)\,. \tag{3.54}$$

The last identities bear the name "Green's function fluctuation-dissipation theorem" in analogy to the FDT known from the linear response theory. In the GF approach, this equilibrium identity mirrors a deep relation between fluctuations (described generally by correlation functions) and dissipation (described by the spectral function). Alternatively, it may be said that the spectral properties of an equilibrium system determine also the statistical information contained in the particle distribution function.

To summarize, the consequence of either of the relations (3.52), (3.54) is that there is only one independent correlation (or Green's) function in equilibrium systems, which is an essential difference from the nonequilibrium situations, for which the knowledge of two independent correlation functions is necessary.

3.3.3. *Orbital representation*

The correlation functions $g^<$, $g^>$ were defined in the coordinate representation. This is natural in a local field theory and, given the structure of the Hamiltonian (3.2), (3.3), this representation is best suited for the general theory, as it will be developed below. In applications, some other orbital representation may be suitable. Consider an orthonormal basis of spin–orbitals $\{\varphi_{\lambda\sigma}(\mathbf{r})\}$. The associated annihilation and creation operators are related to the field operators ψ, $\psi^\dagger$ by

$$\begin{aligned}\psi_\sigma(\mathbf{r}) &= \sum_\lambda \varphi_{\lambda\sigma}(\mathbf{r})\cdot c_{\lambda\sigma} \quad c_{\lambda\sigma} = \int d^3\mathbf{r}\varphi^*_{\lambda\sigma}(\mathbf{r})\psi_\sigma(\mathbf{r})\,,\\ \psi^\dagger_\sigma(\mathbf{r}) &= \sum_\lambda \varphi^*_{\lambda\sigma}(\mathbf{r})\cdot c^\dagger_{\lambda\sigma} \quad c^\dagger_{\lambda\sigma} = \int d^3\mathbf{r}\varphi_{\lambda\sigma}(\mathbf{r})\psi^\dagger_\sigma(\mathbf{r})\,.\end{aligned} \tag{3.55}$$

These relations in the Schrödinger picture are equally valid in the Heisenberg picture. Substituted into the defining relation (3.40) for the particle correlation function $g^<$, they yield

$$\begin{aligned}g^<(1,2) &= \sum_{\lambda_1}\sum_{\lambda_2}\varphi_{\lambda_1\sigma_1}(\mathbf{r}_1)g^<_{\lambda_1\sigma_1;\lambda_2\sigma_2}(t_1,t_2)\varphi^*_{\lambda_2\sigma_2}(\mathbf{r}_2)\,,\\ g^<_{\lambda_1\sigma_1;\lambda_2\sigma_2}(t_1,t_2) &= \langle c^\dagger_{\lambda_2\sigma_2}(t_2)c_{\lambda_1\sigma_1}(t_1)\rangle\,.\end{aligned} \tag{3.56}$$

These results mean two things. First, $g^<$ may be regarded as an operator in the space of single particle states, whose matrix representation transforms according to the usual rules. Second, the matrix elements of $g^<$ in an arbitrary representation can be obtained directly in a mechanical fashion, if the corresponding annihilation and creation operators are known. The same is true for $g^>$, therefore also for the spectral density and for other Green's functions, which are all formed from the two correlation functions $g^<$, $g^>$ by linear operations, as will be seen shortly.

The choice of representation will often be suggested by the symmetry of the system. The best known example is a homogeneous electron gas, for which the translational symmetry points to the momentum representation. In equilibrium, the Green's functions are **k**-diagonal and spin-diagonal. For example, the spectral density becomes

$$A_{\sigma_1\sigma_2}(\mathbf{k}_1,t_1;\mathbf{k}_2,t_2) = A_{\sigma_1}(\mathbf{k}_1;t_1,t_2)\delta_{\mathbf{k}_1\mathbf{k}_2}\delta_{\sigma_1\sigma_2}\,. \tag{3.57}$$

Notice the discrete Kronecker δ for the wave vector. It results from the use of periodic boundary conditions making the system finite, although perhaps large, so that the **k**-vectors form a quasicontinuum.

When setting up a model, the orbital basis is more or less dictated by its structure, without reference to the coordinate representation. Consider, for example, the simplest nanostructure consisting of a molecular island connected by tunneling junctions between two leads. The molecule may be described in a minimum basis set of atomic orbitals, while the leads will be mesoscopic, that is possessing a band of conducting states filled each by a Fermi sea of electrons. The molecular

orbitals (MO) may be considered "relevant" and then we will be interested in just the projection $P_{\rm MO}\cdots P_{\rm MO}$, where $P_{\rm MO}$ is the corresponding projector in the single particle state space and $\cdots$ dots stand for the Green's function in question.[123]

3.4. *Keldysh time contour*

In this section, the basic formalism of the NGFs will be developed. It should be made clear right here that there is no unique "canonical" NGF machinery, although the core of the theory is common to all variants at stock. This core includes the closed time loop as the time range, construction of the Dyson equations, and the transformation of the loop NGF to a matrix Green's function of real time. The main differences concern the perturbation theoretical versus nonperturbative treatment and the ways of properly respecting the initial conditions. Our present choice will be to start with the Keldysh theory of NGF, which employs simple, the so-called "uncorrelated", initial conditions. This permits to develop the theory in an easy manner. We shall proceed in a nonperturbative way, at variance with Keldysh. This way is less laborious and more physical than that based on the traditional many-body perturbation theory (MBPT). Only in the introductory subsection, we shall recapitulate the original Keldysh line of reasoning, and in Sec. 3.4.6, the diagrammatic perturbation expansion will be recovered using the functional derivative technique.

3.4.1. *From equilibrium MBPT to Keldysh nonequilibrium GF technique*

Keldysh entitled his fundamental paper "Diagram technique for nonequilibrium processes". His aim was to modify the Feynman diagrams of the MBPT for the equilibrium Green's function in order to allow for processes reaching arbitrarily far from equilibrium. We shall paraphrase in a heuristic manner the ideas of Keldysh.

Let us contrast the two physical situations for the simplest case of zero temperature, starting from the equilibrium case. The external fields are then switched off, $\mathcal{H}'_{\rm e}(t)=0$ and the Hamiltonian H is time-independent. It is assumed that the system in question is normal, that is, it possesses a nondegenerate ground state $|\Psi\rangle$ with the ground state energy E_g which can be found as an eigensolution of the Schrödinger equation

$$H|\Psi\rangle = E_g|\Psi\rangle\,, \quad H = H_0 + W\,. \tag{3.58}$$

The statistical operator of the system in this ground state is

$$\mathcal{P} = |\Psi\rangle\langle\Psi|\,, \tag{3.59}$$

so that the $g^{>}$, $g^{<}$ functions defined by (3.40), (3.42) are equal to

$$\begin{aligned} g^{>}(1,2) &= \langle\Psi|\psi(1)\psi^{\dagger}(2)|\Psi\rangle\,,\\ g^{<}(1,2) &= \langle\Psi|\psi^{\dagger}(2)\psi(1)|\Psi\rangle\,. \end{aligned} \tag{3.60}$$

There is only one independent Green's function in equilibrium, and for the purpose of the MBPT expansion, the proper one is the *real-time causal GF* formed of $g^{>}$, $g^{<}$ as follows:

$$G^c(1,2) = -i(\theta(t_1 - t_2)g^{>}(1,2) - \theta(t_2 - t_1)g^{<}(1,2)) \tag{3.61}$$

$$= -i\langle\Psi|\,\mathsf{T}(\psi(1)\psi^{\dagger}(2))|\Psi\rangle\,. \tag{3.62}$$

In the first line, $\theta(t)$ is the Heaviside function, i.e., the unit step from 0 to 1 at $t = 0$. The $>$, $<$ superscripts were historically introduced precisely to indicate that G^c is given by $g^{>}$, $g^{<}$ for the time order $t_1 > t_2$, $t_1 < t_2$, respectively. A shorthand for this time-ordering prescription is given in the second line. Although we use the same notation T for the chronological operator as before, its definition (3.20) is extended: If there are also fermion field operators among the operators to be time-ordered, an exchange of their time-order is accompanied by a sign change. As is apparent from the first line of (3.61), for any pair of fermion field operators, the new definition reads

$$\begin{aligned}\mathsf{T}\{A(t)B(t')\} &= A(t)B(t') \quad t > t'\,,\\ \mathsf{T}\{A(t)B(t')\} &= -B(t')A(t) \quad t' > t\,.\end{aligned} \tag{3.63}$$

This reduces to the previous definition (3.20) for operators forming the Hamiltonians like (3.2) or (3.3), because the fermion field operators enter them always in pairs.

Let $t_1 > t_2$. Then the Green's function (3.61) is represented by

$$G^c(1,2) = -i\langle\Psi|\psi(1)\psi^{\dagger}(2))|\Psi\rangle\,, \quad t_1 > t_2\,. \tag{3.64}$$

This relation will be rewritten in the Dirac picture (properly called an interaction picture in this case) introduced in Sec. 3.2.4. The Hamiltonian is split according to Eq. (3.26) with the correspondence

$$\begin{array}{ccc}\mathcal{H} & = & \mathcal{H}_{\mathsf{F}} + \mathcal{H}_{\mathsf{P}}\\ & & \downarrow \quad\ \downarrow\\ \mathcal{H} & = & \mathcal{H}_0 + \mathcal{W}\,.\end{array} \tag{3.65}$$

To make the equation visually close to the notation in the literature, we use the caret for the operators in the Dirac picture and plain S for the Dirac evolution operator:

$$\mathcal{X}_D(t) \to \hat{\mathcal{X}}(t)\,, \quad \mathcal{S}_D(t,t') \to S(t,t')\,. \tag{3.66}$$

With Eqs. (3.65) and (3.66), the Dirac evolution operator (3.29) is written as

$$S(t,t') = \mathsf{T}e^{-i\int_{t'}^{t} d\tau\hat{\mathcal{W}}(\tau)}\,, \quad t > t'\,. \tag{3.67}$$

Let us continue with Eq. (3.64). It becomes

$$G^c(1,2) = -i\langle\Psi|S(t_{\mathrm{I}},t_1)\hat{\psi}(1)S(t_1,t_2)\hat{\psi}^{\dagger}(2)S(t_2,t_{\mathrm{I}})|\Psi\rangle\,, \quad t_1 > t_2\,. \tag{3.68}$$

This equation is still not suitable for the perturbation expansion, because the average is performed over the eigenstates of the full Hamiltonian. This can be overcome (following the inspiration by the quantum field theory) using the adiabatic turning on and off of the perturbation. The underlying *adiabatic hypothesis* or adiabatic theorem is a delicate mathematical problem,[240] but here we present the essence of it following.[9,241] Starting at $t \to -\infty$ from the ground state $|\Phi\rangle$ of the unperturbed, i.e., noninteracting, system, the interaction is adiabatically turned on, until the fully dressed ground state $|\Psi\rangle$ of the interacting system is reached at t_{I}. After that, the interaction is switched off adiabatically again, until at $t \to \infty$ the system returns to the non-interacting ground state $|\Phi\rangle$. Of course, during the process, the wavefunctions acquire phase factors, so that the three stages of the adiabatic process may be formalized as

$$\begin{array}{ccccc} \gamma_2|\Phi\rangle = S(+\infty, t_{\mathrm{I}})|\Psi\rangle & \longleftarrow & \gamma_1|\Psi\rangle = S(t_{\mathrm{I}}, -\infty)|\Phi\rangle & \longleftarrow & |\Phi\rangle \\ t = +\infty & & t = t_{\mathrm{I}} & & t = -\infty \end{array} . \tag{3.69}$$

While the phase factors γ_1, γ_2 are not known individually, if follows from (3.69) immediately that

$$\gamma_1\gamma_2 = \langle\Phi|S(+\infty, -\infty)|\Phi\rangle\,. \tag{3.70}$$

Putting all this together, the expression (3.68) for G^c can be brought to

$$G^c(1,2) = \frac{-i\langle\Phi|S(+\infty, t_1)\hat{\psi}(1)S(t_1, t_2)\hat{\psi}^\dagger(2)S(t_2, -\infty)|\Phi\rangle}{\langle\Phi|S(+\infty, -\infty)|\Phi\rangle}\,, \quad t_1 > t_2\,. \tag{3.71}$$

An analogous result is obtained, if we proceed the same way for $t_2 > t_1$. Together, the two expressions yield the celebrated formula

$$G^c(1,2) = \frac{-i\langle\mathcal{T}\{\hat{\psi}(1)\hat{\psi}^\dagger(2)S(+\infty, -\infty)\}\rangle_0}{\langle S(+\infty, -\infty)\rangle_0} \tag{3.72}$$

as the final result.

We introduce the symbol $\langle\cdots\rangle_0$ for the average over an unperturbed stationary state in general, $\langle\cdots\rangle_0 = \langle\Phi|\cdots|\Phi\rangle$ in Eq. (3.71). This form of G^c is suitable for the perturbation expansion, which also gives a clear interpretation to the symbolic expressions for both the numerator and the denominator. By expanding the evolution operator (3.67) into a power series, which is without problems about commutativity under the $\mathcal{T}$ sign, the numerator becomes

$$-i\sum_n \frac{1}{n!}(-i)^n \int_{-\infty}^{+\infty}\cdots\int_{-\infty}^{+\infty} d\bar{t}_1\cdots d\bar{t}_n\langle\mathcal{T}\{\hat{\psi}(1)\hat{\psi}^\dagger(2)\hat{\mathcal{W}}(\bar{t}_1)\cdots\hat{\mathcal{W}}(\bar{t}_n)\}\rangle_0\,. \tag{3.73}$$

The averages of the time ordered products of operators can be disentangled using the Wick theorem and the bookkeeping of the resulting expressions is best achieved using the Feynman diagrams; these have disconnected parts which are exactly cancelled by the denominator of (3.71) and the result is G^c as a sum over all connected Feynman diagrams. We are not going to follow the details of this classical subject-matter, see, for example, Refs. 17 and 9 for details.

Now we are ready to look into the nonequilibrium process driven by an external field $V_{\rm e}$. The reference time $t_{\rm I}$ will be selected such that $\mathcal{H}'_{\rm e}(t) \neq 0$ for $t > t_{\rm I}$. Prior to $t_{\rm I}$, the system is identical with the equilibrium one, so that we may go over to the interaction picture and start from the Eq. (3.68). The external field term is included in the unperturbed Hamiltonian. The evolution operator is thus given by (3.67) as before, only we have to remember that it incorporates the forces driving the system out of equilibrium through the unperturbed evolution operator which is hidden in the perturbation $\hat{\mathcal{W}}(\tau)$ in the Dirac picture. The whole scenario of the particular Keldysh process we consider starts at $t = -\infty$ from the ground state of the unperturbed system. First, the adiabatic switching on of the interaction leads to the fully dressed ground state, which is reached at $t = t_{\rm I}$. After that, the system is already driven out of equilibrium. The adiabatic mode of evolution holds no more, so the meaning of the state reached by $t = +\infty$ is not clear. It will not be needed, however, if we exactly retrace the evolution back first to $t = t_{\rm I}$ and then further up to $t = -\infty$. This brings the system back to the unperturbed ground state. All this may be summarized by a formula written in two equivalent forms:

$$G^{\rm c}(1,2) = -i\langle S(-\infty,+\infty)\,\mathcal{T}\{\hat{\psi}(1)\hat{\psi}^{\dagger}(2)S(+\infty,-\infty)\}\rangle_0 \tag{3.74}$$

$$= i\langle\Phi|S^{-1}(+\infty,-\infty)\,\mathcal{T}\{\hat{\psi}(1)\hat{\psi}^{\dagger}(2)S(+\infty,-\infty)\}|\Phi\rangle\,. \tag{3.75}$$

The form (3.74) corresponds precisely to the verbal description just given. The time order of the operators seems to be corrupted by the trip in the reverse direction. The factors are ordered correctly, however, if we apply a new rule that the factors coming later into play stand more to the left. This is just the idea of the Keldysh closed time contour. The other form (3.75) is shown as a link to Eq. (3.72). In the equilibrium case, the adiabatic passage permits to take the S^{-1} factor out of the average as a number, a phase factor, into the denominator and the previous expression Eq. (3.72) is recovered.

3.4.2. *Green's functions on the time contour*

In the previous section, it was shown, how the goal of extending the diagrammatic methods of the MBPT to nonequilibrium leads to the Keldysh contour in a natural way. This contour is a special limiting case of the contour introduced by Schwinger.[83] The NGF may be defined on the Schwinger contour without a direct reference to the perturbation expansion. It then serves to describe general nonequilibrium processes in a nonperturbative manner. We shall follow this way of reasoning, turning to the perturbation-theoretical point of view as appropriate.

The Schwinger contour $\mathbb{C}$, commonly but not quite precisely called Schwinger-Keldysh contour today, is sketched in Fig. 1. It has two branches labeled by + and −. The + branch starts at $t_{\rm I}$ and extends to some very large time, $t_\infty \to +\infty$. There the contour makes a U-turn and returns as the − branch back to $t_{\rm I}$. The two branches are depicted as parallel for clarity, but they both lie strictly on the (real) time axis.

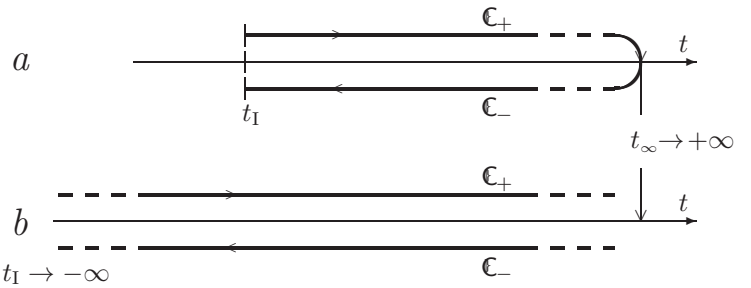


Fig. 1. NGF contour by (*a*) Schwinger; (*b*) Keldysh.

The Keldysh contour is drawn in the conventional manner, as simply stretching from $-\infty$ to $+\infty$ and back. As indicated, this means $t_{\rm I} \to -\infty$. To specify the position of a time variable on either contour, two things are needed: its numerical value and the branch label. Then, two time arguments may be ordered along the contour in an understandable way: If $t < t'$, then the ordering along the contour indicated by the precedence or succession symbols $\prec$, $\succ$ is

$$\begin{aligned} &t \prec t' \quad \text{if } t \text{ is at } \mathbb{C}_+ \quad \text{and } t' \text{ is at } \mathbb{C}_+\,, \\ &t \prec t' \quad \text{if } t \text{ is at } \mathbb{C}_+ \quad \text{and } t' \text{ is at } \mathbb{C}_-\,, \\ &t \succ t' \quad \text{if } t \text{ is at } \mathbb{C}_- \quad \text{and } t' \text{ is at } \mathbb{C}_+\,, \\ &t \succ t' \quad \text{if } t \text{ is at } \mathbb{C}_- \quad \text{and } t' \text{ is at } \mathbb{C}_-\,. \end{aligned} \tag{3.76}$$

The NGF, causal on the contour, is defined by

$$G(1,2) = -i\mathrm{Tr}(\mathcal{P}\,\mathcal{T}_c\{\psi(1|t_{\rm I})\psi^\dagger(2|t_{\rm I})\}) \tag{3.77}$$

with the Heisenberg field operators $\psi(1)$, $\psi^\dagger(2)$ anchored at $t_{\rm I}$, as explicitly shown here and tacitly understood in the following. We shall use this convention also for the Keldysh contour. The time-ordering (or chronological) operator $\mathcal{T}_c$ is acting along the contour $\mathbb{C}$ of Fig. 1 according to the ordering rules (3.76) in a manner similar to the usual time-ordering operator. If A, B denotes field operators,

$$\mathcal{T}_c\{A(t)B(t')\} = A(t)B(t') \quad t \succ t'\,, \tag{3.78}$$

$$\mathcal{T}_c\{A(t)B(t')\} = \mp B(t')A(t) \quad t' \succ t\,. \tag{3.79}$$

where the $-$ sign holds for fermions, $+$ for bosons.

The Green's function $G(1,2)$ defined in Eq. (3.77) contains all necessary ingredients to fully specify a general nonequilibrium process: the initial time $t_{\rm I}$, the initial state $\mathcal{P}$ of the system and the dynamical process driven by the Hamiltonian $\mathcal{H}(t)$ and captured by the Heisenberg field operators. Its physical content is made clear from its decomposition into four real time functions.

The NGF (3.77) defined on the contour comprises in fact four functions of real time (... defined on time axis $-\infty < t < +\infty$) according to the position of the time arguments on the $\mathbb{C}$ contour, as shown in Fig. 2:

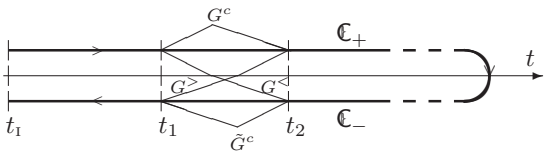


Fig. 2. NGF time contour.

$$G^{++}(1,2) \equiv G^c(1,2) = -i\,\mathrm{Tr}(\mathcal{P}\,\mathsf{T}\{\psi(1)\psi^\dagger(2)\}) \quad t_1, t_2 \text{ at } \mathbb{C}_+\,, \tag{3.80}$$

$$G^{+-}(1,2) \equiv G^<(1,2) = +i\,\mathrm{Tr}(\mathcal{P}\psi^\dagger(2)\psi(1)) \quad t_1 \text{ at } \mathbb{C}_+, \quad t_2 \text{ at } \mathbb{C}_-\,, \tag{3.81}$$

$$G^{-+}(1,2) \equiv G^>(1,2) = -i\,\mathrm{Tr}(\mathcal{P}\psi(1)\psi^\dagger(2)) \quad t_1 \text{ at } \mathbb{C}_-, \quad t_2 \text{at } \mathbb{C}_+\,, \tag{3.82}$$

$$G^{--}(1,2) \equiv \widetilde{G}^c(1,2) = +i\,\mathrm{Tr}(\mathcal{P}\tilde{\mathsf{T}}\{\psi(1)\psi^\dagger(2)\}) \quad t_2, t_1 \text{ at } \mathbb{C}_-\,. \tag{3.83}$$

We know two of these functions already, as $G^>$ and $G^<$ differ from $g^>$ and $g^<$ introduced in Eqs. (3.40) and (3.42) just by a prefactor $\pm i$. The other two quantities are the causal and anti-causal Green's functions. The time-ordering operators $\mathsf{T}, \tilde{\mathsf{T}}$ act in accordance with T_c, see Eq. (3.79), but for real times. T was introduced in Sec. 3.4.1 by Eq. (3.63), $\tilde{\mathsf{T}}$ acts similarly. In an algebraic form,

$$\begin{aligned}
\mathsf{T}\{\psi(1)\psi^\dagger(2)\} &= \theta(t_1 - t_2)\psi(1)\psi^\dagger(2) - \theta(t_2 - t_1)\psi^\dagger(2)\psi(1)\,,\\
\tilde{\mathsf{T}}\{\psi(1)\psi^\dagger(2)\} &= \theta(t_1 - t_2)\psi^\dagger(2)\psi(1) - \theta(t_2 - t_1)\psi(1)\psi^\dagger(2)\,.
\end{aligned} \tag{3.84}$$

It would be possible to work directly with the quadruplet (3.80)–(3.83) already now, but the contour Green's function has important advantageous properties for the formal derivations of the subsequent paragraphs. We shall analyze the decomposition (3.80)–(3.83) in detail in Sec. 3.5.

3.4.3. *Equation of motion for NGF*

The nonperturbative treatment of NGF is based on the method of the equations of motion. This requires a proper treatment of the initial conditions. The reason we are developing the theory for the Keldysh Green's functions first, is that the uncorrelated initial condition in the distant past can be readily satisfied and this permits to proceed with the basic structure of the equations of motion and the ways of their solution. We shall extend the theory to the general case of arbitrary finite time initial conditions in Sec. 4.

The NGF (3.77) on the $\mathbb{C}$ contour can be written with the chronological $\tilde{\mathsf{T}}$ operator expressed in the manner resembling Eq. (3.84):

$$G(t_1, t_2) = \theta_c(t_1, t_2)G^>(t_1, t_2) + \theta_c(t_2, t_1)G^<(t_1, t_2)\,. \tag{3.85}$$

Here, $\theta_c(t_1, t_2)$ is the step function defined on the path $\mathbb{C}$, with reference to (3.76), the definition reads

$$\theta_c(t_1, t_2) = 1 \quad t_1 \succ t_2\,, \quad \theta_c(t_1, t_2) = 0 \quad t_1 \prec t_2\,. \tag{3.86}$$

The equation of motion for the Green's function follows from the Eq. (3.14) for Heisenberg operators. Applied to the field operator, this yields (with the H subscripts suppressed again):

$$\begin{aligned} i\frac{\partial\psi(1)}{\partial t_1} &= [\psi(1), \mathcal{H}(t_1)]_- \\ &= h_0(1)\psi(1) + \int d3w(1,3)\psi^\dagger(3)\psi(3)\psi(1)\,, \\ w(1,3) &\leftarrow w(x_1, x_3)\delta(t_1 - t_3)\,. \end{aligned} \tag{3.87}$$

As indicated, the notation for the interaction w has been changed so as to incorporate its time dependence, i.e., an instantaneous action. The integral then means

$$\int d3 = \int_{\mathbb{C}} dt_3 \int dx_3\,. \tag{3.88}$$

Taking the time derivative of the expression (3.85) and using (3.87), we obtain an equation for the NGF on the $\mathbb{C}$ contour:

$$\left(i\frac{\partial}{\partial t_1} - h_0(1)\right) G(1,2) = \delta_c(t_1, t_2) - i\int d3w(1^+, 3)G_2(1,3,2,3^+)\,. \tag{3.89}$$

A similar "conjugate" equation is derived in the same way and the result is

$$\left(-i\frac{\partial}{\partial t_2} - h_0(2)\right) G(1,2) = \delta_c(t_1, t_2) - i\int d3w(2^+, 3)G_2(1,3,2,3^+)\,. \tag{3.90}$$

Two new functions enter this result. One is the contour δ-function appearing as the time derivative of the contour step function (3.86):

$$\delta_c(t_1, t_2) = \frac{d}{dt}\theta_c(t_1, t_2) = \begin{cases} +\delta(t_1 - t_2) & \text{if } t_1,\, t_2 \text{ are both at } \mathbb{C}^+\,, \\ -\delta(t_1 - t_2) & \text{if } t_1,\, t_2 \text{ are both at } \mathbb{C}^-\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{3.91}$$

The other new function is the two particle NGF G_2 on the $\mathbb{C}$ contour, defined by

$$G_2(1,3,2,4) = (-i)^2\mathrm{Tr}(\mathcal{P}_\mathrm{I}\mathcal{T}_c\{\psi(1|t_\mathrm{I})\psi(3|t_\mathrm{I})\psi^\dagger(4|t_\mathrm{I})\psi^\dagger(2|t_\mathrm{I})\})\,. \tag{3.92}$$

Except for t_2, all time arguments of G_2 in Eq. (3.89) are equal, $t_1 = t_3$ because of the instantaneous interaction w, $t_3 = t_4$ as follows from the equation of motion. In order to preserve the correct order of multiplications, $\psi^\dagger(3)\psi(3)\psi(1)$ under the action of the time-ordering operator, the two arguments are infinitesimally shifted: $t_4 \equiv t_3^+ = t_3 + 0$, $t_3 = t_1^+ \equiv t_1 + 0$. The shifts are along the $\mathbb{C}$ contour, that is, ± 0 in the algebraic sense on $\mathbb{C}_+$, $\mathbb{C}_-$, respectively. Similarly for Eq. (3.90).

Equation (3.89) has the desired form of an equation of motion, but it is not closed, as it contains an unknown Green's function of a higher-order. For this GF, there could be obtained an analogous equation containing a three-particle Green's

function, etc, and in this way an infinite chain of equations would be developed, the so-called Martin–Schwinger hierarchy. Instead, we turn to methods of converting Eq. (3.89) to a closed equation for the single-particle Green's function.

3.4.4. *Auxiliary fields and the technique of functional derivatives*

The method for the derivation of a closed equation of motion for the NGF on the contour is based on a formal device of subjecting the system to an additional fictitious external field traditionally denoted by $U(t)$. The U field is defined along the contour and it may assume different values on its both branches, $U_+(t)$ and $U_-(t)$. The Green's function incorporating this field is defined as

$$G(1,2;U) = -i\frac{\mathrm{Tr}(\mathcal{P}_\mathrm{I}\mathcal{T}_c\{S_U\psi(1)\psi^\dagger(2)\})}{\mathrm{Tr}(\mathcal{P}_\mathrm{I}\mathcal{T}_c S_U)}\,. \tag{3.93}$$

Here,

$$S_U = \mathcal{T}_c e^{-i\int d\bar{1}\psi^\dagger(\bar{1}^+)U(\bar{1})\psi(\bar{1})} \tag{3.94}$$

has the form reminiscent of the S matrix in the interaction representation and the whole Green's function (3.93) may be compared with Eq. (3.72). Presently, the perturbation is the additional external field, so that in the transition to the Dirac picture all field operators have the full Heisenberg time dependence including the interactions. Therefore, they have no hats (carets). The integral in (3.94) is given by (3.88), that is, the time integration extends over the whole $\mathbb{C}$. In the limit of a "physical" disturbance $U_+(t) = U_-(t)$, the denominator of (3.93) would become equal to unity and the whole GF would reduce to the GF with an additional external field written in the Dirac picture. We continue with the general U defined on the contour. The Green's function $G(1,2;U)$ obeys equations of motion extending the Eqs. (3.89) and (3.90) for $G(1,2)$:

$$\left(i\frac{\partial}{\partial t_1} - h_0(1) - U(1)\right) G(1,2;U)$$
$$= \delta_c(t_1,t_2) - i\int d3w(1^+,3)G_2(1,3,2,3^+;U)\,, \tag{3.95}$$

$$\left(-i\frac{\partial}{\partial t_2} - h_0(2) - U(2)\right) G(1,2;U)$$
$$= \delta_c(t_1,t_2) - i\int d3w(2^+,3)G_2(1,3,2,3^+;U)\,. \tag{3.96}$$

$$G_2(1,3,2,4;U) = (-i)^2\frac{\mathrm{Tr}(\mathcal{P}_\mathrm{I}\mathcal{T}_c\{S_U\psi(1)\psi(3)\psi^\dagger(4)\psi^\dagger(2)\})}{\mathrm{Tr}(\mathcal{P}_\mathrm{I}\mathcal{T}_c S_U)}\,. \tag{3.97}$$

The functional derivative with respect to the functional variable U is defined by a relation generalizing the notion of a full differential of a function of many variables expressed in terms of partial derivatives: U is changed by a small variation δU. A

functional $\Phi[U]$ changes by $\delta\Phi$ and the linear part of the variation corresponds to the total differential. It must have the form of a linear functional of δU:

$$\delta\Phi[U] = \int d\bar{1} \frac{\delta\Phi}{\delta U(\bar{1})} \cdot \delta U(\bar{1}) + \text{higher order terms} \tag{3.98}$$

and the coefficients at $\delta U(\bar{1})$ define the functional derivative as a function of the variable $\bar{1} = \{x_1, \bar{t}_1\}$. For example, writing $U(1) = \int d2\delta(1-2)U(2)$, we get from (3.98) the useful identity

$$\frac{\delta U(1)}{\delta U(2)} = \delta(1-2)\,. \tag{3.99}$$

The functional derivative introduced by (3.98) is the physicist's conception of the *Fréchet derivative*. On the same level of mathematical rigor, it may be transformed to the *Volterra derivative*, more convenient in some respects. Its definition is local: let $\delta U(\bar{1}) \neq 0$ only in a small neighborhood of the point 2. Then, by Eq. (3.98),

$$\frac{\Phi[U+\delta U] - \Phi[U]}{\displaystyle\int d\bar{1}\delta U(\bar{1})} = \frac{\delta\Phi}{\delta U(2)} + \text{higher order terms} \tag{3.100}$$

in case that $\delta\Phi/\delta U(1)$ is continuous in a neighborhood of the point 2. Thus the Volterra definition is not suitable for obtaining (3.99).

The main task of this subsection is to deduce the functional derivative of $G(1,2;U)$. By (3.93), G is a ratio of two functionals. The rules for functional derivatives are no different from the usual ones, schematically $(u/v)' = u'/v - uv'/v^2$. Let us sketch the calculation for the denominator of (3.93). It has the explicit form (3.94). The derivative under the chronological operator may be performed ignoring noncommutativity problems:

$$\begin{aligned}
\frac{\delta}{\delta U(3)}\mathrm{Tr}(\mathcal{P}_{\mathrm{I}}\mathcal{T}_c S_U) &= \frac{\delta}{\delta U(3)}\mathrm{Tr}(\mathcal{P}_{\mathrm{I}}\mathcal{T}_c e^{-i\int d\bar{1}\psi^\dagger(\bar{1}^+)U(\bar{1})\psi(\bar{1})}) \\
&= -i\,\mathrm{Tr}(\mathcal{P}_I\mathcal{T}_c e^{-i\int d\bar{1}\psi^\dagger(\bar{1}^+)U(\bar{1})\psi(\bar{1})}\psi^\dagger(3^+)\psi^\dagger(3)) \\
&= -i\,\mathrm{Tr}(\mathcal{P}_{\mathrm{I}}\mathcal{T}_c S_U\psi^\dagger(3^+)\psi^\dagger(3))\,.
\end{aligned} \tag{3.101}$$

The derivative of the whole GF is obtained by similar steps:

$$\frac{\delta G(1,2;U)}{\delta U(3)} = G(3,3^+;U)G(1,2;U) - G_2(1,3;2,3^+;U)\,. \tag{3.102}$$

By this identity, the equation of motion (3.95) becomes a closed differential equation:

$$\begin{aligned}
&\left(i\frac{\partial}{\partial t_1} - h_0(1) - U(1)\right) G(1,2;U) \\
&\quad = \delta_c(t_1,t_2) - i\int d3w(1^+,3)\left(G(3,3^+;U)G(1,2;U) - \frac{\delta G(1,2;U)}{\delta U(3)}\right).
\end{aligned} \tag{3.103}$$

This equation is satisfactory in many respects. It is a nonperturbative equation which closes the Martin–Schwinger hierarchy at the one-particle level. The mean field (Hartree) potential is separated out. For a local spin-independent interaction, like the Coulomb force, we get explicitly:

$$-i\int d3w(1^+,3)G(3,3^+;U) = \int dx_3 w(\mathbf{r}_1-\mathbf{r}_3)\langle n(\mathbf{r}_3,t_1;U)\rangle \equiv V_{\mathrm{H}}(1;U)\,. \tag{3.104}$$

Returning to the physical case $U \to 0$, we may compare the starting equation (3.89) with the final form

$$\left(i\frac{\partial}{\partial t_1} - h_0(1)\right) G(1,2) = \delta_c(t_1,t_2) - i\int d3w(1^+,3)\left(G(3,3^+)G(1,2) - \frac{\delta G(1,2;U=0)}{\delta U(3)}\right). \tag{3.105}$$

While Eq. (3.89) was linear — being a mere first link in the chain of linear Martin–Schwinger equations, the autonomous Eq. (3.105) is nonlinear, as is already seen from the self-consistent nature of the mean field term. The other term involving the functional derivative incorporates everything beyond the mean field, that is all exchange and correlations. This inner many-particle dynamical structure of the GF is seen to be given by a response function probing the reaction of the system to the U field.

There are two serious technical obstacles on the way to the solution of Eq. (3.105). Symptomatically, they are the essential physical constituents of the problem at the same time. One is just $\delta G/\delta U$, the pair correlation function by (3.102), for which unfortunately no methods of direct handling are available. The other technical issue is a proper inclusion of the initial/boundary conditions. Here, we are going to employ the Keldysh initial conditions, as motivated in the introduction to the whole Sec. 3.4: with these initial conditions, several methods how to solve Eq. (3.105) can be developed in a close parallel to analogous procedures known for equilibrium systems.

3.4.5. *Keldysh initial condition*

While the finite time initial condition envisaged for the GF (3.77) on the Schwinger contour is explicit, but requires a complex technical treatment in general, as will be described in Sec. 4, the initial condition for the Keldysh choice is much easier to work with, but needs a precise explanation.

As has been discussed in Sec. 3.4.1, if the interactions are switched off adiabatically as $t_{\mathrm{I}} \to -\infty$, and the external fields do not act yet in that distant past, the Hamiltonian tends to

$$\mathcal{H}_0(t\to-\infty) = \mathcal{T}+\mathcal{V}\,, \tag{3.106}$$

and the system assumes a stationary state $\mathcal{P}_{\rm I}$ of the isolated noninteracting system asymptotically:

$$[\mathcal{P}_{\rm I}, \mathcal{H}_0(t \to -\infty)]_- = 0\,. \tag{3.107}$$

The reference time for both the Heisenberg and Dirac operators coincides with $t_{\rm I} \to -\infty$. An actual value of this elusive time is not critical, because $\mathcal{P}_{\rm I}$ is stationary in the asymptotic region and serves as the Heisenberg state of the system throughout the whole process. All averages similar to (3.77) have the meaning

$$\langle \cdots \rangle = {\rm Tr}(\mathcal{P}_{\rm I} \cdots)\,. \tag{3.108}$$

In the forward time direction, $\mathcal{P}_{\rm I}$ acts as the initial state of both the noninteracting state, and the complete state with interactions included, at $t_{\rm I} \to -\infty$. This initial state often will, but need not, be a state of equilibrium. For example, it may describe a nanostructure + uncoupled leads with a mutual bias, or even with a temperature difference.[136]

This initial condition is imposed on the NGF through the unperturbed GF corresponding to $W = 0$. It is introduced by relations analogous to Eqs. (3.93) and (3.94), but, naturally, with all operators in the interaction representation [cf. Eq. (3.66)]:

$$G_0(1,2;U) = -i\,\frac{{\rm Tr}(\mathcal{P}_{\rm I}\,\mathsf{T}_c\{\hat{S}_U \hat{\psi}(1)\hat{\psi}^\dagger(2)\})}{{\rm Tr}(\mathcal{P}_{\rm I}\,\mathsf{T}_c \hat{S}_U)}\,, \tag{3.109}$$

$$\hat{S}_U = \mathsf{T}_c e^{-i\int d\bar{1}\hat{\psi}^\dagger(\bar{1}^+)U(\bar{1})\hat{\psi}(\bar{1})}\,. \tag{3.110}$$

With G_0 at hand, the differential equation (3.103) for G may be converted to an integral form:

$$\begin{aligned} G(1,2;U) = G_0(1,2;U) - i\iint d4d3 G_0(1,4;U) \\ \times w(4^+,3)\left(G(3,3^+;U)G(4,2;U) - \frac{\delta G(4,2;U)}{\delta U(3)}\right). \end{aligned} \tag{3.111}$$

The function G_0 satisfies the "free" EOM

$$\left(i\frac{\partial}{\partial t_1} - h_0(1) - U(1)\right) G_0(1,2;U) = \delta_c(t_1,t_2)\,, \tag{3.112}$$

$$\left(-i\frac{\partial}{\partial t_2} - h_0(2) - U(1)\right) G_0(1,2;U) = \delta_c(t_1,t_2)\,. \tag{3.113}$$

It is then readily verified that the GF given by (3.111) satisfies the full equation of motion (3.103). The integral form (3.111) incorporates, in addition, the boundary condition set by the free GF G_0. This involves the asymptotic initial condition common to the free GF and to the full GF, and the external fields. The only viable method for solving Eq. (3.111) is to iterate it starting from the zeroth-order solution

$G^{(0)} = G_0$. Let us try the first iteration:

$$G^{(1)}(1,2;U) = G_0(1,2;U) - i\iint d4d3 G_0(1,4;U) \times w(4^+,3)\left(G_0(3,3^+;U)G_0(4,2;U) - \frac{\delta G_0(4,2;U)}{\delta U(3)}\right). \quad (3.114)$$

The key quantity is the functional derivative again. In analogy to Eq. (3.102), it is given by

$$\frac{\delta G_0(1,2;U)}{\delta U(3)} = G_0(3,3^+;U)G_0(1,2;U) - G_{02}(1,3;2,3^+;U) \quad (3.115)$$

with the obvious definition of G_{02}. In the next iteration, G_{03} would enter, etc, invoking gradually the full Martin–Schwinger hierarchy of the unperturbed n-particle Green's functions. This expansion depends entirely on the initial state $\mathcal{P}_\mathrm{I}$ reflecting its inner correlations.

We concentrate on the particular class of initial states having no inner correlations, termed appropriately the *uncorrelated initial states*. We define them as those, for which the free two particle GF factorizes to an anti-symmetric product of a pair of single particle GF. Then the functional derivative of G_0 is expressed in terms of G_0 itself. By (3.115),

$$\frac{\delta G_0(1,2;U)}{\delta U(3)} = G_0(3,3^+;U)G_0(1,2;U) - \{\overbrace{G_0(1,2;U)G_0(3,3^+;U) - G_0(1,3;U)G_0(3^+,2;U)}^{\text{uncorrelated } G_{02}}\},$$

$$\frac{\delta G_0(1,2;U)}{\delta U(3)} = G_0(1,3;U)G_0(3,2;U). \quad (3.116)$$

As a result, the iteration of (3.111) leads to closed expressions for G in terms of G_0 and w in each iteration, and the usual many-body perturbation expansion is possible. This will be shown in the next subsection. In view of the discussion in Sec. 3.4.1, it is then proper to identify the uncorrelated $\mathcal{P}_\mathrm{I}$ states with those which obey the *Keldysh initial condition*, and to call the nonequilibrium processes unfolding from these initial conditions the *Keldysh processes*.

The deeper reason for this result is that the states uncorrelated according to the definition given are those, for which the Wick theorem, properly generalized, works. Let us sketch a simple *ad hoc* proof.

Let us consider the physical case $U \to 0$ for clarity. The field operator in the interaction representation is governed by a simple equation of motion [cf. (3.87)]

$$i\frac{\partial\hat{\psi}(1)}{\partial t_1} = h_0(1)\hat{\psi}(1). \quad (3.117)$$

This equation is easily solved like a single particle Schrödinger equation. We introduce the corresponding evolution operator $s(t,t')$ by

$$i\,\frac{\partial}{\partial t}s(t,t') = h_0(t)\,s(t,t'), \quad s(t',t') = 1_{\rm op} \tag{3.118}$$

and for the initial state we employ the decomposition into the representation of the Hamiltonian (3.106):

$$\mathcal{H}_0(t\to-\infty) = \mathcal{T}+\mathcal{V} = \sum_\alpha \epsilon_\alpha c_\alpha^\dagger c_\alpha\,. \tag{3.119}$$

We get

$$\hat\psi(1) = \sum_\alpha \langle x_1|s(t_1,t_{\rm I})|\alpha\rangle c_\alpha\,, \quad \hat\psi^\dagger(1) = \sum_\alpha c_\alpha^\dagger\langle\alpha|s(t_{\rm I},t_1)|x_1\rangle\,. \tag{3.120}$$

The one-particle GF G_0 is obtained as follows. An initial time $t_{\rm I}$ is selected in the asymptotic region. By Eqs. (3.77), (3.86) and (3.108),

$$\begin{aligned} G_0(1,2) &= -i\,{\rm Tr}(\mathcal{P}_{\rm I}\mathcal{T}_c\{\hat\psi(1)\hat\psi^\dagger(2)\}) \\ &= -i\theta_c(t_1,t_2)\langle\hat\psi(1)\hat\psi^\dagger(2)\rangle + i\theta_c(t_2,t_1)\langle\hat\psi^\dagger(2)\hat\psi(1)\rangle\,. \end{aligned} \tag{3.121}$$

Inserting the expressions (3.120) for the field operators, we obtain

$$\begin{aligned} G_0(1,2) = -i\sum_\alpha\sum_\beta &\langle x_1|s(t_1,t_{\rm I})|\alpha\rangle \\ &\times\{\theta_c(t_1,t_2)\langle c_\alpha c_\beta^\dagger\rangle - \theta_c(t_2,t_1)\langle c_\beta^\dagger c_\alpha\rangle\}\times\langle\beta|s(t_{\rm I},t_2)|x_2\rangle\,. \end{aligned} \tag{3.122}$$

This may be written in a compact transparent form as

$$\begin{aligned} G_0(1,2) = &-i\theta_c(t_1,t_2)\langle x_1|s(t_1,t_{\rm I})(1-\rho_{\rm I})s(t_{\rm I},t_2)|x_2\rangle \\ &+ i\theta_c(t_2,t_1)\langle x_1|s(t_1,t_{\rm I})\rho_{\rm I}s(t_{\rm I},t_2)|x_2\rangle\,, \end{aligned} \tag{3.123}$$

with

$$\rho_{\rm I} = \sum_\alpha\sum_\beta |\alpha\rangle\langle c_\beta^\dagger c_\alpha\rangle\langle\beta|\,. \tag{3.124}$$

This result seems to depend on $t_{\rm I}$, but this dependence is eliminated by the asymptotic stationarity condition (3.107). It is usually assumed that the external fields are turned on at a finite time, say $t_{\rm P}$, so that the stationarity condition holds for $t < t_{\rm P}$. Then Eqs. (3.122) and (3.123) are valid for any $t_{\rm I} < t_{\rm P}$, in particular for $t_{\rm I}\to-\infty$.

The free two-particle Green's function can be obtained in the same way. Its structure is given by the formula (3.125), but with the field operators in the interaction representation again:

$$G_{02}(1,3,2,4) = (-i)^2{\rm Tr}(\mathcal{P}_{\rm I}\mathcal{T}_c\{\hat\psi(1)\hat\psi(3)\hat\psi^\dagger(4)\hat\psi^\dagger(2)\})\,. \tag{3.125}$$

By substitution from Eqs. (3.120), the Green's function is shown to evolve by the action of four evolution operators $\langle x_i|s(t_i,t_{\rm I})|\alpha_i\rangle$ from an initial condition at $t_{\rm I}$.

The initial condition is given by a quadruple sum of averages of four c, $c^\dagger$ operators whose order is given by the order of the corresponding times. Consider the example of time order leading to the two particle density matrix:

$$t_1 \prec t_3 \prec t_4 \prec t_2 \quad \mathrm{IC}\cdots\{+\langle c^\dagger_{\alpha_2} c^\dagger_{\alpha_4} c_{\alpha_3} c_{\alpha_1}\rangle\}\,. \tag{3.126}$$

Next, the requirement that G_{02} factorize [see (3.116)] into

$$G_{02}(1,3,2,4) \to G_0(1,2)G_0(3,4) - G_0(1,4)G_0(3,2)\,, \tag{3.127}$$

brings about a coincident requirement on the initial conditions. It is easy to verify that in our example (3.126) it is required that

$$\begin{gathered} t_1 \prec t_3 \prec t_4 \prec t_2 \\ \langle c^\dagger_{\alpha_2} c^\dagger_{\alpha_4} c_{\alpha_3} c_{\alpha_1}\rangle \stackrel{!}{=} \langle c^\dagger_{\alpha_2} c_{\alpha_1}\rangle\langle c^\dagger_{\alpha_4} c_{\alpha_3}\rangle - \langle c^\dagger_{\alpha_2} c_{\alpha_3}\rangle\langle c^\dagger_{\alpha_4} c_{\alpha_1}\rangle\,. \end{gathered} \tag{3.128}$$

This decomposition is the content of the Wick theorem and it is seen that its validity is equivalent to the decomposition (3.127) of the Green's function. This equivalence has been studied in detail by van Leeuwen, see Ref. 131. It seems to have been clearly stated for the first time by Danielewicz in Ref. 102. This author also established the most general form of an uncorrelated initial density matrix,

$$\mathcal{P}_{\mathrm{I}} = \frac{e^{-A}}{\mathrm{Tr}\, e^{-A}}\,, \quad A = \sum_\alpha A_\alpha c^\dagger_\alpha c_\alpha\,. \tag{3.129}$$

This statistical operator is fully specified by an arbitrary numerical sequence $\{A_\alpha\}$. The grand canonical ensemble is obtained as a special case for $A_\alpha = \epsilon_\alpha - \mu$. The result (3.129) thus crowns the previous work on the Wick theorem in statistical physics.[9,131,242–247] The one-particle density matrix for (3.129) has the form

$$\rho = \sum_\alpha |\alpha\rangle f_\alpha \langle\alpha|\,, \quad f_\alpha = (1+e^{A_\alpha})^{-1}\,. \tag{3.130}$$

The one-particle density matrix thus specifies the uncorrelated initial condition in full. To see the richness of the set of admissible uncorrelated initial conditions, it is enough to choose the various sequences f_α and to recalculate the corresponding $\{A_\alpha\}$. In particular, the N particle ground state is obtained in the limit $f_\alpha \to \theta(\mu - \epsilon_\alpha)$ leading to $A_\alpha \to \pm\infty$ for $\epsilon_\alpha \lessgtr \mu$. By a similar limiting process, any excited Slater determinant of unperturbed one-particle states can be created, etc. In conclusion of this discussion, we mention that Keldysh himself seems to have circumvented the question of uncorrelated initial states in Ref. 89. This he may have done, because the paper was only concerned with spatially homogeneous systems, for which the Wick theorem may be derived under much weaker assumptions, see Ref. 17 for example.

3.4.6. *Perturbation expansion*

Now we are ready to develop the perturbation expansion for the Green's function. The aim is to end up with the Dyson equation for G. By this procedure we depart, in this paragraph, from the general nonperturbative approach of this review. The benefit will be an insight into the relationship of various ways toward the Dyson equation. An outline of the classical method of perturbation expansion in terms of Feynman diagrams was sketched/reminded of in Sec. 3.4.1 at Eq. (3.73). Here, we generate the Feynman diagrams using the alternative technique of functional derivatives. We follow the book of Kadanoff and Baym.[85] Only two equations are needed: Eq. (3.111) slightly rearranged, and the functional derivative (3.116) of G_0:

$$G(1,2;U) = G_0(1,2;U) - \iint d4d3G_0(1,4;U)[iw(4^+,3)]G(3,3^+;U)G(4,2;U) + \iint d4d3G_0(1,4;U) \times [iw(4^+,3)]\frac{\delta G(4,2;U)}{\delta U(3)}\,, \tag{3.131}$$

$$\frac{\delta G_0(1,2;U)}{\delta U(3)} = G_0(1,3;U)G_0(3,2;U)\,. \tag{3.132}$$

The expansion in powers of the interaction w,

$$\begin{aligned} G &= G^{(0)} + G^{(1)} + G^{(2)} + \cdots\,, \\ G^{(0)} &= G_0\,, \end{aligned} \tag{3.133}$$

is obtained successively from the recurrent relation

$$\begin{aligned} G^{(n+1)}(1,2;U) = -\sum_{s=0}^{n} \iint d4d3G_0(1,4;U) \\ \times [iw(4^+,3)]G^{(s)}(3,3^+;U)G^{(n-s)}(4,2;U) \\ + \iint d4d3G_0(1,4;U) \times [iw(4^+,3)]\frac{\delta G^{(n)}(4,2;U)}{\delta U(3)}\,. \end{aligned} \tag{3.134}$$

If all perturbation corrections up to $G^{(n)}$ are expressed in terms of G_0 and w, the same is true for $G^{(n+1)}$ because of Eq. (3.132). It follows by induction that the Green's function is a functional of G_0 and w to all orders of the perturbation expansion, which is called a G_0w expansion therefore. This result is generally taken to mean that simply $G = G[G_0, w]$.

The expansion (3.133) must coincide with the usual perturbation series. Then the individual terms forming together the nth order correction should be represented by standard Feynman diagrams. This will be illustrated by the diagrams of the first-order. There are three elements of the diagrams, the propagator line, the interaction line and a vertex, shown in the table together with their analytical

equivalents:

$G_0(1,2)$	
$iw(1,2)$	
$\int d3$	

(3.135)

By (3.134) and (3.132), the first-order correction is

$$G^{(1)}(1,2;U) = -\iint d4d3 G_0(1,4;U)[iw(4^+,3)]G_0(3,3^+;U)G_0(4,2;U)$$
$$+\iint d4d3 G_0(1,3;U)[iw(3,4)]G_0(3,4^+;U)G_0(4,2;U)\,. \qquad (3.136)$$

The two integrals correspond to the diagrams

(3.137)

Even these simplest examples show the basic overall features of the diagrammatic expansion based on Eqs. (3.134) and (3.132). (a) The diagrams of any order are obtained recurrently following purely mechanical rules which are easy to establish from the analytical equations; (b) a single representant is obtained for each set of topologically equivalent diagrams; (c) all diagrams are connected, i.e., diagrams with disconnected parts, like  , are excluded automatically. Altogether, the present method of functional derivatives leads straight to the *connected diagram expansion* of the Green's function. This is a convenient alternative to the more common direct use of the Wick theorem referred to at the end of Sec. 3.4.1, see, for example Ref. 131.

In order to construct the analytical expressions for the members of the perturbation series starting from the diagrams, it is enough to follow the *General rules for Feynman diagrams*, which are: (a) assign weight 1 to each diagram; (b) use the correspondence (3.135); (c for each closed loop of Fermion lines add a prefactor of -1. Applied to the diagrams (3.137), these rules recover the expressions (3.136). Notice that the (c) rule has to be used for the first (Hartree) diagram.

The whole Green's function is a sum of all (... expressions corresponding to the) Feynman diagrams of the typical form

where the time arrows are left out for simplicity.

Each such diagram consists of a chain of bare (free) propagator lines joined together by inserts consisting of propagator lines and interaction lines and having

exactly two terminal points. The whole diagram is said to be *reducible*, because it can be split into disconnected parts by cutting a single propagator line. The inserts are the *irreducible parts*, called so, because they cannot be split by such a single cut. This distinction is illustrated in the diagram by a few dot–dashed vertical lines. The diagrams may be of various lengths, i.e., have any number of irreducible inserts. Using the notation IR for these irreducible parts, we may write the whole Green's function as a symbolic sum

$$G = G_0 + G_0 \sum_{n=1}^{\infty} \sum_{\mathsf{IR}_1} \cdots \sum_{\mathsf{IR}_n} \mathsf{IR}_1 G_0 \cdots \mathsf{IR}_n G_0 \,. \tag{3.138}$$

The sum may be rearranged to

$$G = G_0 + G_0 \sum_{\mathsf{IR}_1} \mathsf{IR}_1 \left\{ G_0 + G_0 \sum_{n=2}^{\infty} \sum_{\mathsf{IR}_2} \cdots \sum_{\mathsf{IR}_n} \mathsf{IR}_2 G_0 \cdots \mathsf{IR}_n G_0 \right\}. \tag{3.139}$$

All sums involved are infinite and we see that in the last formula $\{\cdots\} = G$ for any IR_1. The outer sum may then be executed with the result

$$G = G_0 + G_0 \Sigma G \,, \tag{3.140}$$

$$\Sigma = \sum_{\mathsf{IR}} \mathsf{IR} \,. \tag{3.141}$$

The first line is a symbolic shorthand for the Dyson equation well-known from the equilibrium theory; the second line defines the

self-energy Σ = sum of all irreducible two terminal diagrams.

As an explicit example, we quote the lowest-order approximation for the self-energy,

$\Sigma^{(1)}(1,2;U) =$ 

$$= -i\delta_c(1,2) \int d3 w(1,3) G_0(3,3^+;U) + i w(1,2) G_0(1,2^+;U) \,. \tag{3.142}$$

It is easy to check that, had we started from Eq. (3.138) with a reverse order of the inner sums, $\mathsf{IR}_n \cdots \mathsf{IR}_1$, the same manipulations would have led to the Dyson equation $G = G_0 + G\Sigma G_0$ with the reverse order of factors, but with the same self-energy. This is an exceedingly important result.

In the standard notation, the final outcome of this analysis is the Dyson equation

$$G(1,2;U) = G_0(1,2;U) + \int d\bar{3} \int d\bar{4} G_0(1,\bar{3};U) \Sigma(\bar{3},\bar{4};U) G(\bar{4},2;U) \tag{3.143}$$

and its conjugate

$$G(1,2;U) = G_0(1,2;U) + \int d\bar{3} \int d\bar{4} G(1,\bar{3};U) \Sigma(\bar{3},\bar{4};U) G_0(\bar{4},2;U) \,. \tag{3.144}$$

To sum up,

- it was shown that the pair interaction can be incorporated into the NGF by means of a perturbation series, whose individual terms are classified by Feynman diagrams identical with those known from the equilibrium many-body theory. This is an important illustration of the rule set by Langreth long ago[95]:

  > "I will not give a set of diagrammatic rules and simply say: use your own rules. They will work here as well!"

  which, as is apparent, should be supplemented by the proviso "... for an uncorrelated initial condition". We shall return to these matters in Sec. 3.4.1.
- In particular, the method of summation of infinite subsets of Feynman diagrams is applicable just as in the equilibrium theory, and it was employed to derive the Dyson equations. These equations have a nonperturbative nature, which will be used below. It should be remembered, however, that this result was obtained to all orders of the perturbation theory only, just like in usual equilibrium statistical physics again.

3.4.7. *Self-energy and Dyson equation*

The self-energy could have been introduced without recourse to the perturbation expansion starting from the equations of motion (3.95) and (3.96), in which the term with the two-particle function G_2 would be replaced by the self-energy using the definitions

$$\begin{aligned} -i\int d3w(1^+,3)G_2(1,3,2,3^+;U) &= \int d3\Sigma(1,3;U)G(3,2;U) \quad \text{in (3.89)}\,, \\ -i\int d3w(2^+,3)G_2(1,3,2,3^+;U) &= \int d3G(1,3;U)\tilde{\Sigma}(3,2;U) \quad \text{in (3.90)}\,, \end{aligned} \tag{3.145}$$

for the self-energy Σ and the conjugate self-energy $\tilde{\Sigma}$. Then the first task would have been to prove that they must be equal, a fact which follows from the diagrammatic analysis directly:

$$\Sigma(1,2;U) = \tilde{\Sigma}(1,2;U)\,. \tag{3.146}$$

The proof can be completed, if the assumption of the uncorrelated initial condition is employed.

Substitution of Eq. (3.145) back in the equations of motion turns them into Dyson equations in differential form. It will be convenient to introduce the inverse Green's functions by the following steps. First, the inverse free Green's function is defined by

$$\begin{aligned} G_0^{-1}(1,2;U) &= \left(i\frac{\partial}{\partial t_1} - h_0(t_1) - U(t_1)\right)\delta_c(1,2)\,, \\ \delta_c(1,2) &\equiv \delta_c(t_1,t_2)\delta(x_1,x_2)\,. \end{aligned} \tag{3.147}$$

It satisfies the equations

$$\begin{aligned}\int d\bar{3}G_0^{-1}(1,\bar{3};U)G_0(\bar{3},2;U) &= \delta_c(1,2)\,,\\ \int d\bar{3}G_0(1,\bar{3};U)G_0^{-1}(\bar{3},2;U) &= \delta_c(1,2)\end{aligned} \tag{3.148}$$

and in this sense is an inverse operator to G_0. The last identities considered as equations for G_0 are solved by any admissible G_0, of course, so that the formal "inverse" G_0^{-1} can only be inverted back in conjunction with a specific initial condition.

With all these prerequisites, we can rewrite the equations of motion (3.95) and (3.96) to the differential Dyson equations in an operator form:

$$\begin{aligned}\int d\bar{3}(G_0^{-1}(1,\bar{3};U)-\Sigma(1,\bar{3};U))G(\bar{3},2;U) &= \delta_c(1,2)\,,\\ \int d\bar{3}G(1,\bar{3};U)(G_0^{-1}(\bar{3},2;U)-\Sigma(\bar{3},2;U)) &= \delta_c(1,2)\,.\end{aligned} \tag{3.149}$$

These equations can also be considered as a definition of the inverse full Green's function:

$$\begin{aligned}G^{-1}(1,2;U) &= G_0^{-1}(1,2;U)-\Sigma(1,2;U)\,,\\ \int d\bar{3}G(1,\bar{3};U)G^{-1}(\bar{3},2;U) &= \int d\bar{3}G^{-1}(1,\bar{3};U)G(\bar{3},2;U) = \delta_c(1,2)\,.\end{aligned} \tag{3.150}$$

Now we turn to the functional equation (3.103) again, this time in order to generate self-consistent equations for the self-energy. We have

$$\begin{aligned}&\int d3\Sigma(1,3;U)G(3,2;U)\\ &\quad = -i\int d3w(1^+,3)\left(G(3,3^+;U)G(1,2;U)-\frac{\delta G(1,2;U)}{\delta U(3)}\right).\end{aligned} \tag{3.151}$$

The identity $\delta G = \delta G(G^{-1}G) = (\delta G G^{-1})G = (-G\delta G^{-1})G$, which follows from (3.150), has the explicit form given by Eq. (3.149)

$$\frac{\delta G(1,2;U)}{\delta U(3)} = -\int d4d5G(1,4;U)\left(\delta_c(3,4)\delta_c(4,5)+\frac{\delta\Sigma(4,5;U)}{\delta U(3}\right)G(5,2;U)\,. \tag{3.152}$$

A closed equation for the self-energy then follows from (3.151). It can be written in two slightly different forms:

$$\begin{aligned}\Sigma(1,2;U) = &\overbrace{-i\int d3w(1^+,3)G(3,3^+;U)\delta_c(1,2)+iw(1,2)G(1,2;U)}^{\Sigma_{\rm HF}(1,2;U)=V_{\rm HF}(x_1,x_2,t_1;U)\delta_c(t_1,t_2)}\\ &+i\int d3d4w(1,4)G(1,3;U)\frac{\delta\Sigma(3,2;U)}{\delta U(4)}\,,\end{aligned} \tag{3.153}$$

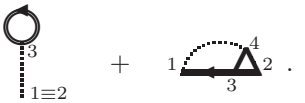
$$\Sigma(1,2;U) = \overbrace{-i\int d3w(1^+,3)G(3,3^+;U)\delta_c(1,2)}^{\Sigma_{\rm H}(1,2;U)} + i\int d3d4w(1,4)G(1,3;U)\overbrace{\left(\delta_c(3,2)\delta_c(3,4)+\frac{\delta\Sigma(3,2;U)}{\delta U(4)}\right)}^{\Gamma(3,2;4;U)}. \quad (3.154)$$

The first form (3.153) collects the two terms which are "singular", i.e., time-local, to the Hartree–Fock self-energy on the first line. The remaining term involves the vertex correction. This equation can be solved by iteration. The full GF is taken as given during the process, so that the iteration leads to a formal expansion of Σ in powers of the interaction w of fixed G. The resulting series can be represented by means of diagrams which are rather similar to those of the plain perturbation expansion of Σ, with two differences: (i) Full lines in the diagrams correspond to G rather than to G_0. (ii) There are no self-energy insertions at these lines.

The important conclusion is that the self-energy is expressed solely in terms of G and w and its U dependence is thus mediated through G. In other words, the self-energy is a functional $\Sigma[G]$ of the Green's function G. This functional dependence complements the Dyson equation (3.149), which is, in fact, just an identity between G_0, Σ and G. A closed equation for G results,

$$\begin{aligned}\int d\bar{3}(G_0^{-1}(1,\bar{3};U)-\Sigma(1,\bar{3})[G])G(\bar{3},2;U)=\delta_c(1,2)\,,\\ \int d\bar{3}G(1,\bar{3};U)(G_0^{-1}(\bar{3},2;U)-\Sigma(\bar{3},2)[G])=\delta_c(1,2)\,.\end{aligned} \quad (3.155)$$

Equation (3.154) preserves the separation of the self-energy into the local mean-field part and the exchange-correlation rest. The expression for Σ may be compared with the lowest-order iteration $\Sigma^{(1)}$ of the perturbation series (3.156). There, two diagrams represent the Hartree term and the Fock exchange term, both expressed in terms of the unperturbed Green's function and of the interaction. The exact self-energy (3.154) is obtained from (3.142) by renormalizing G_0 to G and by renormalizing *one* of the vertices in the exchange term from a simple point-like *bare vertex*, in which two G and one interaction w meet, to a three-point structure of the *full many body vertex*. The *vertex correction* $\delta\Sigma/\delta U$ is responsible for the correlation effects, everything "beyond the Hartree–Fock". This can be represented diagramatically as

$\Sigma(1,2;U) =$  . (3.156)

Once the self-energy functional $\Sigma[G]$ is given, exact or approximate, the auxiliary U field is not needed. A system of self-consistent equations for determination of the NGF can be derived. First, a closed equation for the Γ vertex is obtained. By (3.154)

and (3.152),

$$\Gamma(1,2;3) = \delta_c(1,2)\delta_c(1,3) + \frac{\delta\Sigma(1,2;U)}{\delta U(3)}$$
$$= \delta_c(1,2)\delta_c(1,3) + \int d4d5 \frac{\delta\Sigma(1,2;U)}{\delta G(4,5;U)} \frac{\delta G(4,5;U)}{\delta U(3)} \tag{3.157}$$

and setting $U \to 0$, we obtain the integral equation for Γ

$$\Gamma(1,2;3) = \delta_c(1,2)\delta_c(1,3) + \int d4d5d6d7 \frac{\delta\Sigma(1,2)}{\delta G(4,5)} G(4,6)G(7,5)\Gamma(6,7;3)\,. \tag{3.158}$$

Together with the expression Eq. (3.154) for the self-energy and the Dyson equation (3.149) for G, collected here in a concise form,

$$\Sigma(1,2) = \Sigma_{\rm H}(1,2) + i\int d3d4w(1,4)G(1,3)\Gamma(3,2;4)\,, \tag{3.159}$$

$$\left(i\frac{\partial}{\partial t_1} - h_0(1)\right) G(1,2) = \delta_c(1,2) + \int d3\Sigma(1,3)G(3,2)\,, \tag{3.160}$$

we have a self-consistent system of equations for the GF description of an arbitrary nonequilibrium process starting from a Keldysh initial condition. In order to obtain a solution of the system (3.158)–(3.160), a physical approximation for the four-point vertex $\delta\Sigma/\delta G$ has to be chosen. This is the true heart of the whole task, the rest is technical.

Comparing the results of this part with the perturbative approach of Sec. 3.4.6, we may summarize that there, the self-energy was generated as a functional $\Sigma[G_0]$. This has been superseded by $\Sigma[G]$ presently. The gains from this transition are manifold: the free GF G_0, whose meaning at finite times is spurious, has been eliminated, the relation $G \leftrightarrow \Sigma$ is nonperturbative and self-consistent, the many-body vertex structure is separated from single particle fields.

The transition to the self-consistent formalism may be symbolized simply as going from the G_0w formalism with both the bare GF and the interaction to the Gw formalism, in which the GF is dressed (renormalized), but the interaction remains bare. We sketch now one more step, to the GW formalism, in which the interaction is also renormalized. The procedure is universal. It is inevitable for the Coulomb interaction, where it accounts for the all-important screening effects.

We start from the equation of motion (3.103) and transfer the mean-field part of the right-hand side to the left as the Hartree field $V_{\rm H}(1;U)$ according to Eq. (3.104). We introduce the screened field $U_{\rm eff}(1) = U(1) + (V_{\rm H}(1;U) - V_{\rm H}(1;U=0))$ and get

$$\left(i\frac{\partial}{\partial t_1} - h_0(1) - V_{\rm H}(1;U=0) - U_{\rm eff}(1)\right) G(1,2;U)$$
$$= \delta_c(t_1,t_2) + i\int d3w(1^+,3)\frac{\delta G(1,2;U)}{\delta U(3)}\,. \tag{3.161}$$

$U_{\rm eff}$ will be substituted as the new variational variable instead of U. The integral on the right-hand side equals to $\int d3(\Sigma - \Sigma_{\rm H})G$ by (3.151). We denote the difference of self-energies as $\Sigma_{\rm XC}$ for exchange and correlation:

$$\int d3\Sigma_{\rm XC}(1,3;U)G(3,2;U) = -i\int d3d4w(1^+,3)\frac{\delta U_{\rm eff}(4)}{\delta U(3)}\frac{\delta G(1,2;U)}{\delta U_{\rm eff}(4)}\,. \quad (3.162)$$

Proceeding as before, we obtain

$$\frac{\delta G(1,2;U)}{\delta U(3)} = -\int d4d5G(1,4;U)\Gamma_s(4,5;3)G(5,2;U)\,, \quad (3.163)$$

$$\Sigma_{\rm XC}(1,2) = i\int d3d4w_s(1,4)G(1,3)\Gamma_s(3,2;4)\,, \quad (3.164)$$

with the renormalized interaction w_s and the vertex Γ_s defined by

$$w_s(1,2;U_{\rm eff}) = \int d3w(1^+,3)\frac{\delta U_{\rm eff}(2)}{\delta U(3)}\,, \quad (3.165)$$

$$\Gamma_s(3,2;4;U_{\rm eff}) = \delta_c(3,2)\delta_c(3,4) + \frac{\delta\Sigma_{\rm XC}(3,2;U_{\rm eff})}{\delta U_{\rm eff}(4)}\,. \quad (3.166)$$

Equations (3.164) and (3.166) permit to obtain an expansion of $\Sigma_{\rm XC}$ in terms of G and w_s. In the diagrammatic representation of the resulting series, the diagrams representing insertions between interaction lines are absent and all diagrams correspond to vertex corrections of an ever increasing topological complexity.

The renormalized interaction is given by the equation

$$w_s(1,2) = w(1,2) + \int d3d4w(1,3)\Pi(3,4)w_s(4,2)\,, \quad (3.167)$$

$$\Pi(3,4) = \int d5d6G(3,5)G(6,3)\Gamma_s(5,6;4)\,. \quad (3.168)$$

Equation (3.167) has the structure of a Dyson equation. The quantity Π is the *polarization operator*. It is apparent now that the self-energy is a functional of G again, with no explicit U dependence, so that the final equation closing the self-consistent set for the case of a screened interaction is

$$\Gamma_s(1,2;3) = \delta_c(1,2)\delta_c(1,3) + \int d4d5d6d7\frac{\delta\Sigma_{\rm XC}(1,2)}{\delta G(4,5)}G(4,6)G(7,5)\Gamma_s(6,7;3) \quad (3.169)$$

The equations forming the self-consistent system were already written for $U_{\rm eff} = 0$, that is $U = 0$. These are: (3.164), (3.167), (3.168) and (3.169). Finally, the Dyson equation is added, in the form which follows from Eqs. (3.161) and (3.162):

$$\left(i\frac{\partial}{\partial t_1} - h_0(1) - V_{\rm H}(1)\right)G(1,2;U) = \delta_c(t_1,t_2) + \int d3\Sigma_{\rm XC}(1,3)G(3,2)\,. \quad (3.170)$$

We made this excursion into the GW version of the GF formalism, because it is widely used in the area of electronic structure computations and it is gradually becoming standard also in the nonequilibrium problems. Its approximate formulations include the well-known random phase approximation (RPA) and the popular so-called GW approximation consisting in the neglect of the vertex correction in Eq. (3.164). The reader may be referred to Ref. 131. Here, this direction will not be pursued further.

3.4.8. *A note to approximate theories*

In this review, we are concerned primarily with the general structure of the NGF theory and do not analyze in detail properties of the inevitable approximations which make the whole formalism tractable. On the whole, two classes of approximations are in use, one class is formed by approximations of the decoupling type, which are usually of an *ad hoc* nature, based on physical motivation. The best known example is the Hartree–Fock theory. The other class encompasses the approximations of a systematic nature, usually based on the existence of small parameters, which serve for a systematic expansion and offering ways of testing and/or improving an approximation of certain degree. Here, we have to mention the RPA method as a classical example and the GW approximation as the technique on the rise and promising further improvement.

It is clear that very often there is no quantitative criterion to judge an approximation. It is then essential to use only (or at least as much as possible) approximate theories which are physically consistent, in other words, which are qualitatively correct and do not contain an inner contradiction.

Here, we only briefly mention several consistency requirements, which approximate theories have to fulfill. The reader can find a useful overview of these topics here.[129,131]

To ensure proper physical meaning of calculated observables, approximations must lead to conservation laws for observables like the number of particles and total energy, total momentum and total angular momentum. Within the framework of NGF approach this is closely related to the so-called Ward identities and ϕ derivable approximations for the self-energy. The conserving approximations for the NGF were thoroughly discussed by Kadanoff and Baym.[85,248,249] Ward identities, including their nonequilibrium variants, are discussed in the following articles.[125,162,250–253]

3.5. *Matrix Green's function of real time*

The formalism of the NGF's defined on the time loop has an equivalent reformulation working with functions of real time, as we have mentioned preliminarily in Sec. 3.4.2. There are several variants of this matrix representation which have been used in the literature and a brief overview follows.

3.5.1. *Matrix representation for general functions on the contour*

In Sec. 3.4.2, Eqs. (3.80)–(3.83) and Fig. 2, it was shown on the example of the Green's function, how a single function of double times produces four real time functions. For further work, this quadruplet is conveniently arranged into a 2×2 matrix. In the case of the Green's function, we have

$$G \leftrightarrow \breve{\mathbf{G}} \equiv \begin{vmatrix} G^c & G^< \\ G^> & \tilde{G}^c \end{vmatrix} \equiv \begin{vmatrix} G^{++} & G^{+-} \\ G^{-+} & G^{--} \end{vmatrix} \equiv \begin{vmatrix} G^{11} & G^{12} \\ G^{21} & G^{22} \end{vmatrix}. \tag{3.171}$$

The first representation is descriptive, peculiar to the Green's function, and we shall return to it in Sec. 3.5.2. The $\pm$ notation originates from Keldysh and the signs refer to the two branches of the time contour. The numerical labels have the same meaning and we shall use the third variant for the formal developments now. In general, for a function $F(s,t)$ of two times s, t on the contour, the correspondence is

$$F(s,t) \leftrightarrow \breve{\mathbf{F}} \equiv \begin{vmatrix} F^{11}(s,t) & F^{12}(s,t) \\ F^{21}(s,t) & F^{22}(s,t) \end{vmatrix} \equiv \begin{vmatrix} F(s^+,t^+) & F(s^+,t^-) \\ F(s^-,t^+) & F(s^-,t^-) \end{vmatrix}, \tag{3.172}$$

where on the right all times run from $-\infty$ to $+\infty$. These matrices are denoted by boldface characters and are — just for the present discussion — tagged by the $\supset$ symbol as a reminder of the time loop. The functions on the loop can be added and multiplied one with another and their assembly contains a neutral element for addition, zero, represented simply by the zero function, and also a neutral element for multiplication, unity, represented by the delta function $\delta_c(s,t)$ — if such functions, singular at $s = t$, are also admitted. Altogether, the functions on the loop form a (unitary) ring $\mathfrak{C}$.[a] On going to the matrix representation, it appears that addition is mapped on the matrices trivially, but for multiplication, say $D = BC$, we obtain

$$D(s,u) = \int_{\mathfrak{C}} dt B(s,t)C(t,u)\,, \tag{3.173}$$

$$\begin{aligned} \leftrightarrow D^{\alpha\beta}(s,u) &= \int_{-\infty}^{+\infty} dt\, B^{\alpha 1}(s,t)C^{1\beta}(t,u) + \int_{+\infty}^{-\infty} dt\, B^{\alpha 2}(s,t)C^{2\beta}(t,u) \\ &= \int_{-\infty}^{+\infty} dt\, B^{\alpha 1}(s,t)C^{1\beta}(t,u) - \int_{-\infty}^{+\infty} dt\, B^{\alpha 2}(s,t)C^{2\beta}(t,u) \qquad (3.174) \\ &= \int_{-\infty}^{+\infty} dt\, (\breve{\mathbf{B}}(s,t)\tau_3\, \breve{\mathbf{C}}(t,u))^{\alpha\beta}, \quad \tau_3 = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}. \qquad (3.175) \end{aligned}$$

Here, τ_3 is one of the Pauli matrices; for the rest, we use a corresponding notation,

$$\tau_0 = \begin{vmatrix} 1 & 0 \\ 0 & 1 \end{vmatrix}, \quad \tau_1 = \begin{vmatrix} 0 & 1 \\ 1 & 0 \end{vmatrix}, \quad \tau_2 = \begin{vmatrix} 0 & -i \\ i & 0 \end{vmatrix}. \tag{3.176}$$

[a]Remaining axioms of a ring, commutativity of addition, associativity of multiplication, distributivity of multiplication, are all verified by inspection.

We are thus led to work with matrices

$$\overrightarrow{\overrightarrow{\mathbf{F}}} = \tau_3 \overrightarrow{\overleftarrow{\mathbf{F}}} = \begin{vmatrix} F^{11} & F^{12} \\ -F^{21} & -F^{22} \end{vmatrix} . \tag{3.177}$$

Their set is closed with respect to addition and multiplication, i.e., Eq. (3.173) becomes

$$\overrightarrow{\overrightarrow{\mathbf{D}}}(s,u) = \int_{-\infty}^{+\infty} dt\; \overrightarrow{\overrightarrow{\mathbf{B}}}(s,t)\, \overrightarrow{\overrightarrow{\mathbf{C}}}(t,u) . \tag{3.178}$$

In other words, the set is algebraically isomorphic with the original ring of functions on the contour. It is possible to multiply more factors consecutively, so that, for example, the Dyson equation (3.143) reads

$$\overrightarrow{\overrightarrow{\mathbf{G}}} = \overrightarrow{\overrightarrow{\mathbf{G_0}}} + \overrightarrow{\overrightarrow{\mathbf{G_0}}}\, \overrightarrow{\overrightarrow{\mathbf{\Sigma}}}\, \overrightarrow{\overrightarrow{\mathbf{G}}} . \tag{3.179}$$

The matrix representation of the delta-function follows from Eq. (3.91):

$$\delta_c(t_1,t_2) \leftrightarrow \overrightarrow{\overleftarrow{\boldsymbol{\delta}}}(t_1,t_2) = \tau_3\delta(t_1-t_2) \leftrightarrow \overrightarrow{\overrightarrow{\boldsymbol{\delta}}}(t_1,t_2) = \tau_0\delta(t_1-t_2) . \tag{3.180}$$

By the last transformation, a plain delta-function is thus obtained, so that, for example, the definition (3.147) of the inverse free Green's function has the form

$$\begin{gathered} \overrightarrow{\overrightarrow{\mathbf{G}}}_{\mathbf{0}}^{-1}(1,2;U) = \left(i\frac{\partial}{\partial t_1} - h_0(1) - U(1) \right) \tau_0\delta(1,2) \equiv G_0^{-1}(1,2;U)\delta(1,2) , \\ \delta(1,2) \equiv \delta(t_1-t_2)\tau_0\delta(x_1,x_2) . \end{gathered} \tag{3.181}$$

3.5.2. *G-like functions*

The definition (3.77) of the Green's function, repeated here for convenience,

$$G(1,2) = -i\mathrm{Tr}(\mathcal{P}\,\mathsf{T}_c\{\psi(1|t_\mathrm{I})\psi^\dagger(2|t_\mathrm{I})\}) .$$

implies several symmetry properties of G as a function on the contour discussed here following Danielewicz[102]:

- *Symmetry with respect to the branches of the contour*

We introduce the following notation. Let t_1 be at a branch of the contour. Then t_1^{T} lies oppositely on the other branch. Further, if $t_1,\ x_1 \equiv 1$, then $t_1^{\mathsf{T}},\ x_1 \equiv 1^{\mathsf{T}}$. The symmetry of G reads:

$$\begin{aligned} &\text{Let } t_1 > t_2 \text{ algebraically. Then } t_2 \prec t_1,\ t_1^{\mathsf{T}} \Rightarrow G(1,2) = G(1^{\mathsf{T}},2) . \\ &\text{Let } t_1 < t_2 \text{ algebraically. Then } t_1 \prec t_2,\ t_2^{\mathsf{T}} \Rightarrow G(1,2) = G(1,2^{\mathsf{T}}) . \end{aligned} \tag{3.182}$$

These rules lead to the form (3.85) for G, which in turn is equivalent with the first matrix form of G in Eq. (3.171).

Other quantities also obey the symmetry rules (3.182), and together they constitute the *class of G-like functions* we shall denote as $\mathfrak{K}$. The general structure of functions from $\mathfrak{K}$ is

$$F(t_1,t_2) = \theta_c(t_1,t_2)F^{>}(t_1,t_2) + F^{\delta} + \theta_c(t_2,t_1)F^{<}(t_1,t_2)\,, \tag{3.183}$$

where $F^{>}$, $F^{<}$ are arbitrary and

$$F^{\delta}(t_1,t_2) = f_0(t_1)\delta_c(t_1,t_2) + f_1(t_1)\delta_c'(t_1,t_2) + \cdots \tag{3.184}$$

is the singular component already introduced for a general F in the preceding paragraph.

It turns out that the G-like functions (3.183) form a subset of all functions on the contour, which is closed with respect to addition and multiplication, and contains unity δ_c. In other words, $\mathfrak{K}$ is a (unitary) sub-ring of $\mathfrak{C}$. If the inverse to an $F \in \mathfrak{K}$ exists, then it also belongs to this class of G-like functions. In particular, for the self-energy we get the important result that $\Sigma \in \mathfrak{K}$, explicitly

$$\Sigma(1,2) = \theta_c(t_1,t_2)\Sigma^{>}(1,2) + V_{\mathrm{HF}}(1,2)\delta_c(t_1,t_2) + \theta_c(t_2,t_1)\Sigma^{<}(1,2)\,. \tag{3.185}$$

Note: The set of G-like functions is referred to as Keldysh space in Ref. 131 and other works of R. van Leeuwen and coworkers. In Ref. 129 even the whole $\mathfrak{C}$ ring is called the Keldysh space. It should be noted that this terminology is at variance with most other literature, where the term Keldysh space is reserved, probably starting from the influential review (Ref. 104), to the representation of contour functions by matrices of real time functions. Even if this latter convention is not accepted universally, we are going to adhere to it.

- *Symmetry with respect to complex conjugation*

Another symmetry of G which follows directly from the definition (3.77) or from Eq. (3.85) and Eqs. (3.81)–(3.82) can be written in two equivalent forms:

$$[G(1,2)]^{*} = -G(2^{\mathsf{T}},1^{\mathsf{T}})\,, \tag{3.186}$$

$$t[G(1,2)]^{\dagger} = -G(1^{\mathsf{T}},2^{\mathsf{T}})\,. \tag{3.187}$$

The important functions from $\mathfrak{K}$, like G_0, G_0^{-1}, G^{-1} and Σ, all may be shown to obey the same symmetry condition

$$\begin{aligned} [F(1,2)]^{*} &= -F(2^{\mathsf{T}},1^{\mathsf{T}})\,,\\ [F(1,2)]^{\dagger} &= -F(1^{\mathsf{T}},2^{\mathsf{T}})\,. \end{aligned} \tag{3.188}$$

For an F function of the general form (3.183), the conditions (3.188) yield the explicit relationships

$$\begin{aligned} [F^{\delta}(1,2)]^{*} &= F^{\delta}(2,1) \quad & [F^{\gtrless}(1,2)]^{*} &= -F^{\gtrless}(2,1)\,,\\ [F^{\delta}(1,2)]^{\dagger} &= F^{\delta}(1,2) \quad & [F^{\gtrless}(1,2)]^{\dagger} &= -F^{\gtrless}(1,2)\,, \end{aligned} \tag{3.189}$$

where $F^{\gtrless}$ are functions of real time.

3.5.3. *G-like functions in the Keldysh space*

In analogy to (3.171), a function $F \in \mathfrak{K}$ is mapped on

$$F \leftrightarrow \vec{\mathbf{F}} \equiv \begin{vmatrix} F^c & F^< \\ F^> & \tilde{F}^c \end{vmatrix} \equiv \begin{vmatrix} F^{++} & F^{+-} \\ F^{-+} & F^{--} \end{vmatrix} \equiv \begin{vmatrix} F^{11} & F^{12} \\ F^{21} & F^{22} \end{vmatrix} \tag{3.190}$$

and the matrix elements, by Eqs. (3.183) and (3.184), are

$$\begin{aligned} F^{11}(1,2) &= F^\delta(1,2) + \theta(t_1 - t_2)F^>(t_1,t_2) + \theta(t_2 - t_1)F^<(t_1,t_2)\,, \\ F^{12}(1,2) &= F^<(1,2)\,, \\ F^{21}(1,2) &= F^>(1,2)\,, \\ F^{22}(1,2) &= -F^\delta(1,2) + \theta(t_1 - t_2)F^<(t_1,t_2) + \theta(t_2 - t_1)F^>(t_1,t_2)\,. \end{aligned} \tag{3.191}$$

Four matrix elements are expressed by three functions, which are reflected by the identity

$$F^{11} + F^{22} = F^{12} + F^{21}\,. \tag{3.192}$$

As a special quantity, the *Keldysh function* is defined by

$$F^K = F^{12} + F^{21}\,. \tag{3.193}$$

Other functions in common use are

$$F^R = F^{11} - F^{12} = F^{12} - F^{22}\,, \tag{3.194}$$

$$F^A = F^{11} - F^{21} = F^{21} - F^{22}\,. \tag{3.195}$$

These are the retarded component (3.194) and the advanced component (3.195), respectively. Their explicit form follows from the relations (3.191):

$$\begin{aligned} F^R(1,2) &= F^\delta(1,2) + \theta(t_1 - t_2)(F^>(t_1,t_2) - F^<(t_1,t_2))\,, \\ F^A(1,2) &= F^\delta(1,2) - \theta(t_2 - t_1)(F^>(t_1,t_2) - F^<(t_1,t_2))\,. \end{aligned} \tag{3.196}$$

Finally, F^R, F^A satisfy the *spectral identity*

$$A^F \equiv i(F^R - F^A) = i(F^{21} - F^{12})\,, \tag{3.197}$$

by which another important quantity, the *spectral density* A^F, is introduced.

The action of complex conjugation may be demonstrated on the example of the Green's function for which $G^\delta = 0$. Combining Eq. (3.189) and the explicit expressions (3.191), we get

$$\begin{aligned} [G^c(1,2)]^* &= -\tilde{G}^c(2,1)\,, \\ [G^<(1,2)]^* &= -G^<(2,1)\,, \quad [G^>(1,2)]^* = -G^>(2,1)\,, \\ [G^K(1,2)]^* &= -G^K(2,1)\,, \\ [G^R(1,2)]^* &= -G^A(2,1)\,, \quad [G^A(1,2)]^* = -G^R(2,1)\,, \\ [A(1,2)]^* &= +A(2,1)\,. \end{aligned} \tag{3.198}$$

3.5.4. *Isomorphic transformations of the Keldysh space*

Now we return to Sec. 3.5.1. It was shown there that in order to obtain an isomorphic mapping of contour functions onto the matrix functions of real time, the correspondence should not be $F \mapsto \overset{\supset}{\mathbf{F}}$ but rather should involve matrices we denoted there by $\overset{\rightrightarrows}{\mathbf{F}}$:

$$F \mapsto \tau_3 \overset{\supset}{\mathbf{F}} = \begin{vmatrix} F^{++} & F^{+-} \\ -F^{-+} & -F^{--} \end{vmatrix} \equiv \overset{\rightrightarrows}{\mathbf{F}} . \tag{3.199}$$

This simplest transformation is recommended e.g., by Kita,[126] and the matrix (3.199) is the representation of choice for general formal work.

Often, it turns out as more convenient to take into account the linear dependence of the four matrix elements, Eq. (3.192), and to eliminate one of them by means of a linear transformation. A popular variant was introduced by Keldysh himself in Ref. 89. By a unitary transformation (known as "*Keldysh rotation*") with the matrix

$$\mathsf{L} = \frac{1}{\sqrt{2}}(\tau_0 - i\tau_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} 1 & -1 \\ 1 & 1 \end{vmatrix} , \tag{3.200}$$

he obtained the GF matrix in the form

$$G \mapsto \mathsf{L}\, \overset{\supset}{\mathbf{G}} \mathsf{L}^{-1} = \begin{vmatrix} 0 & G^A \\ G^R & K \end{vmatrix} . \tag{3.201}$$

A modification proposed by Larkin and Ovchinikov[254] yields a more convenient upper triangular $\mathbf{F}$ matrix. The same unitary matrix (3.200) is employed, but the basic transformation (3.199) is performed first. The GF matrix, self-energy matrix, etc, all obtain as

$$F \mapsto \mathsf{L}\tau_3 \overset{\supset}{\mathbf{F}} \mathsf{L}^{-1} = \begin{vmatrix} F^R & F^K \\ 0 & F^A \end{vmatrix} \equiv \mathbf{F}_K . \tag{3.202}$$

This "KLO" form of matrix functions is also widely used in the literature. We shall denote it by the $\mathbf{K}$ label. It should be warned that the Keldysh, and the Larkin Ovchinnikov, transforms are often mutually confused in the literature.

Yet another representation was proposed and developed in detail by Langreth and Wilkins[94] and popularized by Langreth in his famous lecture.[95] This variant employs a similarity transformation which is not unitary and this leads to an asymmetric result, in which the Keldysh function is replaced by $F^<$:

$$F \mapsto M\tau_3 \overset{\supset}{\mathbf{F}} M^{-1} = \begin{vmatrix} F^R & F^< \\ 0 & F^A \end{vmatrix} \equiv \mathbf{F} , \tag{3.203}$$

with

$$M = \tau_0 + \frac{1}{2}(\tau_1 - i\tau_2) = \begin{vmatrix} 1 & 0 \\ 1 & 1 \end{vmatrix} . \tag{3.204}$$

This transformation was introduced, because it is particularly well suited for transport problems including the derivation of quantum transport equations. For the same reason, it will be employed in the rest of this review predominantly. The associated dialect of NGF will be referred to as LW for brevity and the Langreth–Wilkins matrices will be used without label.

The LW representation is intuitively appealing, because it operates with the propagators and the particle correlation function, and these quantities have an immediate physical meaning. The formal advantage of LW formalism emerges when two matrix functions are multiplied:

$$\begin{aligned} \mathbf{B} = \mathbf{CD} &= \begin{vmatrix} C^R & C^< \\ 0 & C^A \end{vmatrix} \begin{vmatrix} D^R & D^< \\ 0 & D^A \end{vmatrix}, \\ \mathbf{B} &= \begin{vmatrix} B^R & B^< \\ 0 & B^A \end{vmatrix} = \begin{vmatrix} C^R D^R & C^R D^< + C^< D^A \\ 0 & C^A D^A \end{vmatrix}. \end{aligned} \tag{3.205}$$

The resulting multiplication formulae are widely known as the so-called *Langreth rules*. They have been derived in a number of ways, originally by a distortion of the Keldysh trajectory to another shape with two U-turns.[95] For a purely analytical derivation see, e.g., Ref. 131. Here, they are seen as a corollary to the algebraic structure of the LW representation. The rules are easily extended to more factors:

$$\begin{aligned} (\mathbf{CDEF}\cdots)^R &= C^R D^R E^R F^R \cdots, \\ (\mathbf{CDEF}\cdots)^A &= C^A D^A E^A F^A \cdots. \end{aligned}$$

For the *less*-component, the pattern already emerges for three factors:

$$(\mathbf{CDE})^< = C^R D^R E^< + C^R D^< E^A + C^< D^A E^A. \tag{3.206}$$

From a comparison of Eq. (3.202) with (3.203) it is apparent that the KLO multiplication rules are identically structured with the LW rules. We have, in particular:

$$\begin{aligned} B &= CD && \text{on } \mathbb{C}, \\ B^< &= C^R D^< + C^< D^A && \text{LW}, \\ B^K &= C^R D^K + C^K D^A && \text{KLO}, \\ B^> &= C^R D^> + C^> D^A. \end{aligned} \tag{3.207}$$

The fourth line is obtained by subtracting the second line from the third one.

3.5.5. *Dyson equation — various representations*

The Dyson equation in the basic representation (3.199) has already been given in Eq. (3.179). In the differential form, this equation and its conjugate read

$$\vec{\vec{\mathbf{G}}}_{\mathbf{0}}^{-1}\, \vec{\vec{\mathbf{G}}} = \vec{\vec{\delta}} + \vec{\vec{\mathbf{\Sigma}}}\, \vec{\vec{\mathbf{G}}}, \tag{3.208}$$

$$\vec{\mathbf{G}}\,\vec{\mathbf{G}}_{\mathbf{0}}^{-1} = \vec{\delta} + \vec{\mathbf{G}}\,\vec{\mathbf{\Sigma}}\,. \tag{3.209}$$

The inverse $\vec{\mathbf{G}}_{\mathbf{0}}^{-1}$ of the free GF is given by (3.181) with $U = 0$.

- *Kadanoff–Baym equations*

It is enough to consider two of the matrix components of either of the equations (3.208)–(3.209), because of the relations (3.191) valid both for $G \in \mathfrak{K}$ and $\Sigma \in \mathfrak{K}$. Choosing the off-diagonal elements and using the specific correspondence (3.85), (3.185), we are led to two equivalent pairs of equations for $G^{>}$ and $G^{<}$, one arising from Eq. (3.208),

$$\begin{aligned}
&\left(i\frac{\partial}{\partial t_1} - h(1)\right) G^{>}(1,2) - \int dx_3 V_{\mathrm{HF}}(1,3^{+}) G^{>}(3,2) \\
&\quad = \int_{-\infty}^{t_1} d3[\Sigma^{>}(1,3) - \Sigma^{<}(1,3)] G^{>}(3,2) \\
&\qquad - \int_{-\infty}^{t_2} d3\Sigma^{>}(1,3)[G^{>}(3,2) - G^{<}(3,2)]\,, \\
&\left(i\frac{\partial}{\partial t_1} - h(1)\right) G^{<}(1,2) - \int dx_3 V_{\mathrm{HF}}(1,3^{+}) G^{<}(3,2) \\
&\quad = \int_{-\infty}^{t_1} d3[\Sigma^{>}(1,3) - \Sigma^{<}(1,3)] G^{<}(3,2) \\
&\qquad - \int_{-\infty}^{t_2} d3\Sigma^{<}(1,3)[G^{>}(3,2) - G^{<}(3,2)]\,,
\end{aligned} \tag{3.210}$$

the other one arising from the conjugate Eq. (3.209):

$$\begin{aligned}
&\left(-i\frac{\partial}{\partial t_2} - h(2)\right) G^{>}(1,2) - \int dx_3 G^{>}(1,3) V_{\mathrm{HF}}(3,2^{+}) \\
&\quad = \int_{-\infty}^{t_1} d3[G^{>}(1,3) - G^{<}(1,3)] \Sigma^{>}(3,2) \\
&\qquad - \int_{-\infty}^{t_2} d3 G^{>}(1,3)[\Sigma^{>}(3,2) - \Sigma^{<}(3,2)]\,, \\
&\left(-i\frac{\partial}{\partial t_2} - h(2)\right) G^{<}(1,2) - \int dx_3 G^{<}(1,3) V_{\mathrm{HF}}(3,2^{+}) \\
&\quad \int_{-\infty}^{t_1} d3[G^{>}(1,3) - G^{<}(1,3)] \Sigma^{<}(3,2) \\
&\qquad - \int_{-\infty}^{t_2} d3 G^{<}(1,3)[\Sigma^{>}(3,2) - \Sigma^{<}(3,2)]\,.
\end{aligned} \tag{3.211}$$

These are the well-known *Kadanoff–Baym equations*, best represented in Ref. 85. We have a minimum set of two coupled integro-differential equations for the elemental quantities $G^>$, $G^<$ as the two unknowns. The discontinuities of G^c and $\tilde{G}^c$ come out here as the finite upper integration limits taking care of causality. On the whole, the KB equations leave the field theoretic idiom and are written in a manner close to the transport equations. In Sec. 5, we shall combine Eqs. (3.210) and (3.211) to a proto-transport equation called the Generalized Kadanoff–Baym equation (GKBE). A certain drawback of the KB equations is that the spectral and statistical aspects are not distinct and there is no direct way of separating both. This is better treated in the LW equations working explicitly with the set of propagators and the particle correlation function.

• *Dyson equation in the LW representation*

The Dyson equations in the KLO representation and in the LW representation are handled in the same manner, and we shall work out the LW case. Performing the transformation (3.203) on the "left" and "right" Dyson equations (3.208), (3.209), we get

$$\mathbf{G_0^{-1}G} = \boldsymbol{\delta} + \boldsymbol{\Sigma}\mathbf{G}\,, \tag{3.212}$$

$$\mathbf{GG_0^{-1}} = \boldsymbol{\delta} + \mathbf{G}\boldsymbol{\Sigma}\,. \tag{3.213}$$

Here, $\mathbf{G_0^{-1}} = \vec{\vec{\mathbf{G}}}_{\mathbf{0}}^{-1}$ and $\boldsymbol{\delta} = \vec{\vec{\boldsymbol{\delta}}}$, because these matrices are diagonal, see Eqs. (3.180) and (3.181). By matrix multiplication or by the Langreth rules (3.205), the Dyson equations for the R, A components are found as

$$\begin{aligned} G_0^{-1}G^R &= \delta + \Sigma^R G^R\,, \quad G_0^{-1}G^A = \delta + \Sigma^A G^A\,, \\ G^R G_0^{-1} &= \delta + G^R\Sigma^R\,, \quad G^A G_0^{-1} = \delta + G^A\Sigma^A\,. \end{aligned} \tag{3.214}$$

It suffices to treat one of these equations explicitly. By left-multiplying by G_0^R, the left equation for G^R is transformed to an integral equation, assuming, of course, the self-energy Σ^R to be known:

$$G^R = G_0^R + G_0^R\Sigma^R G^R\,. \tag{3.215}$$

The integral equation incorporates the boundary condition through the free propagator. It is important to realize that these boundary conditions do not depend on the initial condition specific for the selected uncorrelated initial state. To see that, it is enough to inspect the equation of motion for G_0^R:

$$G_0^{-1}G_0^R = \delta \cdots \left(i\frac{\partial}{\partial t_1} - h_0(1) - U(1)\right) G_0^R(1,2) = \delta(1,2)\,, \tag{3.216}$$

with the boundary condition

$$G_0^R(1,2) = 0 \quad \text{for } t_1 < t_2\,. \tag{3.217}$$

The solution is fixed by the jump conditions at equal times and the initial condition does not enter at all. In fact, the free propagator depends on the internal and external fields, but as concerns various initial conditions, it is universal for all of them. Explicitly,

$$G_0^R(1,2) = -is(1,2)\theta(t_1 - t_2)\,. \tag{3.218}$$

The evolution operator s has been defined by (3.118).

The *less*-component of $\mathbf{G}$ is governed by the equations

$$G_0^{-1}G^< = \Sigma^R G^< + \Sigma^< G^A\,, \tag{3.219}$$

$$G^< G_0^{-1} = G^R\Sigma^< + G^<\Sigma^A\,. \tag{3.220}$$

These equations are, in fact, identical with the second Kadanoff–Baym equation (3.210), as can be verified with the use of relations (3.196), and its conjugate. The form (3.219) is well suited for a numerical integration. More importantly, it permits a formal explicit solution in a closed form. For this, the right Dyson equation for G^R is needed. From (3.213) or (3.214), it follows that $G^R(G_0^{-1} - \Sigma^R) = \delta$. With this identity, Eq. (3.219) multiplied by G^R from the left becomes

$$G^< = G^R\Sigma^< G^A\,. \tag{3.221}$$

This exceedingly simple result is another one of the NGF relations most frequently quoted — and used. It was seemingly obtained without invoking the initial conditions in three steps: first – G_0^R from (3.217); second – G^R from the Dyson equation; finally, in the third step, G^R alone is enough to specify the solution of Eq. (3.219) uniquely. This was only made possible by the Keldysh initial conditions. These enter the solution implicitly through the self-energies Σ^R, $\Sigma^<$, which incorporate the uncorrelated initial condition in the present case. Returning to Eq. (3.221), the following features are apparent: (a) The $<$ component of the *integral* Dyson equation is, in fact, a formula. (b) Neither the initial conditions nor the unperturbed GF enter the result. (c) The expression for $G^<$ has the causal structure $R\cdots<\cdots A$, and the finite integration limits, explicit in the KB equations, are imposed by the boundary conditions for both propagators. (d) Finally, we quote the KLO equivalent of Eq. (3.221). As expected,

$$K = G^R\Omega G^A\,; \quad K \equiv G^K\,, \quad \Omega \equiv \Sigma^K\,, \tag{3.222}$$

where we use the conventional Keldysh notation.

4. Finite Time Initial Conditions

In the previous chapter, we were able to present in some detail ways of handling the NGFs of the Keldysh type, that is defined on the Keldysh contour extending to an infinitely remote past and obeying an uncorrelated initial condition there. In this chapter, we will be concerned with the same task, but for the general case of

Green's functions defined on a Schwinger contour with an arbitrary, typically finite, initial time $t_{\rm I}$ and starting from an arbitrary initial many-body state $\mathcal{P}_{\rm I}$.

The problem of general initial conditions is often stated as a problem of *correlated* initial conditions. This may be understood in two ways: either as a requirement that at any finite time the description of the system takes account of the particle correlations, or simply as opposite to the Keldysh initial conditions. This second interpretation is more than a trivial logical figure, because it points to the basic formal difficulty that the Wick theorem does not hold in the correlated case. See the discussion in Sec. 3.4.5. This means in turn that neither the perturbative expansion based on Feynman diagrams of Sec. 3.4.6, nor its nonperturbative equivalents of Sec. 3.4.7 are valid, and the whole theory has to be reconsidered anew.

Historically, the problem of general initial conditions was not fully appreciated at first, partly because it has little importance for the steady state nonequilibrium quantum transport, the topic in focus of the early NGF work. We cannot review here the beginnings of the investigations on the finite time initial conditions started by Fujita,[193] Hall,[194] Craig[92] and Kukharenko and Tikhodeev.[195] The modern period in this field was opened by the work[102] of Danielewicz, which we had occasion to cite several times already. There is a vast literature devoted to the finite time initial conditions. Here are some of the important citations.[102,110,118,125,129,131,154,167,168,171,196–210]

There are two basic approaches in current use, as sketched in Fig. 3.

A. A direct construction of the NGF with arbitrary initial conditions on the Schwinger contour, Fig. 3.
B. A perturbative treatment of the correlated initial condition on an extended contour, the so-called Kadanoff–Baym trajectory. This is the Schwinger countour extended by an imaginary time stretch beyond the final time $t_{\rm I}^-$, as shown in Fig. 3(b). This is, without doubt, the most widely used technique in the field.
C. An extension of the Schwinger contour to the full Keldysh contour, Fig. 3(c), can be used for the same purpose, yielding simple and physically transparent results.

First, the case A will be introduced briefly. It is remarkable that the NGF problem can be attacked directly from the definition, so to say, for an initial many-body state $\mathcal{P}_{\rm P}$ which may be arbitrary, that is, no temperature, chemical potential, etc can need be ascribed to it. The only condition is that it is normalized to a prescribed particle number,

$$\mathrm{Tr}(\mathcal{P}_{\rm P}\mathcal{N}) = N\,. \tag{4.1}$$

The task of finding the Green's function from the definition (3.77) might seem hopeless, but, in fact, several practicable algorithms have been devised for it. A fully self-consistent approach based on the functional derivative method has been developed and partly applied with success.[197,201,207,208] A parallel treatment is the very basic procedure employing the perturbation expansion. It was outlined in Ref. 102

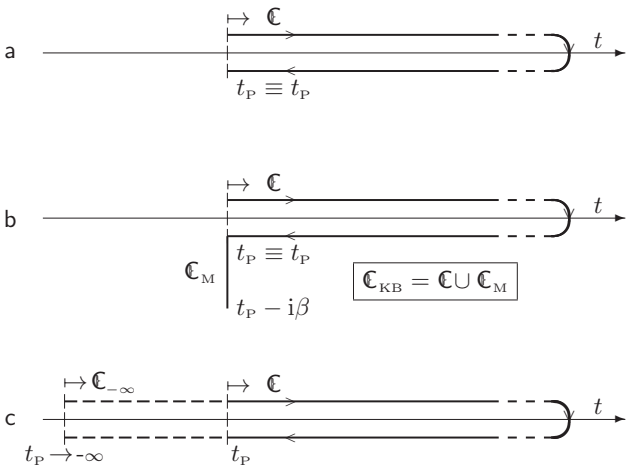


Fig. 3. The contours used to deal with finite time initial conditions. The time $t_{\rm P}$ marks the onset of the relevant nonequilibrium process. (a) *Schwinger trajectory* $\mathbb{C}$ of the process under study. The initial time $t_{\rm I}$, at which the trajectory is starting and ending, coincides with $t_{\rm P}$. (b) *Extended* (Kadanoff–Baym) trajectory $\mathbb{C}$ consists of the Schwinger trajectory $\mathbb{C}$ and of its extension to imaginary times $\mathbb{C}_{\rm M}$; the label M stands for "Matsubara". The trajectory is not closed, but still it involves the excursion to "$+\infty$" and back. (c) *Keldysh* trajectory $\mathbb{C}_{-\infty}$ for a "host" process starting at $t_{\rm I} \to -\infty$ and partitioned at $t_{\rm P}$ marking the onset of the physical process in question, and the end of a "prelude" unfolding in the "past".

and worked out in detail in recent years[247] with the outcome of a generalized Wick theorem according to which the perturbation expansion gradually incorporates also the initial condition in the form of the correlation parts of the reduced density matrices of ever increasing order. An uncorrelated initial state then falls back to the standard Wick expansion in an automatic fashion. The self-consistent equations have a diagrammatic representation too, with the GF lines dressed, $G_0 \to G$, while the correlation inserts remain intact. All these matters are excluded from the present review, in which we concentrate rather on the cases B and C. Even there, the presentation will be but brief.

4.1. *Extended (Kadanoff–Baym) contour*

This method was originally discovered for the initial condition given by the grand-canonical ensemble (3.51) with a prescribed temperature and chemical potentials. We shall briefly outline this important case and mention possible extensions only at the end.

4.1.1. *Green's function on the extended contour*

For the grand canonical thermal average, the Green's function becomes

$$G(1,2) = -i\frac{{\rm Tr}[e^{-\beta(\mathcal{H}_{\rm eq}-\mu\mathcal{N})}\,\mathcal{T}_c(\psi(1)\psi^\dagger(2))]}{{\rm Tr}\,e^{-\beta(\mathcal{H}-\mu\mathcal{N})}}\,, \tag{4.2}$$

where the times t_1, t_2 are on the real time Schwinger contour so far and

$$\mathcal{H}_{\rm eq} = \mathcal{H}(t_{\rm P}) = \mathcal{H}_0(t_{\rm P}) + \mathcal{W} = \mathcal{T} + \mathcal{V} + \mathcal{W}\,, \tag{4.3}$$

is the equilibrium Hamiltonian of the stand alone system before the external fields $\mathcal{H}'_{\rm e}(t)$ are turned on, see Eq. (3.1). The statistical operator obeys the Matsubara analogy with the evolution operator of a constant Hamiltonian and can be formally attached to the evolution operator on the loop as its extension beyond the end point $t_{\rm P}^-$, that is for times $t_{\rm P}^- - i\tau$, $0 \le \tau \le \beta$. The evolution operator is defined on the whole extended contour in Fig. 3(b) by

$$\begin{aligned}
\mathcal{S}(t,t') &\equiv \mathcal{S}(t,t') && \text{for } t,t' \in \mathbb{C} \\
&= \mathcal{S}_{\rm M}(t,t_{\rm P})\mathcal{S}(t_{\rm P},t') && \text{for } t \in \mathbb{C}_{\rm M}, t' \in \mathbb{C} \\
&= \mathcal{S}_{\rm M}(t,t') && \text{for } t,t' \in \mathbb{C}_{\rm M} \\
&\quad \text{etc} \\
\mathcal{S}_{\rm M}(t,t') &= e^{-i(t-t')\mathcal{H}_{\rm M}}\,, && \mathcal{H}_{\rm M} = \mathcal{H}_{\rm eq} - \mu\mathcal{N} \equiv \mathcal{H}_{\rm M0} + \mathcal{W}\,.
\end{aligned} \tag{4.4}$$

It is important to define the GF for time arguments on the whole extended contour $\bar{\mathbb{C}} = \mathbb{C} \cup \mathbb{C}_{\rm M}$. To this end, we have to modify the definition of the Heisenberg operators by restricting it to the second form of Eq. (3.15) which is suitable for both real and imaginary times:

$$\mathcal{X}_{\rm H}(t) \equiv \mathcal{X}(t) = \mathcal{S}(t_{\rm I},t)\mathcal{X}(t)\mathcal{S}(t,t_{\rm I})\,. \tag{4.5}$$

With the definition (4.4), the GF (4.2) becomes

$$G(1,2) = -i\,\frac{{\rm Tr}[\mathcal{S}(t_{\rm I}-i\beta,t_{\rm I})\mathcal{T}_c(\psi(1)\psi^\dagger(2))]}{{\rm Tr}\,\mathcal{S}(t_{\rm I}-i\beta,t_{\rm I})}\,, \tag{4.6}$$

where the range of the time-ordering operator $\mathcal{T}_c$ is now also extended to the whole $\bar{\mathbb{C}}$ contour and the times from the $\mathbb{C}_{\rm M}$ extension come later than all times on the basic real time contour.

4.1.2. *Kubo–Martin–Schwinger conditions*

The so-called Kubo–Martin–Schwinger (KMS) conditions are boundary conditions for the Green's function (4.6). They have been derived originally for the equilibrium Green's functions. Quite remarkably, they can be extended to the systems out of equilibrium. The boundary condition they represent links the values of the Green's function at the initial time $t_{\rm I}$ and at the final time $t_{\rm I} - i\beta$:

$$\begin{aligned}
G(x_1,t_{\rm I}-i\beta,2) &= -i\,\frac{{\rm Tr}[\psi(x_1)\mathcal{S}(t_{\rm I}-i\beta,t_2)\psi^\dagger(x_2)\mathcal{S}(t_2,t_{\rm I})]}{{\rm Tr}\,\mathcal{S}(t_{\rm I}-i\beta,t_{\rm I})} \\
&= -i\,\frac{{\rm Tr}[\mathcal{S}(t_{\rm I}-i\beta,t_2)\psi^\dagger(x_2)\mathcal{S}(t_2,t_{\rm I})\psi(x_1)]}{{\rm Tr}\,\mathcal{S}(t_{\rm I}-i\beta,t_{\rm I})} \\
&= -G(x_1,t_{\rm I},2)\,.
\end{aligned} \tag{4.7}$$

In a similar fashion, the other KMS relation can be derived:

$$G(1, x_2, t_{\rm I} - i\beta) = -G(1, x_2, t_{\rm I})\,. \tag{4.8}$$

As is seen, these conditions express the anti-periodicity of the Green's function along the imaginary time axis.

4.1.3. *Perturbation expansion on the extended contour*

Our task will be to transform the Green's function (4.6) into the interaction picture in the literal sense, with the interaction $\mathcal{W}$ playing the role of the perturbation, like in Sec. 3, but on the extended contour $\bar{\mathbb{C}}$. We recall the notation with carets over the operators in the interaction picture and plain S for the evolution operator in the interaction picture introduced in Sec. 3.4.1. Then

$$\mathcal{S}(t, t_{\rm P}) = \mathcal{S}_0(t, t_{\rm P}) S(t, t_{\rm P})\,. \tag{4.9}$$

The free evolution operator is defined in analogy with Eq. (4.4), but for the free Hamiltonian. In particular,

$$\mathcal{S}_0(t_{\rm P} - i\beta, t_{\rm P}) = e^{-\beta \mathcal{H}_{\rm M0}}\,. \tag{4.10}$$

The unperturbed statistical operator is thus equal to

$$\mathcal{P}_0 = \frac{\mathcal{S}_0(t_{\rm P} - i\beta, t_{\rm P})}{\mathrm{Tr}\,\mathcal{S}_0(t_{\rm P} - i\beta, t_{\rm P})}\,. \tag{4.11}$$

Finally, we define

$$S = \mathcal{T}_{\bar{c}}\, e^{-i\int d\tau \hat{\mathcal{W}}(\tau)}\,, \qquad \boxed{\int = \int_{\bar{\mathbb{C}}}}\,. \tag{4.12}$$

With all this notation, it is easy to bring (4.6) to

$$G(1,2) = -i\,\frac{\mathrm{Tr}[\mathcal{P}_0\,\mathcal{T}_c(\psi(1)\psi^\dagger(2)S)]}{\mathrm{Tr}[\mathcal{P}_0 S)]}\,. \tag{4.13}$$

The structure of this formula is the same as that of the ground state expression (3.72). The average is now taken over the free grand canonical ensemble, which is clearly an uncorrelated state. Expanding the expression (4.12) for S in terms of $\mathcal{W}$, we obtain a power series both in the numerator and in the denominator, to which the Wick theorem applies. The resulting expansion is organized according to the standard connected Feynman diagrams, only the integrals involved now run over the whole extended contour.

4.1.4. *Functional derivatives*

It is illuminating to see, how the same result can be obtained by a procedure closely following Sec. 3.4.6. An auxiliary external scalar field is introduced into the system,

so that the Green's function is U-dependent. Equation (3.131)

$$G(1,2;U) = G_0(1,2;U) - \iint dd4d3 G_0(1,4;U)[iw(4^+,3)]G(3,3^+;U)G(4,2;U)$$
$$+ \iint d4d3 G_0(1,4;U) \times [iw(4^+,3)] \frac{\delta G(4,2;U)}{\delta U(3)} \,. \tag{4.14}$$

can be derived as before, because the initial conditions are not used in the derivation. Now comes the critical point. This equation should serve as a basis for the iterative procedure yielding G as series in powers of iw. In order to get the conventional Feynman diagrams, the simple expression for the functional derivative of G_0 is needed:

$$\frac{\delta G_0(1,2;U)}{\delta U(3)} = G_0(1,3;U)G_0(3,2;U) \,. \tag{4.15}$$

In Sec. 3.4.6, the latter relation was valid as a consequence of the uncorrelated Keldysh initial conditions. Following Kadanoff and Baym,[85] we may try to derive it from the identity $G_0^{-1}G_0 = 1$:

$$\delta[G_0^{-1}G_0] = \delta(G_0^{-1})G_0 + G_0^{-1}\delta G_0 = 0 \,. \tag{4.16}$$

We are tempted to conclude that

$$\delta G_0 = -G_0 \delta(G_0^{-1}) G_0 \,. \tag{4.17}$$

This conclusion is too rash, because to δG_0 in (4.16), an arbitrary solution of the homogeneous equation may be added

$$\left(-i\frac{\partial}{\partial t_1} - h_0(1)\right) Q(1,2) = 0 \,. \tag{4.18}$$

The result (4.17) follows also from the other relation, $G_0 G_0^{-1} = 1$, so that Q should also satisfy the conjugate equation. At this point enter the KMS conditions, which hold for $\delta G_0/\delta U$ as a corollary to (4.7), (4.8) and finally determine that $Q = 0$. Thanks to that, the whole iterative procedure becomes possible, the self-energy can be uniquely defined as the sum of all irreducible two-point diagrams and the Dyson equations of the extended loop follow.

4.1.5. *Matrix Green's function*

Just like in Sec. 3.5.3, it is important for a practical work with the NGF to rewrite the formalism on the extended $\bar{\mathbb{C}}$ contour into equations for the components. Now, there are three stretches of the contour, $+$, $-$ and M, so that we get nine combinations of the time arguments:

$$\mathbf{G} = \begin{vmatrix} G^{++} & G^{+-} & G^{+\mathrm{M}} \\ G^{-+} & G^{--} & G^{-\mathrm{M}} \\ G^{\mathrm{M}+} & G^{\mathrm{M}-} & G^{\mathrm{MM}} \end{vmatrix} = \begin{vmatrix} G^{c} & G^{<} & G^{\rceil} \\ G^{>} & \tilde{G}^{c} & G^{\rceil} \\ G^{\lceil} & G^{\lceil} & G^{\mathrm{M}} \end{vmatrix} . \tag{4.19}$$

In the second form of the matrix, we use the more common notation nowadays, in particular the symbols $\lceil$ and $\rceil$ for the "mixed" components, whose one time argument is real, the other imaginary. This notation also makes explicit that $G^{\mathrm{M}+} = G^{\mathrm{M}-}$ and similarly the other pair; the reason is that the imaginary stretch follows in contour ordering both the + branch and the − branch of the contour. For $\mathbf{G}$, the multiplication rules have to be extended, but are still called the Langreth–Wilkins rules. For example, if $C = AB$ on the extended contour, then

$$C^{<} = A^{R}B^{<} + A^{<}B + A^{\rceil}B^{\lceil}\,, \tag{4.20}$$

$$C^{R} = A^{R}B^{R}\,, \tag{4.21}$$

$$C^{\lceil} = A^{\lceil}B^{A} + A^{\mathrm{M}}B^{\lceil}\,, \tag{4.22}$$

with the products meaning the appropriate integrations. Correspondingly enriched are the Kadanoff–Baym equations.

4.1.6. *Notes to the extended contour*

The first remark concerns terminology. The extended contour has been given various names, like Schwinger–Keldysh, which appears as somewhat inappropriate; in the book,[131] the authors coin the name of Konstantinov and Perel, which would be just a tribute to the very early work of these authors,[255] where the extended contour is a central concept. We prefer to call the extended contour the Kadanoff–Baym contour. It is true that neither in the famous papers,[248,249] nor in the book,[85] the contour is introduced at all. Yet it can be construed from these works in the hindsight, as pointed out by Langreth in Ref. 95.

The method of Kadanoff and Baym is very different from the present understanding of the use of the extended contour. They start from a Matsubara-like Green's function of imaginary times, but with an external field U included, which depends on time analytically. This nonequilibrium function is found to satisfy the KMS boundary conditions just like in equilibrium, and these boundary conditions serve to fix uniquely the analytical continuation of both pieces of the causal function from the imaginary axis to real times; they are identified with $G^{>}$ and $G^{<}$, and the two functions are shown to be controlled by the Kadanoff–Baym equations. The initial value problem is obviated by sending t_{P} to $-\infty$, together with the imaginary time stretch. The evolution operator is, naturally, the same in the whole complex time plane, and this gives the left KMS condition the form

$$G(x_1, t_{\mathrm{I}} - i\beta, 2) = -e^{\beta\mu}G(x_1, t_{\mathrm{I}}, 2)$$

and similarly for the right one. Reminiscences of this technique appear from time to time in the literature in phrases like "derive the LW rules by analytical continuation" used for contemporary quite remote techniques.

It has appeared clearly from the derivations in Sec. 4.1.1 that the $\mathbb{C}_{\mathrm{M}}$ extension of the Schwinger loop is simply an additional integration range contiguous with the

return track of the loop, not necessarily lying in a complex time plane; in that sense, the idea of the extended contour is more general, admitting initial conditions having nothing in common with the dynamics of the system for real times. This has been brought to an extreme by Wagner,[196] who proposed the following construction. Take an arbitrary initial state $\mathcal{P}_\mathrm{I}$ which is positive definite, and a real positive number λ (the case of positive semidefinite states, like a pure state $|\psi\rangle\langle\psi|$, seems to be overstretched). Then a self-adjoint operator $\mathcal{B}$ exists such that

$$\mathcal{P}_\mathrm{I} = e^{-\lambda\mathcal{B}}\,. \tag{4.23}$$

Further a single particle "Hamiltonian" $\mathcal{B}_0$ can be introduced, and their difference is the "interaction" $\mathcal{Y}$. Making now the replacements

$$\begin{aligned} \mathcal{H}_\mathrm{M} &\dashrightarrow \mathcal{B} \\ \mathcal{H}_\mathrm{M0} &\dashrightarrow \mathcal{B}_0 \\ \mathcal{W} &\dashrightarrow \mathcal{Y} \\ \beta &\dashrightarrow \lambda \end{aligned} \tag{4.24}$$

in Eq. (4.4), we may define a generalized version of NGF on the extended contour and continue up to Eq. (4.13) without change. Then, of course, the excessive generality causes a problem. The formal interaction $\mathcal{Y}$ involves instantaneous collisions of arbitrarily large clusters in general, and an attempt to generate a perturbation expansion is bound to fail.

There is a restricted choice of $\mathcal{B}$, however, which is tractable with an effort similar to the basic case (4.4). Namely, as proposed by Danielewicz in Ref. 102, the initial state is taken to correspond to a Hamiltonian with pair interactions only, but the interaction term $\mathcal{Y}$ may be chosen at will, for example stronger than $\mathcal{W}$, or stronger in certain parts of the phase space. This will produce an overcorrelated initial state. This concept should be understood relative to the "true" dynamics with the interaction $\mathcal{W}$, according to which the system will relax. Similarly, the one-particle Hamiltonian defining the initial state may be selected different from that acting on the loop. For example, the system may be squeezed initially, and then released. We see that the extended contour permits a wide flexibility in the admissible initial conditions.

4.2. *Folding down the Keldysh contour* (*time partitioning*)

Finally, we briefly introduce a third method of respecting the finite time initial conditions, as it was defined in Fig. 3(c). The goal is to construct a NGF with an initial time t_P, at which the correlated initial state is $\mathcal{P}_\mathrm{P}$. This initial state is not arbitrary, but it coincides with the state at which an antecedent ("preparation") process has arrived at the initial time. Beyond that time, the evolution will continue as the dynamical process in question ("measurement" or "observation").

This interpretation of the two stages as the past and the future with respect to the initial time is entirely subjective and our task is, in fact, to compare two

processes differing only in their time definition range, as shown in the figure. The process under study evolves along the Schwinger–Keldysh trajectory $\mathbb{C}$ starting and ending at $t_{\rm P}$ and is described by the Green's function we denote $\mathbf{G}$ suppressing the subscript. This process is augmented by a preparatory stage running between $t_{\rm I} \to -\infty$ and $t_{\rm P}$. Together, an extended host process results with the $\mathbb{C}_{-\infty}$ trajectory, and $\mathbf{G}_{-\infty}$ the associated NGF. The $\mathbb{C}_{\rm P}$ process is *embedded* in the $\mathbb{C}_{-\infty}$one. Both processes describe the same evolution beyond $t_{\rm P}$. This coincidence permits to build up the NGF of the shorter process starting from that of the long process. Once this is done, the $t_{\rm P}$ process may be viewed as an autonomous "restart" process which is being restarted from a frozen initial state $\mathcal{P}_{\rm P} = \mathcal{P}_{-\infty}(t_{\rm P})$ at $t_{\rm P}$. The perturbation scheme is based on the time partitioning method. We will not go to details of its derivation here.[168] We will, however, mention at the beginning a principle, which lies in foundations of this method, namely the invariance of the NGF with respect to the restart time. In this section, we will work with the NGF of real time rather than on the contour. The advantages will be apparent.

4.2.1. *Invariance of the NGF with respect to the restart time*

Now we will demonstrate that the NGF is invariant with respect to the choice of the initial time. To this end, we compare two NGFs differing by their initial times and, hence, by their definition ranges D_{t_0}, $D_{t_{-\infty}}$ [Fig. 4(a)]. We consider the *less* correlation function; $G^{>}$ would be treated similarly and the R, A components are their combinations. The two correlation functions define also the whole GF on the contour by Eq. (3.85). We have

$$\begin{aligned} G^{<}_{t_{-\infty}}(1,1') &= -i\,\mathrm{Tr}(\mathcal{P}_{t_{-\infty}}\psi^{\dagger}(1'|t_{-\infty})\psi(1|t_{-\infty}))\,, \\ G^{<}_{t_0}(1,1') &= -i\,\mathrm{Tr}(\mathcal{P}_{t_0}\psi^{\dagger}(1'|t_0)\psi(1|t_0))\,, \end{aligned} \tag{4.25}$$

in the respective definition ranges $D_{t_{-\infty}}\{t,t' \geq t_{-\infty}\}$ and $D_{t_0}\{t,t' \geq t_0\}$.

The Heisenberg field operators are evolving from the respective initial times according to the full many-particle unitary evolution operator $\mathcal{K}(t,t')$

$$\begin{aligned} \psi(1|t_{-\infty}) &= \mathcal{K}(t_{-\infty},t)\psi(x)\mathcal{K}(t,t_{-\infty})\,, \quad & \psi^{\dagger}(1'|t_{-\infty}) &= \dots\,, \\ \psi(1|t_0) &= \mathcal{K}(t_0,t)\psi(x)\mathcal{K}(t,t_0), & \psi^{\dagger}(1'|t_0) &= \dots\,, \end{aligned} \tag{4.26}$$

while the two initial states, over which the trace is performed, are mutually related by

$$\mathcal{P}_{t_0} = \mathcal{K}(t_0,t_{-\infty})\mathcal{P}_{t_{-\infty}}\mathcal{K}(t_{-\infty},t_0) \tag{4.27}$$

see Fig. 4.

Introducing all these relations into the definition (4.25), we find that, in fact, the values of the two GF's are identical over the common definition range D_{t_0} and can be denoted by $G^{<}$ without the time label:

$$\begin{aligned} G^{<}(1,1') &\equiv G^{<}_{t_{-\infty}}(1,1')\,, \quad & t,t' &\geq t_{-\infty}\,, \\ G^{<}(1,1') &\equiv G^{<}_{t_0}(1,1')\,, & t,t' &\geq t_0\,. \end{aligned} \tag{4.28}$$

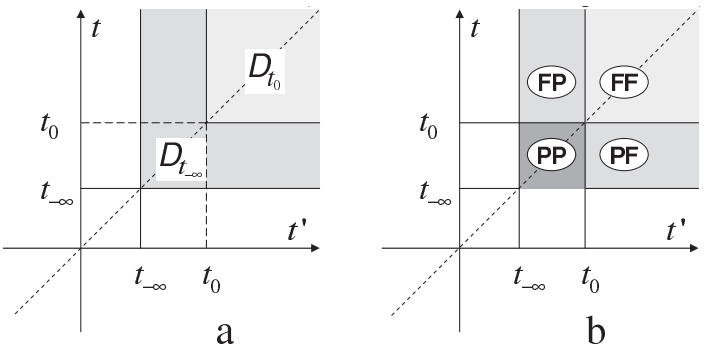


Fig. 4. (a) Definition ranges $D_{t_{-\infty}}$ of the full process and D_{t_0} of the restarted process are the first quadrants with the initial times specifying their lower left corners, see (4.25). (b) In the partitioning language the whole $D_{t_{-\infty}}$ range is cut into four partitions at the crossing point $[t_0, t_0]$. The future–future partition coincides with the restart process time range D_{t_0}.

The restart time may be an arbitrary time later than $t_{-\infty}$ and the result (4.28) thus proves that the definition of the GF for an embedded process is invariant with respect to shifting its initial ("restart") time t_0.

4.2.2. *Dyson equation with initial conditions*

The NGF for a general finite time initial condition satisfies Dyson equations, but with a self-energy having additional terms singular at the initial time. In this section, we will arrive at this structure of the NGF and its self-energy on the basis of the relationship between the host process and the embedded process. For definiteness, we first summarize the expected structure of the Dyson equation working on general terms. The NGF satisfies the Dyson equation on the finite time contour, but it is convenient to use the real time matrix form. The new feature is that now the self-energy $\mathbf{\Sigma}$ is replaced by the self-energy $\mathbf{\Sigma}_{\rm IC}$ having additional terms, so that the Dyson equation reads

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0 \mathbf{\Sigma}_{\rm IC} \mathbf{G}\,. \tag{4.29}$$

The properties of the self-energy are quite different for different components and we will consider them separately.

The Dyson equation for the propagators $G^{R,A}$ retains its structure. The mean field G_0 is not changed at all; the effect of the self-energy is gradual, so that we have

$$G^{R,A} = G_0^{R,A} + G_0^{R,A} \Sigma^{R,A} G^{R,A}\,, \quad \text{etc}\,, \tag{4.30}$$

with the self-energies being "regular" two-time functions.

The *less*-component of the Dyson equation, in contrast, has the form

$$G^{<}_{t_{\rm P}}(t,t') = \int_{t_{\rm P}}^{t} d\bar{t} \int_{t_{\rm P}}^{t'} d\bar{\bar{t}} G^R \Xi^< G^A\,, \quad \boxed{t \geq t_{\rm P}, t' \geq t_{\rm P}}\,, \tag{4.31}$$

where

$$\Xi^< = {}_\circ\Sigma^<_\circ + \Sigma_{\rm IC}\,, \quad \Sigma_{\rm IC} = {}_\circ\Sigma^<_\bullet + {}_\bullet\Sigma^<_\circ + {}_\bullet\Sigma^<_\bullet\,. \tag{4.32}$$

Note that the integrations in (4.31) start at $t_0 = t_{\rm P}$. The four terms have a varying degree of singularity at the initial time. The open circles indicate a time variable fixed at $t_{\rm P}$, the filled ones a time variable continuous in $(t_{\rm P}, \infty)$. The regular term ${}_\bullet\Sigma^<_\bullet$ corresponds to the Dyson equation as it is usually written for $t_{\rm P} \to -\infty$, namely $G^< = G^R\Sigma^< G^A$. The other terms play each a specific role. In particular, ${}_\circ\Sigma^<_\bullet$ and ${}_\bullet\Sigma^<_\circ$ (the self-energies Σ^c, Σ_c of Ref. 102) are related to the initial correlations. They have the form

$$\begin{aligned} {}_\bullet\Sigma^<_\circ(t,t') &= \Lambda^<_\circ(t,t_{\rm P})\delta(t'-t^+_{\rm P})\,,\\ {}_\circ\Sigma^<_\bullet(t,t') &= {}_\circ\Lambda^<(t_{\rm P},t')\delta(t+t^+_{\rm P})\,, \quad \boxed{t^+_{\rm P} = t_{\rm P}+0} \end{aligned} \tag{4.33}$$

and are thus equivalent to single-time continuous functions $\Lambda^<_\circ(t,t_{\rm P})$, ${}_\circ\Lambda^<(t_{\rm P},t')$ dependent on $t_{\rm P}$ as on a parameter. For the correlated initial conditions, these two functions must be determined in addition to the regular *less* self-energy.

The last term,

$$\begin{aligned} {}_\circ\Sigma^<_\circ(t,t') &= i\rho(t_{\rm P})\delta(t-t^+_{\rm P})\delta(t'-t^+_{\rm P})\,,\\ \rho(t) &= -iG^<(t,t)\,, \end{aligned} \tag{4.34}$$

represents the uncorrelated part of the initial conditions. This is the only part of $\Xi^<$ which enters the free particle correlation function

$$G^<_0 = G^R_0\,{}_\circ\Sigma^<_\circ G^A_0\,. \tag{4.35}$$

To verify the uncorrelated IC limit of Eq. (4.31), let us write $\Sigma^<$ for ${}_\bullet\Sigma^<_\bullet$ and use the uncorrelated, that is unperturbed, $\rho(t_{\rm P}) \to \rho_0(t_{\rm P}) = iG^<_0(t_{\rm P},t_{\rm P})$ to transform

$$G^R\,{}_\circ\Sigma^<_\circ G^A \to G^R(i\rho_0(t_{\rm P}))G^A = G^R[G^R_0]^{-1}G^R_0(i\rho_0(t_{\rm P}))G^A_0[G^A_0]^{-1}G^A \equiv f^<$$

and finally set ${}_\circ\Sigma^<_\bullet$ and ${}_\bullet\Sigma^<_\circ$ to zero. Equation (4.31) becomes

$$\begin{aligned} G^< &= f^< + G^R\Sigma^< G^A\,,\\ f^< &= (1+G^R\Sigma^R)G^<_0(1+G^A\Sigma^A)\,. \end{aligned} \tag{4.36}$$

This is identical with the famous form of the Dyson equation with uncorrelated initial conditions for $G^<$ given by Keldysh.[109]

4.2.3. *Time partitioning and equations for NGF*

The details of the derivation of the time partitioning formulas will be skipped. The basic idea is simple: it is required that the host and the embedded Green's function coincide according to the invariance theorem (4.28). The host GF has its "usual" Dyson equation, while the embedded GF has the $<$ self-energy according to (4.32), whose correction singular terms serve to compensate for the left-out effect of the past. Combining all that, the partitioning expressions are obtained.

To present the partitioned form of $G^<$, it is convenient to introduce the decomposition (4.32) into the Dyson equation (4.31) and write the latter in an explicit form:

$$\begin{aligned} G^<_{t_\mathrm{P}}(t,t') &= iG^R(t,t_\mathrm{P})\rho(t_\mathrm{P})G^A(t_\mathrm{P},t') \\ &\quad + G^R(t,t_\mathrm{P}) \times \int_{t_\mathrm{P}}^{t'} du\, {}_\circ\Lambda^<(t_\mathrm{P},u)G^A(u,t') \\ &\quad + \int_{t_\mathrm{P}}^{t} dv G^R(t,v)\Lambda^<_\circ(v,t_\mathrm{P}) \times G^A(t_\mathrm{P},t') \\ &\quad + \int_{t_\mathrm{P}}^{t} dv \int_{t_\mathrm{P}}^{t'} du G^R(t,v)\, {}_\bullet\Sigma^<_\bullet(v,u)G^A(u,t'), \\ &\quad t > t_\mathrm{P}\,, \quad t' > t_\mathrm{P}\,. \end{aligned} \tag{4.37}$$

Notice that the lower integration limit is t_P, while t_I has been shifted to the remote past at the onset of the preparatory stage. The whole host process is partitioned into the past prior to t_P and into the future after t_P. This *partitioning* is reflected in the form of the components of the less self-energy entering Eq. (4.37),

$$\begin{aligned} {}_\circ\Lambda^<(t_\mathrm{P},u) &= i\int_{t_\mathrm{I}}^{t_\mathrm{P}} d\bar{t}\{G^R\Sigma^< + G^<\Sigma^A\}\,, \\ \Lambda^<_\circ(v,t_\mathrm{P}) &= -i\int_{t_\mathrm{I}}^{t_\mathrm{P}} d\bar{\bar{t}}\{\Sigma^<G^A + \Sigma^RG^<\}\,, \\ {}_\bullet\Sigma^<_\bullet(v,u) &= \Sigma^<(v,u) \\ &\quad + \int_{t_\mathrm{I}}^{t_\mathrm{P}} d\bar{t}\int_{t_\mathrm{I}}^{t_\mathrm{P}} d\bar{\bar{t}}\{\Sigma^RG^R\Sigma^< + \Sigma^RG^<\Sigma^A + \Sigma^<G^A\Sigma^A\} \\ &\quad \Sigma^RG^R\Sigma^< \mapsto \Sigma^R(u,\bar{t})G^R(\bar{t},\bar{\bar{t}})\Sigma^<(\bar{\bar{t}},v)\,, \text{etc.} \end{aligned} \tag{4.38}$$

By these relations, the self-energy of the embedded process is expressed by integrals involving time blocks of the Green's functions and the self-energies of the host process. The external arguments u, v refer to the process in the future and are always greater than t_P, while the integration variables, denoted by $\bar{t}, \bar{\bar{t}}$ for clarity, belong entirely to the past and are less than t_P. The propagation takes place entirely in the past. The history and the future are interconnected by the off-diagonal blocks of the self-energies. The singular components of the self-energy have no analogue in the host process, while the regular term ${}_\bullet\Sigma^<_\bullet$ has two parts

$${}_\bullet\Sigma^<_\bullet = \Sigma^<(t,t') + \widehat{\Sigma}_{t_\mathrm{P}}{}^<(t,t')\,. \tag{4.39}$$

The first term comes from the host process without change (where it would enter the Dyson equation in the usual form, $G^< = G^R\Sigma^<G^A$). It is supplemented by the second term, $\widehat{\Sigma}_{t_\mathrm{P}}{}^<(t,t')$, which takes the finite time initial condition into account.

4.2.4. *Notes to the time partitioning method*

The infinite Schwinger–Keldysh contour can accommodate an extremely rich class of processes bearing the generic name of the *Keldysh switch-on processes*. These processes start from general uncorrelated states, become correlated as the interactions are switched on and are driven by an endless variety of external influences. It may be said that the intermediate states passed through by the system in the course of such processes form in their entirety the class of *all physically attainable states* of the system, including states out of equilibrium and incorporating correlations of widely different nature and strength. Any of these states may be used as an initial state for the transient process we wish to study. Thus, we can start the transient from "all" physically meaningful initial states. Still, the direct method of including finite time initial conditions[247] admits, in principle at least, quite arbitrary initial states, including those which are artificially overcorrelated etc. Such states fall out of our scope by definition.

The formal tool for using an arbitrary Keldysh switch-on process as preparatory for the relevant process starting at a finite time $t_{\rm P}$ is the time partitioning. It is clear that the time partitioning is universal and does not depend on any assumptions, like equilibrium, about the "past". We may thus place the splitting time to any convenient time instant.

It is essential, however, that the "past" preparatory stage and the envisaged embedded "relevant" transient are a part of one uninterrupted host process. Just as in the method of the extended Kadanoff–Baym contour, the mixed components of the GF and the self-energy played a crucial role, the time partitioning expressions contain the coupling between the past and the future with respect to the dividing time $t_{\rm P}$. Fortunately, the time depth of the coupling is typically quite restricted. According to the Bogolyubov principle, the mutual correlation will die out within a time of the order of the collision duration time.

Within the NGF formalism, the Bogolyubov principle is translated into the assumption about the behavior of the system expressed in terms of self-energies, as will be discussed further in Sec. 6.1: All components of the host self-energy should be concentrated to a strip

$$|t - t'| < \mathcal{O}(\tau^\star) \quad \tau^\star = \mathcal{O}(\tau_c, \tau_{\rm Q})\,.$$

The two times appearing at the right-hand side are: τ_c, often called the collision duration time in transport theory, relevant for $\Sigma^<(t,t')$, and $\tau_{\rm Q}$, usually called the quasiparticle formation time, characteristic for $\Sigma^{R,A}(t,t')$. This is illustrated in Fig. 5. To conclude, we have presented two methods of incorporating the finite time initial conditions, both of which transform the inclusion of the complex many-body initial condition at a single time to invoking the single particle GF for all times in the past with respect to the dividing time point; we have proposed to distinguish these methods as *diachronous* as opposed to the *synchronous* direct methods defined as case A at the beginning of the whole Sec. 4.

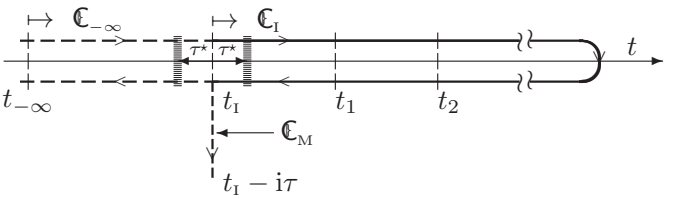


Fig. 5. A finite-time Schwinger–Keldysh contour and its diachronous extensions. $\mathbb{C}$: The closed time contour for a transient starts at the initial time $t_{\rm P}$, goes to $+\infty$ and returns to $t_{\rm P}$. $\mathbb{C}_{\rm M}$: Extension by a Matsubara-like imaginary time interval according to Refs. 107 and 102 or Refs. 196 and 66. $\mathbb{C}_{-\infty}$: Extension of $\mathbb{C}$ along the time axis to the past. The resulting contour starts at $t_{\rm I}$. The dashed segment preceding $t_{\rm P}$ accommodates the preparation process. The two adjoining processes form together the host process, in which the transient is embedded. For $t_{\rm I} \to -\infty$, the host process with an uncorrelated initial condition becomes a Keldysh switch-on process. Two diffuse boundaries bracketing $t_{\rm P}$ at the distance $\sim \tau^\star$: If a finite correlation decay time $\tau^\star$ exists, the lower boundary indicates the depth of coupling between the preparation process and the transient, the upper one marks the extent of penetration of the initial correlations into the future, cf. Sec. 6.1.

5. Reconstruction Theorems

The aim of this section is to introduce the so-called reconstruction theorems. Their name derives from the fact that they are built over the better known reconstruction equations (REs)[109,110,116,118,125,129,154,171,211] and make them an integral part of an alternative system of NGF equations. These equations are exact, but one of their features is that they are suggestive of the approximations leading to quantum kinetic equations of the GME type. In fact, the way to the exact reconstruction technique was just the reverse: it was inspired and motivated by a simplified description of quantum dynamics based on the quantum transport theory, in which all dynamics is expressed in a kinetic equation governing a single-particle single-time density matrix.

Throughout the whole section, we confine the considerations to the Keldysh initial condition without correlations. Only in the last subsection, the modifications brought about by correlated initial conditions will be indicated.

5.1. *Generalized Kadanoff–Baym equation*

We will start the way toward reconstruction theorems by aiming at a quantum kinetic equation for the single particle density matrix $\rho(t)$ from the NGF equations.

5.1.1. *Precursor kinetic equation*

The well-known starting point on the way from the double time NGF to single time kinetic equations is the differential equation called the GKBE. This equation is obtained directly from the Dyson equation.

First, we subtract the Dyson equations (3.219), (3.220) one from another. Second, we use the Dyson equation (3.214) in the form

$$[G^{R,A}]^{-1} = [G_0^{R,A}]^{-1} - \Sigma^{R,A}\,. \tag{5.1}$$

After easy manipulations we get the identity

$$G_0^{-1}G^< - G^<G_0^{-1} = \Sigma^R G^< - G^<\Sigma^A - G^R\Sigma^< + \Sigma^<G^A\,. \tag{5.2}$$

This (still exact) equation is the GKBE. It has already a structure closely related to transport equations: its left-hand side contains information about the drift of free particles, the four terms on the right-hand side represent the generalized collision terms. The equation still has the double time structure, however.

In order to obtain an equation for $\rho(t)$, we make the limit $t_1 = t = t_2$ of Eq. (5.2) and recall that at equal times, $t_1 = t = t_2$, the one particle density matrix ρ is given by the time-diagonal of $G^<$

$$G^<(t,t) = i\rho(t)\,. \tag{5.3}$$

Using the explicit expression (3.181) for G_0^{-1},

$$G_0^{-1}(t_1,t_2) = \{i\partial t_1 - h_0(t_1)\}\delta(t_1-t_2) = \{-i\partial t_2 - h_0(t_2)\}\delta(t_1-t_2) \tag{5.4}$$

the left-hand side of the (5.2) is transformed to an unrenormalized drift of the one-particle density matrix ρ:

$$\text{left-hand side of (5.2)} \xrightarrow{t_1=t=t_2} \frac{\partial\rho}{\partial t} + i[h_0(t),\rho]_-\,. \tag{5.5}$$

This already has the form consistent with a QTE, in which $h_0(t)$ is the mean field one-particle Hamiltonian, and the whole equation (5.2) becomes the desired *Precursor Quantum Kinetic Equation* (PKE):

$$\frac{\partial\rho}{\partial t} + i[h_0(t),\rho]_- = (\Sigma^R G^< - G^<\Sigma^A)_{t_1=t=t_2} - (G^R\Sigma^< - \Sigma^<G^A)_{t_1=t=t_2}\,. \tag{5.6}$$

The "generalized collision" terms on the right-hand side still involve double time *less* quantities. The related integrals preserve causality extending only to the past because of the presence of the propagator factors.

5.1.2. *On the way to the quantum kinetic equation*

To convert the precursor kinetic equation to a true closed kinetic equation for ρ, we first have to specify the *physical approximation for the self-energies* in the form

$$\mathbf{\Sigma} = \mathbf{\Sigma}[\mathbf{G}]\,, \tag{5.7}$$

that is

$$\mathbf{\Sigma}^{R,A} = \mathbf{\Sigma}^{R,A}[G^{R,A}, G^<]\,, \quad \mathbf{\Sigma}^< = \mathbf{\Sigma}^<[G^{R,A}, G^<]\,. \tag{5.8}$$

Next comes the crucial point, $G^<$ is expressed in the functional form

$$G^< = G^<[\rho, G^{R,A}]\,. \tag{5.9}$$

By introducing (5.9) into (5.8) and directly into Eq. (5.6), the double time function $G^<$ is eliminated in favor of its time diagonal ρ, and by this, a true kinetic equation is obtained.

We will deal with the question of an actual implementation of this program in the following subsections. Here we only note that the first successful (approximate) attempt in this direction was connected with the famous KBA (Sec. 6.2.1), which was followed by other Ansatzes, a parallel derivation of the REs, and culminated by formulation of the reconstruction theorems.[116,118,125,154,168,171]

5.2. *Concept of reconstruction theorems*

The general plan of constructing quantum transport equations within the NGF scheme, as outlined at the end of the preceding subsection, is to transform the GKBE (5.6) (... precursor kinetic equation) to a closed kinetic equation for the single particle distribution function. We may assume a more abstract position and detach the construction of transport equations from the more fundamental issue formulated already in the Introduction as the *reconstruction problem*:

> Can the full description of a many-body interacting system be built up from its single-particle characteristics, and if yes, then under which conditions?

It appears, and has been documented in this paper, that virtually all relevant information about a nonequilibrium many-body system can in principle be unfolded from its properly chosen reduced characteristics, such as the pair of double-point quantities, $G^<$ and $G^>$. Now we touch at the possibility that, actually, it may be enough to know or control even less: just a function of a single time variable, the one-particle density matrix.

5.2.1. *Various approaches to reconstruction problem*

Let us begin by a look at several alternative approaches *vis-à-vis* the reconstruction problem. This will help us to grasp the NGF reconstruction hypothesis properly.

First of these approaches is based on *the Bogoluybov postulate*[38–40]:

> In an autonomous system, the evolution is controlled by a hierarchy of times (2.9) and for times past the initial decay of correlations, a transport equation of the form (2.17) is valid.

which we properly recall here once more. It should be noted that this postulate has no universal proof, but its validity has been verified for a whole row of systems of a rather different nature. The postulate is related to the reconstruction problem in the following sense. After the decay of initial correlations the systems is expected to assume a state characterized by a set of robust observables, which can be reconstructed from the knowledge of the sole one-particle distribution function. The

related reconstruction has a rather symbolic form

$$\mathcal{P} = \tilde{\Phi}[\rho]\,, \quad t > t_0 + \tau_c\,. \tag{5.10}$$

A complementary stream of research closely related to the reconstruction questions, although distinct in some respect, is the so-called *inversion problem*. It stems from the fundamental paper by Schwinger[83] on the use of the generating functional in nonequilibrium physics. The key concept is the functional inversion (or substitution) based on the Legendre transformation. It has been amply used in the field theoretical studies of many-body problems and it found its best known application in the density functional theory (DFT) first in equilibrium, then in the extension to the TDDFT.[59–69]

Schwinger introduced, as discussed already, the closed time path $\mathfrak{C}$ and the generating functional dependent on an external field $U^{\pm}(t)$ depending on the branch of the contour,

$$e^{iW(U^+,U^-)} = \mathrm{Tr}\,\mathcal{P}(t_{\mathrm{I}})\tilde{\mathbf{T}}\, e^{+i\int_{t_I}^{\infty} d\tau(\mathcal{H}-U^-(\tau)X)}\mathbf{T}\, e^{-i\int_{t_I}^{\infty} \mathrm{d}\tau(\mathcal{H}-U^+(\tau)X)}\,. \tag{5.11}$$

For a local field U, the response of local density of particles could be obtained by functional derivatives, and this solved the related transport problem in a closed form:

$$\bar{n}(x,t) = \left.\frac{\delta W}{\delta U^+(x,t)}\right|_{U^+=U^-=U} = -\left.\frac{\delta W}{\delta U^-(x,t)}\right|_{U^+=U^-=U}\,. \tag{5.12}$$

It comes immediately to mind that the latter relations could be *inverted*, so that the field U would be expressed in terms of $\bar{n}$. Introducing this back into the time derivative of (5.12) should lead to a transport equation. This can be further formalized by working with a Legendre transform of the Schwinger functional. All this has been thoroughly investigated, e.g., by the Fukuda group.[256,257]

This is one of the classical cases of the inversion expressed symbolically by the relation

$$U(t), \{t_{\mathrm{I}} \le t < \infty\} \rightleftharpoons \bar{n}(t)\,, \quad \{t_{\mathrm{I}} \le t < \infty\}\,. \tag{5.13}$$

The importance of the inversion consists in the following: Starting from $\bar{n}$, an ultimately reduced data set, we may go, by (5.13), in the *inverse* direction to U. This, in the "forward" direction, implemented by means of any quantum transport formalism, defines uniquely, i.e., reconstructs, the behavior of the whole many-body system. Thus, whenever the inversion is possible, it proves and clarifies the Bogolyubov symbolic reconstruction loop (5.10).

This is similar to the well-known development for equilibrium systems, where the famous DFT is based on the Hohenberg–Kohn theorem stating that in equilibrium the bijection (5.13) is valid.

The foundations of the time dependent extension of DFT have long lagged behind its intuitive introduction and use, based on the simplest approximations for the effective potentials.

The TDDFT analogue to the Kohn–Hohenberg theorem, established relatively long ago, is the **Runge–Gross Theorem**: Let $U(t)$ be a local potential smooth in time. Then, for a fixed initial state $|\mathbf{\Psi}_0\rangle$, the functional relation $\bar{n}[U]$ is bijective and can be inverted.

A consistent time dependent counterpart to the Kohn–Sham energy functional has only been found recently in the Schwinger functional for effective noninteracting particles moving in an effective potential local in space and time. We will not follow the details of this developing field, see Refs. 69 and 131.

5.2.2. *NGF approach to reconstruction problem*

Now it is possible to sum up some lessons. Within the NGF context, there is an exact formal theory, which permits, in principle at least, to obtain a complete description of the evolution of a nonequilibrium system. Our present aim is to recast the theory to a form, where the decisive quantity, sufficient for a complete reconstruction of the NGF results, would be the single particle density matrix.

In Sec. 5.1, we have outlined one part of the program, namely the reduction of GKBE to a kinetic equation. There, the problem of initial conditions was avoided by using the Keldysh IC. The Bogolyubov postulate warns us that the simple method may work in the saturated kinetic regime only, while the early stage of the decay of correlations may be difficult. On the other hand, the Runge–Gross theorem should be valid in the whole time range starting from t_{I}, which is encouraging. Of course, this theorem is existential, not operational, so that it suggests no way to follow. It is well-known that all DFTs involve an introduction of ill-controlled approximations for the exchange and correlations. Besides, the reciprocity theorems of the DFTs use pairs of variables like local potential — local particle density. The theories based on the use of the reduced density matrix (RDDMFT) also exist, but they offer no truly viable alternative. There should be no surprise that the technique which is really inspirational here, is the inversion technique of Schwinger as represented by (5.13).

Let us summarize the requirements on a reconstruction technique in the NGF theory:

- The central quantity will be the single particle density matrix ρ;
- The technique should represent a complete operational scheme;
- It should be exact in principle, not based on *ad hoc* approximations;
- It should incorporate general finite time initial conditions.

All these requirements are fulfiled by the REs we are going to discuss in the next subsection.

5.3. *Reconstruction equations*

An integral part of the reconstruction formalism are the REs, which permit an exact reconstruction of $G^<$ from ρ.[109,110,116,118,125,154,168,171,211]

If the Keldysh initial condition is assumed, they easily follow from the Dyson equations. To derive the RE, we first split the exact $G^<$ as follows:

$$G^<(t_1,t_2) = G^<_R(t_1,t_2) - G^<_A(t_1,t_2)\,, \tag{5.14}$$

$$G^<_R(t_1,t_2) = \theta(t_1-t_2)G^<(t_1,t_2)\,, \tag{5.15}$$

$$G^<_A(t_1,t_2) = -\theta(t_2-t_1)G^<(t_1,t_2) = [G^<_R(t_2,t_1)]^\dagger\,. \tag{5.16}$$

It is convenient to calculate

$$\begin{aligned}\{G^R\}^{-1}G^<_R|_{t_1,t_2} &= (G_0^{-1}-\Sigma^R)G^<_R|_{t_1,t_2}\\ &= \delta(t_1-t_2)\rho(t_2)\\ &\quad +\theta(t_1-t_2)(\{G^R\}^{-1}G^< + \Sigma^R G^< - \Sigma^R G^<_R)|_{t_1,t_2}\\ &= \delta(t_1-t_2)\rho(t_2) + \theta(t_1-t_2)(\Sigma^< G^A + \Sigma^R G^<_A)|_{t_1,t_2}\,,\end{aligned} \tag{5.17}$$

where Dyson equations (5.1), (3.221) and definition of G_0 were employed. Multiplication by G^R from the left yields the first equation for $G^<_R$, which coincides with $G^<$ in the $t_1 > t_2 > -\infty$ wedge. In the complementary time region $-\infty < t_1 < t_2$, an analogous equation for $G^< = G^<_A$ results. The two equations are conjugate, as it holds $G^<(t_1,t_2) = -[G^<(t_2,t_1)]^\dagger$.

In other words, we have obtained the REs in the form

$$\begin{array}{cc} \boxed{t>t'} & \boxed{t<t'} \\ \multicolumn{2}{c}{G^<(t,t') =}\end{array}$$

$$\begin{array}{l|l} -G^R(t,t')\rho(t') & +\rho(t)G^A(t,t') \\ +\displaystyle\int_{t'}^{t} d\bar{t}\int_{-\infty}^{t'} d\bar{\bar{t}}\, G^R(t,\bar{t})\Sigma^<(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t') & +\displaystyle\int_{t}^{t'} d\bar{\bar{t}}\int_{-\infty}^{t} d\bar{t}\, G^R(t,\bar{t})\Sigma^<(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t') \\ +\displaystyle\int_{t'}^{t} d\bar{t}\int_{-\infty}^{t'} d\bar{\bar{t}}\, G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{\bar{t}})G^<(\bar{\bar{t}},t') & +\displaystyle\int_{t}^{t'} d\bar{\bar{t}}\int_{-\infty}^{t} d\bar{t}\, BG^<(t,\bar{t})\Sigma^A(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t') \end{array} \tag{5.18}$$

These equations represent the most important step on the way to the NGF reconstruction theorem.

5.3.1. *Properties of reconstruction equations*

The REs are inhomogeneous and their source terms contain ρ as an input. The unknown $G^<$ is also contained in both integral terms: in the second one explicitly, in the first one through the functional dependence $\Sigma^< = \Sigma^<[G^<]$.

By solving Eqs. (5.18), the double time correlation function $G^<(t_1, t_2 \neq t_1)$ is generated from the knowledge of its time-diagonal part, the one-particle single-time density $\rho(t) \propto G^<(t,t)$, and of the propagators taken also as known. The role

of propagators will be discussed in detail below. The integrals are written down explicitly to show the complicated interplay of the integration limits leading to an integration range consisting of two off-diagonal blocks.

We have to warn that the REs alone do not solve the reconstruction problem:

- For $t = t'$, they turn into the tautology $\rho = \rho$, thus an independent input of ρ is required.
- This input is not arbitrary: while the equations would lead to a formal solution $G^<$ for a wide range of input $\rho(t)$, the two functions need not be compatible as constituents of the same Green's function, however. This would lead to unphysical, invalid results. In particular, this would impair the conservation laws.

The compatibility is provided by the precursor kinetic equation (5.6). Recall now that also the PKE is a consequence of the Dyson equation for $G^<$. In fact, RE and PKE together are equivalent with the Dyson equation:

$$\boxed{\begin{array}{c}\text{Dyson equation for } G^< \\ \text{Eq. (3.221)}\end{array}} \Longleftrightarrow \begin{cases} \text{REs for } G^<, \text{ Eq. (5.18)} \\ \text{Precursor kinetic equation for } \rho, \text{ Eq. (5.6)} \end{cases}. \tag{5.19}$$

5.4. *Reconstruction theorems*

The preceding subsection set the stage for a compact formulation of the reconstruction theorem. It will be done in three consecutive steps, first for the correlation function $G^<$, then for the complete NGF assuming the Keldysh initial condition, and, finally, the finite time initial conditions will be incorporated.

5.4.1. *Reconstruction of $G^<$*

The use of the Dyson equation split into two parts according to the right-hand side of the scheme (5.19) clearly hints at a cyclic solution for $G^<$, giving rise to the cycle

$$\boxed{\text{RE}} \rightleftharpoons \boxed{\text{precursor kinetic equation}} \tag{5.20}$$

constituting a new alternative for generating the full $G^<$ correlation function.

The REs are thus not stand-alone equations, but one part of a linked twin process whose other constitutive part is the precursor kinetic equation: $G^<$ is substituted from the REs the kinetic equation is solved for the density matrix $\rho(t)$ and this in turn enters the RE as an input.

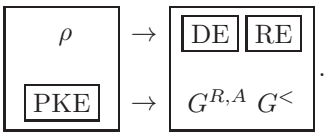
Before going to discuss general formulation of reconstruction theorems, we make a point, which will be important in the next section. Equation (5.18) can be used in two alternative ways:

(1) They are perfectly suited for a direct numerical solution aiming at $G^<$ connected with a particular physical situation.
(2) They provide an efficient tool for generating transport equations.

5.4.2. *Reconstruction theorem*

The new reformulation of the NGF method starts from putting ρ at the hub. The whole process of finding the complete NGF, including $G^<$ and the propagator pair G^R, G^A, is restructured to a dual task:

NGF Reconstruction Scheme



(5.21)

In one (the upper) stream, the single-particle distribution ρ is introduced into the REs for $G^<$ and the Dyson equations for propagators so that the NGF is reconstructed from a known ρ. In the reverse stream, the NGF components are introduced into the PKE, which then acts as a quantum kinetic equation, and yields ρ. These two mutually coupled streams thus complete the reconstruction cycle.

This scheme gives a full description of the NGF reconstruction procedure in operational terms. On a more abstract level, this result may be summarized as a mathematical statement central in the present context:

NGF Reconstruction Theorem:

> For a nonequilibrium process starting from the Keldysh initial condition, the complete double-time NGF **G** and the single-time single-particle density matrix ρ are in a bijective relationship,
>
> $$\{G^<, G^R, G^A\} \rightleftharpoons \rho\,. \tag{5.22}$$

This theorem satisfies all requirements set at the end of Sec. 5.2.2. It should be compared with the alternative schemes listed in the preceding section. Let us start with the Runge–Gross theorem. First, on one side of our dual relation stands the full ρ rather than its space diagonal $\bar{n}$. This may appear as a weaker result, but, in fact, the Legendre duality behind the NGF theorem extends to arbitrary nonlocal fields U and thus covers a class of physical situations much wider than those limited to the local external fields. Second, in comparison with the Runge–Gross *existence* theorem, the present theorem has a constructive algorithmic nature. The validity of the theorem is thus established in each specific case by an actual reconstruction process. Third, the dual relation (5.22) links ρ with the NGF rather than with the external field U in the vein of Eq. (5.13). It may be said that, in this sense, the NGF reconstruction theorem makes true the Bogolyubov conjecture (5.10), albeit in a realistically restricted form.

An important question remains about the feasibility of the reconstruction scheme (5.21). Several procedures offer themselves, all based on some type of successive approximations:

(1) *NGF solver.* The equations have a structure suitable for a novel type of the NGF solver.[144,187] With all equations cast in the differential form, the solution

proceeds in steps incremental in time. This may appear as abandoning the kinetic equation approach, but, in fact, this solver would permit to implement a still unemployed concept: an auto-adaptive scheme NGF/QKE, in which the full NGF solver would only be acting when necessary, like at the instant of a rapid transient, while it would downgrade to the quantum kinetic equation when possible, like over the long periods of autonomous relaxation.

(2) *Interaction strength as small parameter.* Iteration of the REs is less promising for computations than a solver, but it has a more basic context. It permits various interpretations. For noninteracting particles, the self-energies vanish and the particle correlation function is given by the absolute term of Eqs. (5.18) exactly. Thus, the iteration can be interpreted as a perturbation expansion in the particle interaction strength. This has the advantage that the reconstruction is turned into a systematic procedure and also brought close to the direct methods of deriving the QKE. The drawback of this expansion is that it mixes two consecutive levels by respecting the many-particle correlations and the kinetic behavior simultaneously.

(3) *Collision duration time as small parameter.* This choice is fully consistent with the present approach, as it clearly separates the many-body level and the kinetic behavior. The theory then may work with dressed GF, so that it is fully renormalized. It is true that the collision duration time is not an *a priori* well-defined quantity. It may be argued, however, that the REs serve to offer an operational definition of the collision duration time in the course of their solution. For this, a special feature of the RE (5.18), namely their off-diagonal integration range, may be employed. This in turn reflects the time/spectral structure of the self-energies. This is sketched in an idealized representation in Fig. 6. The "small parameter" measuring the corrections to the GKBA in the RE is the triangular overlap region of the integration range and of the strip around the time diagonal in which the values of self-energies are significant. The effective width of the strip is identified with the quasi-particle formation time τ_Q for Σ^R and with the collision duration time τ_c for $\Sigma^<$. The two times may be different, but both should be "small". It is known that rather than the interaction strength alone, it is the whole inner dynamics of build-up processes induced in the system during a nonequilibrium evolution, whose subtle details are decisive for the magnitude of these characteristic times, and, thus, for the iteration procedure. Even if the strips are less sharply defined, the iteration provides clues as to the effective values of τ_Q and τ_c. To conclude, this approach parallels neatly other transport theories, in particular, it is a NGF implementation of the Bogolyubov principle.

5.5. *Generalized reconstruction theorem: Correlated initial state*

In the case of a *correlated initial state at a finite initial time*, the process is similar as in the case of the Keldysh initial condition already treated, but it is more involved. Both the precursor kinetic equation and the REs are modified.

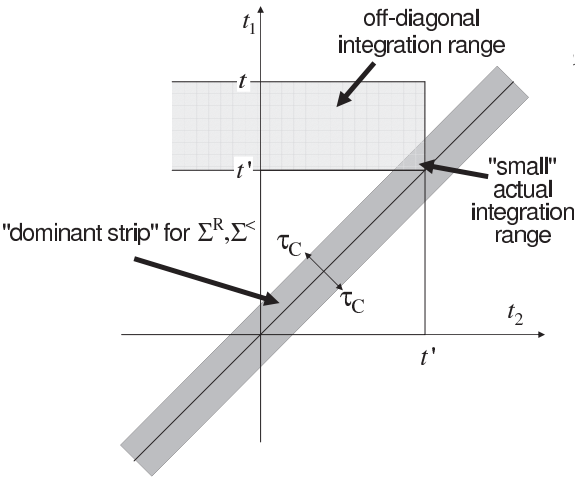


Fig. 6. Integration range for the REs (retarded part).

5.5.1. *Precursor quantum kinetic equation with initial conditions*

The starting point on the way from the double time NGF to single time transport equations is the GKBE. We have already introduced the GKBE for the special case of Keldysh initial conditions in Sec. 5.1. We will now generalize GKBE for the more general initial conditions. As in the previous case, we begin with a differential equation obtained from Eq. (4.31) combined with Eq. (4.30) written as $[G^{R,A}]^{-1} = [G_0^{R,A}]^{-1} - \Sigma^{R,A}$.

$$G_0^{-1}G^< - G^<G_0^{-1} = \Sigma^R G^< - G^<\Sigma^A - G^R\Xi^< + \Xi^<G^A\,. \tag{5.23}$$

Again, this (exact) equation has already a structure closely related to transport equations. The four terms on the right-hand side represent the generalized collision terms. The equation still has the double time structure, however, and, in contrast to common transport equations, it also incorporates the initial conditions through the self-energy $\Xi^<$. Using Eq. (4.31) and splitting the self-energy $\Xi^<$ into the self-energy $\Sigma^<$ of the host process and the remainder $\Theta^<$ including all contributions from the initial correlations,

$$\Theta^<_{t_0} = {}_\circ\Sigma_\circ + {}_\circ\Sigma_\bullet + {}_\bullet\Sigma_\circ + \widehat{\Sigma}_{t_\mathrm{P}}{}^<(t,t')\,, \quad \widehat{\Sigma}_{t_\mathrm{P}}{}^<(t,t') = {}_\bullet\Sigma_\bullet - \Sigma^<(t,t')\,,$$

we can rewrite Eq. (5.23) into the following form:

$$G_0^{-1}G^< - G^<G_0^{-1} = \Sigma^R G^< - G^<\Sigma^A - G^R\Sigma^< + \Sigma^<G^A - G^R\Theta^<_{t_0} + \Theta^<_{t_0}G^A\,. \tag{5.24}$$

Finally, we arrive at the precursor kinetic equation generalizing Eq. (5.6),

$$\begin{aligned}\frac{\partial\rho}{\partial t}+i[h_0(t),\rho]_- &= (\Sigma^R G^< - G^<\Sigma^A)_{t_1=t=t_2}\\ &\quad -(G^R\Sigma^< - \Sigma^< G^A)_{t_1=t=t_2}\\ &\quad -(G^R\Theta^<_{t_0}+\Theta^<_{t_0}G^A)_{t_1=t=t_2}\,. \end{aligned}\tag{5.25}$$

Notice again that according to (4.39) the fully nonsingular term of self-energy ${}_\bullet\Sigma_\bullet$ contains also the part $\widehat{\Sigma}_{t_{\rm P}}{}^<(t,t')$ which is dependent on initial correlations and is dying out with time.

5.5.2. *Reconstruction equations with finite time initial conditions*

We write down the exact REs for $G^<$ extended so as to incorporate the finite time initial conditions right away. They are an exact consequence of the Dyson equation (4.31) like in the uncorrelated case before. They have the appearance of an integral equation serving to reconstruct full $G^<$ from the inhomogeneous term which coincides with the analogous term in Eq. (5.18)

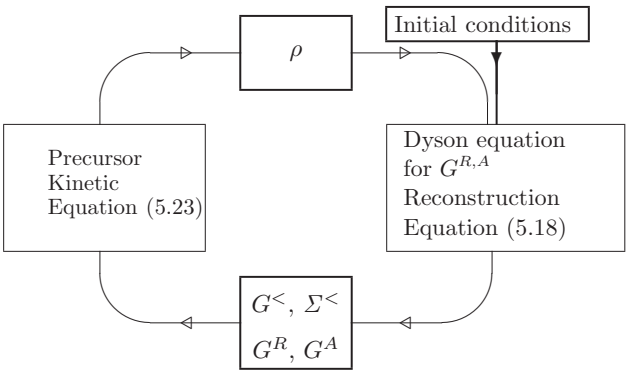
$$\begin{aligned}G^<(t,t') &= -G^R(t,t')\rho(t') \quad \boxed{t\geq t'\geq t_{\rm I}}\\ &\quad +\int_{t'}^{t}d\bar{t}\int_{t_{\rm I}}^{t'}d\bar{\bar{t}}G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{\bar{t}})G^<(\bar{\bar{t}},t')\\ &\quad +\int_{t'}^{t}d\bar{t}\int_{t_{\rm I}}^{t'}d\bar{\bar{t}}G^R(t,\bar{t})\Xi^<(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t')\,,\\ G^<(t,t') &= \rho(t')G^A(t,t')+\cdots \quad \boxed{t'\geq t\geq t_{\rm I}}\end{aligned}\tag{5.26}$$

In other words, Eq. (5.26) serves to reconstruct a full double time function from the knowledge of its time diagonal $i\rho$ (and propagators). Unfortunately, the integral terms involve also the $\Xi^<$ self-energy, see (4.32), with all initial time corrections and this is a problem in general. In the uncorrelated case, these corrections vanish and the self-energy can be obtained from Eq. (5.7). This defines the reconstruction procedure of the preceding section.

5.5.3. *Reconstruction scheme with initial conditions*

The generalized reconstruction theorem states that the solution of the Dyson equation for $G^<$ can be obtained according to the scheme, which represents a substantial modification of the scheme for the Keldysh case, because of the necessity to include the initial conditions. We draw the scheme in a slightly different format from the

diagram (5.21), but the core of the process remains the same and is easily identified:



(5.27)

The basic cycle is indicated by open arrows. The cycle follows the true physical process under investigation. It starts at $t_{\rm I}$ and is incremental in time. The initial conditions — correlated or uncorrelated alike — have to be fed in from outside, as shown symbolically by a box "initial conditions" in the top right corner of Eq. (5.27).

We have to distinguish the uncorrelated initial condition from the correlated one, however. The uncorrelated initial conditions amount just to the initial one-particle density matrix, which is known. This would be enough to reconstruct the initial correlation function and its self-energy in terms of initial ρ (right-hand box). These enter the precursor transport equation and the result would be ρ for the first incremental time (left-hand box). This cycle would then proceed on and on. This is the practical use of the reconstruction theorem, by which the Dyson equation is solved for all times using the already known section of ρ as a function of time.

In the correlated case, the initial conditions which have to be input during each cycle in addition to $\rho_{\rm I}$ involve basically the initial time corrections to $\Xi^<$. The reconstruction cycle may become practicable, if it will be supplemented by the corresponding algorithm, which will depend on the method of incorporating the initial conditions. We are not aware of a practical attempt to make use of the scheme for correlated initial conditions, and do not enter into details for that reason.

6. Long Time Asymptotics: Quantum Kinetic Equations

This section will be devoted to the second main theme of this review, namely the use of the NGFs as a reliable tool for derivation and justification of simplified quantum kinetic equations, both of the type of transport equations, augmenting the Boltzmann equation for extended systems and of the type of generalized master equation extending the common Pauli equation to systems with some quantum memory.

We will introduce two schemes how to construct quantum kinetic equations for a single time distribution function within the NGF approach: the first one is based on the quasiclassical expansion and leads to various versions of quantum Boltzmann equation, the second one is related to a short time expansion and it enables us to

describe time-dependent processes via the GME type of kinetic equations. Both these schemes are approximate only, and are based on certain type of decoupling schemes which are commonly known under the name of "Ansatzes". The way toward the Boltzmann equation is based on the use of the *Kadanoff–Baym Ansatz*, while the derivation of the GME uses the *Generalized Kadanoff–Baym Ansatz*. Both schemes start from the PKE as introduced in Secs. 5.1.1 and 5.5.1.

6.1. *Assumptions about the time structure of the self-energy*

For convenience, we repeat here Eq. (5.24):

$$\begin{aligned} G_0^{-1}G^< - G^<G_0^{-1} = \Sigma^R G^< - G^<\Sigma^A \\ - G^R\Sigma^< + \Sigma^< G^A \\ - G^R\Theta^<_{t_0} + \Theta^<_{t_0} G^A \,. \end{aligned}$$

We intend to use it for times of steady external conditions. More precisely, for times which are sufficiently separated from the time $t_{\rm Last}$ of the last abrupt ("jerky") perturbation of the system. To understand how this can simplify the precursor equation, we have to review once more the time structure of the self-energies.

The assumption we make is that there exists a time $\tau^\star$, such that

$$\Sigma^\natural(t,t') \approx 0 \text{ for } |t-t'| > \tau^\star\,, \quad \natural = R, A, > \ . \tag{6.1}$$

This condition should not be taken too literally, as e.g., the band edges lead to weak power law tails. Still, it captures in a simple manner the essential feature of a typical self-energy, to be concentrated along the time diagonal, and is in agreement with the notion of the decay of correlations, as explained above. We will use (6.1) for convenience and simplicity. The finite range of the IC corrections is just a corollary.

To see, how the condition (6.1) works, we note that the time $t_{\rm Last}$ plays the role of the initial time for the smooth phase of the system evolution we consider. The system quickly loses the memory of the disturbance, which means that the last two generalized collision terms of Eq. (5.24), which take the initial conditions into account explicitly, become zero as the running time t exceeds $t_{\rm Last} + 2\tau^\star$. This is in accord with the Bogolyubov conjecture. Thus, it is enough to wait for just $2\tau^\star$ past $t_{\rm Last}$, and the precursor QTE becomes free of any IC terms:

$$\begin{aligned} G_0^{-1}G^< - G^<G_0^{-1} = \Sigma^R G^< - G^<\Sigma^A \\ + \Sigma^< G^A - G^R\Sigma^<\,, \quad t_1, t_2 > t_{\rm Last} + 2\tau^\star\,. \end{aligned} \tag{6.2}$$

In the remaining collision terms, the time integration range is restricted by the condition (6.1) to a finite interval $(t-\tau^\star, t)$. This is the memory depth of the system. For a typical term in Eq. (6.2), $\Sigma^R G^<$, this means

$$\{\Sigma^R G^<\}(t,t) = \int_{t-\infty}^{t} d\bar{t}\Sigma^R(t,\bar{t})G^<(\bar{t},t)$$

$$\stackrel{\tau^\star}{\to} \int_{t-\tau^\star}^{t} d\bar{t}\Sigma^R(t,\bar{t})G^<(\bar{t},t)\,. \tag{6.3}$$

For $t > t_{\rm Last} + 3\tau^\star$, the self-energy in (6.3) extends already over the steady time span, and while the turbulent past may be reflected in the values of $G^<$, it will in no case show in the form of the EOM (6.2). And this is all the Bogolyubov conjecture says.

Equation (6.2) is just the GKBE (5.6). This is the equation, which enabled Kadanoff and Baym to derive the quantum Boltzmann equation.

6.2. *Kadanoff–Baym Ansatz and quantum Boltzmann equation*

To arrive at a quantum generalization of the Boltzmann equation, it is natural to convert the transport equation (6.2) for correlation function $G^<$ to the form which contains explicitly spectral properties of the system and has a shape which is more suitable for quasi-classical approximation. To this end, we first introduce into (6.2) spectral functions A and Γ by separating the imaginary and real parts of retarded and advanced functions

$$A = i(G^R - G^A)\,, \quad G = \frac{1}{2}(G^R + G^A)\,, \tag{6.4}$$

$$\Gamma = i(\Sigma^R - \Sigma^A)\,, \quad \Sigma = \frac{1}{2}(\Sigma^R + \Sigma^A)\,. \tag{6.5}$$

In the second step with the help of the following identities

$$i(G^R\sigma^< - \sigma^< G^A) = i[G,\sigma^<]_- + \frac{1}{2}[A,\sigma^<]_+\,, \tag{6.6}$$

$$i(\Sigma^R g^< - g^< \Sigma^A) = i[\Sigma,g^<]_- + \frac{1}{2}[\Gamma,g^<]_+\,, \tag{6.7}$$

where $[A,B]_\pm = AB \pm BA$ are anticommutators or commutators, we rearrange (6.2) into the following equation

$$-i[G_0^{-1} - \Sigma, g^<]_- - i[G,\sigma^<]_- = \frac{1}{2}[A,\sigma^<]_+ - \frac{1}{2}[\Gamma,g^<]_+\,. \tag{6.8}$$

Here we used instead of $G^<$ its counterpart $g^<$ given by (3.40), and correspondingly $\sigma^<$.

This equation is just a different form of the GKBE and it is thus also often called the GKBE.

6.2.1. *Kinetic equation for quasi-particle distribution function: Kadanoff–Baym approach*

Our aim is to find a quantum generalization of the BE, in a controlled way, i.e., we want to find a kinetic equation for a distribution function $f(k,r,t)$ from the GKBE

as an asymptotic equation. Naturally, the first step is to introduce the Wigner representation of the correlation function

$$\mathbf{g}^{<}(\omega,k,r,t)=\int dxd\tau \mathrm{e}^{i\omega\tau-ikx} \times g^{<}\left(r+\frac{x}{2},t+\frac{\tau}{2},r-\frac{x}{2},t-\frac{\tau}{2}\right), \tag{6.9}$$

where $(r+(x/2),t+(\tau/2))\equiv 1$ and $(r-(x/2),t-(\tau/2))\equiv 2$ in the cumulative variable notation. From now on, we will use Roman types for operators in the cumulative variable representation and Sans-serif types for operators in Wigner's representation.

The expression for Wigner's distribution function,

$$\rho(k,r,t)=\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}\mathbf{g}^{<}(\omega,k,r,t)\,, \tag{6.10}$$

has the essential property that it includes contributions from all independent energies ω. Thus, a perturbation scheme constructed for $\mathbf{g}^{<}$ instead for ρ will enable us to keep the energy as an independent variable until we select how to determine the energy of a particle from its position in phase space. By this step, we will find a proper distribution function avoiding the problems with the high momenta tails of Wigner's function. The existence of the independent energy permits to distinguish two very different contributions in the transport equations for the correlation function $\mathbf{g}^{<}$. First, the on-shell contributions, for which a dispersion relation between the energy and the position of the particle in phase space holds. Second, the off-shell contributions, for which no such relation exists. As we will see later, the possibility of this distinction leads to a formulation of the perturbation schemes which better suit the demands of the kinetic equations. To summarize this philosophy, we will close the perturbative expansion for $\mathbf{g}^{<}$. A quantum kinetic equation will be derived as an asymptotic limit of the equation for $\mathbf{g}^{<}$. This asymptotic equation is not closed for the Wigner distribution, but only for the on-shell part of $\mathbf{g}^{<}$ which can be interpreted as the quasi-particle distribution. The observables will be obtained from $\mathbf{g}^{<}$ in the second step via (6.10).

6.2.2. *Quasi-classical approximation*

To proceed on the way to a kinetic equation, we now need to convert the GKBE (6.8) to the Wigner representation. For matrix products, $C=AB$, it reads

$$\mathbf{c}=\exp\left(\frac{i}{2}\left(\frac{\partial}{\partial\omega}\frac{\partial}{\partial t'}-\frac{\partial}{\partial t}\frac{\partial}{\partial\omega'}-\frac{\partial}{\partial k}\frac{\partial}{\partial r'}+\frac{\partial}{\partial r}\frac{\partial}{\partial k'}\right)\right) \mathbf{a}(\omega,k,r,t)\mathbf{b}(\omega',k',r',t')_{\omega'=\omega,k'=k,r'=r,t'=t}\,. \tag{6.11}$$

The Boltzmann equation is known to be valid only for slowly varying fields. For this case we can expect that a dependence on the hydrodynamical variables r and t will be proportional to gradients of the external fields, i.e., small. In this situation,

the gradient expansion (6.11) can be approximated by its lowest-order terms. The anticommutator is even in gradients, thus it is approximated by a simple product, $C = (1/2)[A, B]_+$,

$$\mathbf{c} = \mathbf{ab}\,. \tag{6.12}$$

The commutator is odd in gradients and it thus turns to the Poisson bracket, $C = -i[A, B]_-$,

$$\mathbf{c} = [\mathbf{a}, \mathbf{b}] \equiv \frac{\partial \mathbf{a}}{\partial \omega}\frac{\partial \mathbf{b}}{\partial t} - \frac{\partial \mathbf{a}}{\partial t}\frac{\partial \mathbf{b}}{\partial \omega} - \frac{\partial \mathbf{a}}{\partial k}\frac{\partial \mathbf{b}}{\partial r} + \frac{\partial \mathbf{a}}{\partial r}\frac{\partial \mathbf{b}}{\partial k}. \tag{6.13}$$

Using (6.12) and (6.13) we find the GKBE (6.8) in the gradient approximation

$$[\omega - \epsilon - U_{\rm eff} - \sigma, \mathbf{g}^<] + [\mathbf{g}, \sigma^<] = \mathbf{a}\sigma^< - \gamma \mathbf{g}^<. \tag{6.14}$$

This equation is a good starting point for quantum generalizations of the BE.

6.2.3. *Kadanoff–Baym Ansatz*

Contrary to the KB equation, which is the equation for $\mathbf{g}^<(\omega, k, r, t)$, any kinetic equation of the Boltzmann type is an equation for a distribution function $f(k, r, t)$, so that there is no independent energy variable in it. Therefore, any construction of an asymptotic kinetic equation from the KB equations means to find an auxiliary functional $\mathbf{g}^<[f]$ by which the independent energy becomes fixed and related to the phase-space variables. Kadanoff and Baym suggested as a starting point for their construction of the auxiliary functional the relation

$$\mathbf{g}^<(\omega, k, r, t) \approx \phi(\omega, k, r, t)\mathbf{a}(\omega, k, r, t)\,, \tag{6.15}$$

i.e., they assumed that the relation between the correlation function $\mathbf{g}^<$, the spectral function $\mathbf{a}$ and the Fermi Dirac distribution $f_{\rm FD}$, in the form

$$\begin{aligned} \mathbf{g}^<(k, \omega, r, t) &\overset{\text{equil.}}{\equiv} \mathbf{g}^<(k, \omega) \\ &= f_{\rm FD}(\omega) \times A(k, \omega)\,, \end{aligned} \tag{6.16}$$

which is exact in equilibrium, was approximately valid near to equilibrium also for a nonequilibrium function ϕ. In the following step they eliminated the energy argument from ϕ by the assumption that the scattering rate was small, so that the spectral function had a singularity

$$\mathbf{a}(\omega, k, r, t) \approx 2\pi\delta(\omega - \epsilon - U_{\rm eff}(r, t))\,. \tag{6.17}$$

The energy argument of ϕ can be replaced by the mean-field energy $\epsilon + U_{\rm eff}$. Kadanoff and Baym proposed to approximate $\mathbf{g}^<$ as

$$\mathbf{g}^<(\omega, k, r, t) \approx f(k, r, t)\mathbf{a}(\omega, k, r, t) \tag{6.18}$$

$$\approx f(k, r, t)2\pi\delta(\omega - \epsilon - U_{\rm eff}(r, t))\,. \tag{6.19}$$

Taking the approximation (6.18), one does not obtain the BE, since this approximation leads to the violation of energy conservation of individual scattering events. Kadanoff and Baym thus used the (mean-field) nonrenormalized pole approximation (6.19), which is called the KBA.

6.2.4. *BE in the mean-field approximation*

From the KB equation (6.14) and the KBA (6.19) of $\mathbf{g}^<$ we get

$$\begin{aligned} &2\pi\delta(\omega-\epsilon-U_{\rm eff})[\omega-\epsilon-U_{\rm eff}-\sigma,f]+[\mathbf{g},\sigma^<] \\ &\quad=2\pi\delta(\omega-\epsilon-U_{\rm eff})(\sigma^<-\gamma f)\,, \end{aligned} \tag{6.20}$$

where we used $[\omega-\epsilon-U_{\rm eff},\delta(\omega-\epsilon-U_{\rm eff}]=0$, and the δ–function can be extracted from the first Poisson bracket.

At this point, Kadanoff and Baym adopted an idea that only the pole terms, in other words only the terms with the δ-function, contributed to the BE. They completely neglected the Poisson bracket $[\mathbf{g},\sigma^<]$. By this step, Kadanoff and Baym eliminated the ω-dependence using the pole value, $\omega=\epsilon+U_{\rm eff}$ and they derived the following kinetic equation:

$$\frac{\partial f}{\partial t}+\frac{\partial\epsilon}{\partial k}\frac{\partial f}{\partial r}-\frac{\partial U_{\rm eff}}{\partial r}\frac{\partial f}{\partial k}=I_{\rm in}[f]-I_{\rm out}[f]\,, \tag{6.21}$$

where the scattering integrals are given by

$$I_{\rm in}[f]=\sigma^<_{\omega=\epsilon+U_{\rm eff}}\,, \tag{6.22}$$

$$I_{\rm out}[f]=f\gamma_{\omega=\epsilon+U_{\rm eff}}\,. \tag{6.23}$$

There are various generalization of the KBA, which go beyond the mean-field approximation, the most advanced of which is the so-called extended quasiparticle approximation. It is out of scope of this article to discuss them.[106,258–267] Instead we will deal with its generalizations in different direction, in which the starting point is the GKBA.

6.3. *Generalized Kadanoff–Baym Ansatz and generalized master equation*

In this subsection, the GKBA will be defined, its salient properties will be analyzed, and the Ansatz will be finally used as a tool for deriving the GME. As mentioned the GKBA has originally been introduced as an alternative to the KBA. We shall follow this line of reasoning now. The KBA is given by

$$G^<(t_1,t_2)=f\left(\frac{t_1+t_2}{2}\right)\left[-G^R(t_1,t_2)+G^A(t_1,t_2)\right]. \tag{6.24}$$

The GKBA has been written as

$$G^<(t_1,t_2)=-G^R(t_1,t_2)\rho(t_2)+\rho(t_1)G^A(t_1,t_2)\,. \tag{6.25}$$

In comparison with the KBA it differs in four constitutive properties:

***Causal structure*:** The two propagators are now separated and each is multiplied by its own distribution function corresponding to the earlier time argument, depending on the retarded or advanced propagation.

***Equal time limit*:** The distribution function is the true one-particle density matrix, not the quasiparticle distribution. Thus, at equal times, the GKBA for $G^<$ obeys identity (3.41). This implies an automatic particle number conservation.

***General representation*:** The order of factors corresponds to the products interpreted as a matrix multiplication. Therefore, a diagonal representation for Green's functions is not assumed.

***Arbitrary nonequilibrium*:** No assumptions about slowly varying disturbances, small deviations from equilibrium, or quasiparticle approximation are built in, the Ansatz is formally quite general.

In addition, there is a basic difference, which distinguishes the GKBA from the KBA. Namely, while both Ansatzes are but approximate constructions, only the expression (6.25) can serve as a starting approximation for a process leading to an exact reconstruction of $G^<$. The GKBA thus has an important meaning, independent of and going beyond the restricted context of transport equations: it offers a path to the reconstruction problem as discussed in the previous section devoted to the reconstruction theorem.

The GKBA particle correlation function perfectly fits into the formal NGF scheme. It was constructed in this manner in order to overcome the limitations of the KBA. When inserted into the machinery of deriving quantum transport equations from the NGF, it leads to the GME, rather than to the BE like quantum kinetic equations.

6.3.1. *Towards GME*

To derive a GME, i.e., to obtain a single time kinetic equation, we proceed in three steps:

1st step: We recall the PKE (5.6). In other words on the way to GME we start from

$$\frac{\partial \rho}{\partial t} - \text{drift} = [-G^R\Sigma^< + \Sigma^< G^A + \Sigma^R G^< - G^<\Sigma^A]_{\text{equal times}}\,. \tag{6.26}$$

2nd step: A self-consistent *physical approximation* (5.7) is selected, that is, the self-energy is expressed in terms of the GF,

$$\mathbf{\Sigma} = \mathbf{\Sigma}[\mathbf{G}]\,.$$

A typical approximation could be RPA for interacting electrons, or the Migdal approximation for an electron–phonon system.

3rd step: The left-hand side of (6.26) already has the desired GME form. The right-hand side contains a number of double time quantities, which have to be eliminated.

In this final step, use is made of the GKBA in order to eliminate $G^<$ in favor of its time diagonal ρ:

$$G^<(t,t') = -\underset{t>t'}{G^R(t,t')\rho(t')} + \underset{t<t'}{\rho(t)G^A(t,t')}\ . \tag{6.27}$$

When introduced into the PKE (6.26), this leads finally to the quantum kinetic equation represented by a closed GME for ρ:

$$\begin{aligned}\frac{\partial\rho}{\partial t} + i[h_0,\rho]_- \quad & \boxed{\Sigma^< = \Sigma^<[\rho|G^R, G^A]} \\ &= -i\int_{-\infty}^{t} d\bar{t}(G^R(t,\bar{t})\Sigma^<(\bar{t},t) - \Sigma^<(t,\bar{t})G^A(\bar{t},t)) \\ &\quad + i\int_{-\infty}^{t} d\bar{t}(\Sigma^R(t,\bar{t})\rho(\bar{t})G^A(\bar{t},t) + G^R(t,\bar{t})\rho(\bar{t})\Sigma^A(\bar{t},t))\,.\end{aligned} \tag{6.28}$$

The memory kernel at the right-hand side is seen to be the generalized collision term; the role of the propagators is essential, and this will be further accented by the discussion in the following subsections.

The result (6.28) is still very general. If it is specified that h_0 corresponds to an extended system of electrons moving in a single band under the influence of a strong dc or ac homogeneous electric field, we find that an equivalent equation, usually referred to as the Levinson equation,[268] has originally been derived by the density matrix techniques. Its derivation from the NGF has been the first success of the GKBA. In fact, it re-established the Green functions as a serious contender in the everlasting competition with the more direct density matrix approach. Namely, the GME obtained previously with the help of the KBA failed to describe correctly even the ac linear response in the weak scattering limit, as it predicted spurious subharmonic frequencies in the induced current. This artifact of the approximations was not appearing for the original Levinson equation; it was eliminated in the NGF method by simply using the GKBA instead of the KBA.

To summarize, a closed transport equation for ρ was derived in three steps,

$$\frac{\partial\rho}{\partial t} - \text{drift} = \Phi[\rho(\tau);\tau<t|G^R,G^A]\,, \tag{6.29}$$

having precisely the form (2.17), only here the functional dependence on the propagators is explicitly indicated.

With the aid of GKBA, the program for deriving GME like equations outlined in Sec. 5.1.2 has been successfully completed.

6.3.2. *GME and the quantum BE compared*

The GME resembles the BE since it has the drift term on the left-hand side and interaction term similar to the scattering integrals on the right-hand side. In detail, however, there are three basic differences between both equations: the GME captures more of the quantum dynamics, it is not limited to the quasiclassical limit,

and it is not conditional on the quasiparticle picture. This mirrors in some obvious features of the GME. First, it is a non-Markovian equation, thanks to the time integration in interaction terms. Second, its drift term does not include the quasiparticle energy renormalization. Finally, it is an equation directly for the reduced density matrix, so in comparison to the BE it does not need any accompanying functional serving to calculate observables. The first right-hand side integral describes the back scattering of electrons. In (6.28), it is still kept in the closed symbolic form. Its expanded form will depend on the specific approximation used for $\Sigma^<[G^<]$. We will not discuss here any specific interaction. The second, forward scattering integral, on the other hand, has a sufficiently explicit structure to be compared with the BE.

7. GKB Ansatz, its Variants and GME

The GKBA has been introduced in Sec. 6.3 in an intuitive manner on the basis of several physically motivated requirements. Then we concentrated on demonstrating its use in deriving the quantum kinetic equations. In this last section of the whole review, we intend to seek for a better justification of the Ansatz both from the formal and the physical point of view. It may be pointed out that GKBA has been applied to a number of problems with an excellent or at least a good success. In this sense, it has already been accepted as a reliable tested part of the inventory of the tools of condensed matter theory. A purely theoretical background of its use may still be important. In particular, we will find that a detailed study of the properties of GKBA suggests its possible modifications promising improved reconstruction schemes or offering a hindsight justification of the reconstruction schemes which have been employed in practice.

7.1. *GKBA and the reconstruction equations*

The GKBA and the REs are intimately related, as is seen at a single glance; for convenience, we repeat here one half of the RE, Eq. (5.18). For $t_1 > t_2$ we have

$$\begin{aligned} G^<(t_1,t_2) = &-G^R(t_1,t_2)\rho(t_2) \\ &+\int_{t_2}^{t_1} d\bar{\bar{t}} \int_{-\infty}^{t_2} d\bar{t} G^R(t_1,\bar{\bar{t}})\Sigma^<(\bar{\bar{t}},\bar{t})G^A(\bar{t},t_2) \\ &+\int_{t_2}^{t_1} d\bar{\bar{t}} \int_{-\infty}^{t_2} d\bar{t} G^R(t_1,\bar{\bar{t}})\Sigma^R(\bar{\bar{t}},\bar{t})G^<(\bar{t},t_2)\,. \end{aligned} \tag{7.1}$$

The absolute term of this inhomogeneous equation is identical with the corresponding part of the GKBA formula (6.25). If the integral terms of (7.1) could be neglected, the Ansatz would be justified. An iteration of this equation would yield a corrected GKBA, but this still would represent $G^<$ as a functional of ρ and the propagators, which could be used for the same reconstruction mechanism as the

Ansatz itself. There are two drawbacks of such procedure. One is practical. Computation of the double integrals may be truly time consuming. In a steady state, some simplifications would be possible, but for transient processes the computational effort would be prohibitive. The other difficulty is fundamental. The special feature of the Ansatz is the factorization of $G^<$ at one sharp instant of time, and, of course, any integral corrections would blur that sharply time local factorization over some range, most likely on the order of the collision duration time.

7.2. *GKBA and the multiplicative rule for propagators*

In this section the GKBA will be illuminated from a different angle, following Ref. 138. The dynamic nature of the GKBA will be linked with the so-called semi-group character of the single-particle propagation.

7.2.1. *Noninteracting particles*

For independent particles, it holds

$$G_0^<(t_1,t_2) = iG_0^R(t_1,t_0)\rho(t_0)G_0^A(t_0,t_2)\,. \tag{7.2}$$

The propagators $G_0^{R,A}$ are proportional to the unitary single-particle evolution operator. They obey a multiplication rule (have the "*semi-group property*"). For G_0^R, which obeys

$$G_0^R(t_1,t_0) = iG_0^R(t_1,t_2)G_0^R(t_2,t_0)\,, \quad t_1 > t_2 > t_0\,. \tag{7.3}$$

Using this semi-group property in (7.2) we obtain, for $t_1 > t_2 > t_0$,

$$\begin{aligned} G_0^<(t_1,t_2) &= -G_0^R(t_1,t_2)G_0^R(t_2,t_0)\rho(t_0)G_0^A(t_0,t_2) \\ &= -G_0^R(t_1,t_2)\rho(t_2)\,, \end{aligned} \tag{7.4}$$

which is just the retarded half of the GKBA. The advanced half for the converse order of times can be obtained by Hermitian conjugation. The GKBA appears here as an exact identity based on the semi-group property of free particle propagators.

7.2.2. *Interacting particles*

In the case of interacting particles we follow the heuristic argument of Ref. 138 and start from the Dyson–Keldysh equation (3.221):

$$G^<(t_1,t_2) = \int_{-\infty}^{t_1} dt_3 \int_{-\infty}^{t_2} dt_4 G^R(t_1,t_3)\Sigma^<(t_3,t_4)G^A(t_4,t_2)\,. \tag{7.5}$$

Let $t_1 > t_2 > t_0 \to -\infty$. The formal integration region shown in Fig. 7 is a rectangle with corners at t_0, t_1, t_2. Following Sec. 6.1, it will be assumed that the actual integration involves only an intersection with the strip of a width $2\tau_c$ along the time diagonal $t_1 = t_2$, where the self-energy $\Sigma^<$ is significantly different from zero, cf. Eq. (6.1). If the "small" area C is neglected, the integral extends only over

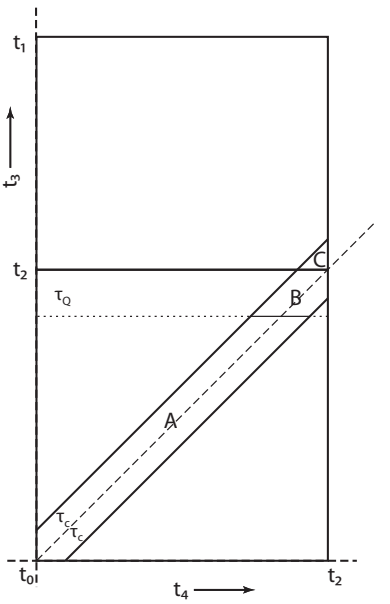


Fig. 7. Schematic structure of integration regions for deriving the GKBA from (7.5). To obtain $G^<(t_1, t_2)$, the integration region is the big rectangle. The actual integration range is the strip of the width $2\tau_c$ flanking the time diagonal. The effective integration region for obtaining the GKBA is the diagonal square. The propagators should be factorized according to the semi-group rule at its top side. The initial time t_0 should be set to $-\infty$ at the end. Derivation of the QKBA runs along similar lines; for details, see the main text.

the square $t_3 < t_2, t_4 < t_2$. Notice that neglecting the contribution of C is identical with setting the first integral correction in the RE (7.1) to zero.

In the remaining square integration range, let us assume an approximate validity of the semi-group rule generalized from (7.3) to

$$G^R(t_1, t_0) \approx iG^R(t_1, t_2)G^R(t_2, t_0)\,, \quad t_1 > t_2 > t_0\,. \tag{7.6}$$

Then Eq. (7.5) is reduced to the form of the GKBA

$$G^<(t_1, t_2) = -G^R(t_1, t_2)\rho(t_2)\,, \quad t_1 > t_2\,, \tag{7.7}$$

where

$$\begin{aligned}\rho(t_2) &= -iG^<(t_2, t_2) \\ &= -i\int_{-\infty}^{t_2} dt_3 \int_{-\infty}^{t_2} dt_4 G^R(t_2, t_3)\Sigma^<(t_3, t_4)G^A(t_4, t_2)\,,\end{aligned} \tag{7.8}$$

according to Eq. (7.5) for $t_1 = t_2$.

In deriving the GKBA, three assumptions were invoked. Two have a general character: an uncorrelated initial condition (not essential), and a uniformly small particle correlation time. The third one, the semi-group rule, is specific for this consideration. We have found that the semi-group property (7.6) is equivalent to

an elimination of the second integral term from the RE (7.1). Due to the interactions, the semi-group condition for the propagators cannot be valid exactly. The conclusion is that the Ansatz for $G^<$ can be checked or improved by the study of the multiplicative properties of propagators $G^{R,A}$.

7.3. *Quasiparticle GKBA*

We have seen the link between the GKBA and the semigroup property of propagators. In interacting systems, validity of this semigroup property is doubtful. A modified multiplication rule and a related modification of the Ansatz can be motivated, however, if the quasi-particle picture is known to work.

7.3.1. *Quasiparticle multiplication rule for G^R*

Consider first an equilibrium quasiparticle. The propagator $G^R(t_1, t_2)$ is characterized by three quantities: the pole energy $E_W = E - i\tau^{-1}$, the renormalization constant z and the time of formation τ_Q, which corresponds to the time spread of the kernel of the retarded self-energy Σ^R, just like τ_c is related to $\Sigma^<$. In order to achieve the correct hierarchy of the characteristic times, the so-called quasiparticle condition, $\tau_Q \ll \tau_r$, is required, see Ref. 116. Here, τ_r is the transport relaxation time which is comparable with the quasiparticle life-time τ . Then

$$G^R(t_1, t_2) = \begin{cases} \text{QP formation process} & t_1 < t_2 + \tau_Q \,, \\ z G^R_W(t_1, t_2) & t_1 > t_2 + \tau_Q \,, \end{cases} \tag{7.9}$$

$$G^R_W(t_1, t_2) = -i \exp(-iE(t_1 - t_2) - \tau^{-1}(t_1 - t_2)) \,,$$

with G^R_W the Weisskopf–Wigner propagator. This propagator obeys, as a defining property, the exact multiplication rule

$$G^R_W(t_1, t_2) = i G^R_W(t_1, \tilde{t}) G^R_W(\tilde{t}, t_2) \,. \tag{7.10}$$

For the following hierarchy of times,

$$t_1 > \tilde{t} > t_2 + \tau_Q > t_2 > t_0 \,, \tag{7.11}$$

the modified multiplication rule for G^R is obvious:

$$G^R(t_1, t_2) = i G^R_W(t_1, \tilde{t}) G^R(\tilde{t}, t_2) \,. \tag{7.12}$$

In contrast, the original semigroup factorization (7.3) is not satisfactory: at $t_1 = \tilde{t}$, a spurious kink appears because of a repeated quasiparticle formation.[138,141,144] For times $t_1 > \tilde{t} + \tau_Q$, the factorized expression has the value $z^2\, G^R_W(t_1, t_2)$ rather than the correct one as given by (7.9).

The rule may now be generalized to nonequilibrium by postulating that, to the true propagator G^R, a time of formation τ_Q and a construct called $G^R_W(t_1, t_2)$ characterized by (7.10) exists such that for times satisfying (7.11) the modified composition rule (7.12) holds. The conditions for validity of this rule, presently just postulated, are discussed in Ref. 218.

7.3.2. *Quasiparticle Ansatz for $G^<$*

On the way to the new Ansatz we continue as above in Sec. 7.2.2. We start from the exact relation (7.5) and substitute everywhere G^R by its factorized form. Only now we use (7.12) instead of (7.6). Integration regions are sketched in Fig. 7 again. The newly invoked feature is the dashed horizontal line at $t_3 = t_2 - \tau_Q$. Below this line, the rule (7.12) is exact. The quasidiagonal integration strip is thus divided into three regions, A, B and C. In A, our transformation is exact. The top region C reaching above t_2 has to be neglected again and the region B remains as the principal source of error caused by (7.12). Ignoring this, we obtain

$$G^<(t_1, t_2) = -G^R_W(t_1, t_2)\rho(t_2)\,, \quad t_1 > t_2\,, \tag{7.13}$$

where ρ is given by the exact expression (7.8), just as before.

7.4. *GKBA, QKBA and family of causal Ansatzes*

The main problem of the GKBA is the uncertain role of the involved unknown propagators. We have already seen that one of the possibilities is to use quasiparticle propagators in the structure of the GKBA. We will now first summarize properties of the GKBA before we discuss variants of generalization of the GKBA and their role in generation of GME.

The GKBA fits well into the general formal and physical structure of the NGF theory. Its basic property is the correct causal structure. In addition, the GKBA has the particle-hole symmetry, the correct equal time limit, the correct asymptotic behavior for $|t_1 - t_2| \gg \max\{\tau_c, \tau_Q\}$. It is correct in the true Boltzmann limit. In the limit of noninteracting particles, it is exact for excitations arbitrarily far from equilibrium. Thus, it emerges as an interpolation scheme between two crucial exact limits. Furthermore, the GKBA does not depend on the quasi-classical expansion in space, and, in fact, it is not associated with any specific representation for the GF. All these qualitatively correct features do not guarantee that the GKBA, as a truncation, is satisfactory also quantitatively.

However, practical experience with this "standard approach" based on the GKBA has covered with good success several areas of physics including the hot electron transport (Levinson equation), and the response of electrons in semiconductors to sub-picosecond pulses (quantum optical Bloch equations). Computed properties and processes were in an excellent qualitative and very good quantitative agreement with experimental data.

A closer look offers an explanation for these good results. It was naturally not practicable to compute the exact propagators entering the GKBA, and the propagators constructed on model grounds worked well, most likely compensating the error of the Ansatz itself.

Such approach, seemingly a pragmatic expedient, has, in fact, a deep meaning. In reality, the Ansatz used was not the GKBA proper, but its modification employing rather the quasiparticle propagators, the "QKBA". We meet here an instance of

an Ansatz scheme possessing the same general properties as the GKBA. A whole family of such "causal Ansatzes" already exists. Our goal in the next part of the paper will be to discuss the means of their systematic generation, comparison and assessment. This is also due to the general concept of the reconstruction procedure discussed above.

Clearly, neither the GKBA (7.7), nor the QKBA (7.13) have been proven, but first, both have been linked with the related multiplication rule for propagators. Second, their physical motivation has been put on the same footing. In fact, the QKBA appears as somewhat better justified than the GKBA proper once the quasiparticle behavior of the system can be assumed. Third, the two Ansatzes appear as two instances of a general factorization $G^<_X = G^R_X \rho$ with the subscript $_X$ meaning an arbitrary choice of the effective propagator. If this propagator satisfies basic requirements, the corresponding "Ansatz" will possess the general properties listed for the GKBA like causal Ansatzes.

7.4.1. *Causal Ansatzes*

We have already discussed that the GKBA ansatz has many useful properties. On the whole, the GKBA has a number of important properties which make it consistent with the general NGF scheme. It would be natural to take this set of properties as requirements to be fulfilled by any other Ansatz approximation scheme. We will term any approximation a **causal Ansatz**, if it fullfills the same following characteristics as the GKBA:

- Its basic property is that of possessing the correct causal structure.
- In addition, the GKBA has the particle-hole symmetry,
- the correct equal time limit,
- the correct asymptotic behavior for $|t_1 - t_2| \gg \max\{\tau_c, \tau_Q\}$.
- It coincides with the KBA in the true Boltzmann limit. In the limit of noninteracting particles.
- It is exact for excitations arbitrarily far from equilibrium (cf. Sec. 7.2.1).
- Thus, it emerges as an interpolation scheme between two crucial exact limits.
- As it is said already, it fits not only into the physical framework, but also into the formal structure of the exact NGF equations.
- Furthermore, the GKBA does not depend on the quasiclassical expansion in space, and, in fact, it is not associated with any specific representation for the GF.

A wide family of causal Ansatzes already exists. The GKBA, in addition to its direct importance, is the primary member of this family. Still, all these qualitative properties do not guarantee that the GKB approximation, amounting to the first term of an asymptotic expansion, will be quantitatively satisfactory.

Finally, we have in this section outlined a simple and graphic way to the causal Ansatz family, which offers new possibilities of devising, improving and analyzing its further members.

7.5. *Causal Ansatzes and various GME*

We will now shortly show how variants of the GKBA can influence the related form of corresponding GME.

To this end we first shortly summarize the general method of generating a quantum transport equation from the precursor transport equation:

- We will start from the precursor quantum transport equation:

$$\frac{\partial \rho}{\partial t} + i[H_0, \rho]_- = -(\Sigma^R G^< - G^< \Sigma^A) + (G^R \Sigma^< - \Sigma^< G^A) + \Theta^<_{t_0} G^A - G^R \Theta^<_{t_0} . \tag{7.14}$$

  This already has the form of a QTE, in which $H_0(t)$ is the mean field one-particle Hamiltonian. The "generalized collision" terms on the right-hand side still involve double time *less* quantities. The related integrals extend only to the past because of the presence of the propagator factors.
- We will apply the Keldysh initial conditions at $t_0 \to t_{\rm I}$,
- The double-time $G^<(t,t')$ is replaced by an approximate "Ansatz" expression involving only its time diagonal $\rho(t) = -iG^<(t,t)$ and propagators.
- This expression is also introduced into the self-energy, for which a self-consistent approximation specifying the self-energy in terms of the Green's function is assumed.
- As a parallel input the knowledge of the propagator components of the Green's function in necessary. In general, the components of the NGF are interconnected, but often this is of a lesser importance and the propagators can be found beforehand once forever.

7.5.1. *From an Ansatz to the GME*

The resulting transport equation depends on the approximate replacement of $G^<$.

As we already discussed, the historically first one is the famous KBA, schematically $G^< = 1/2[\rho, G^A - G^R]_+$. This choice was connected with the subsequent quasi-classical expansion made by Kadanoff and Baym. This is irrelevant for systems with discrete levels

We will concentrate on the so-called XKBA, belonging to the general class of the causal Ansatzes, and exemplified by the original GKBA $G^< = -G^R\rho + \rho G^A$. This ansatz is exact for independent particles governed by a one-particle Schrödinger equation. In general, it is an approximation and other XKBA variants have been considered:

$$G^<_X = -G^R_X \rho + \rho G^A_X . \tag{7.15}$$

Some more important examples are summarized in the table:

Abbr.	Ansatz
GKBA	$G^<_{\rm G} = -G^R_{\rm G}\rho + \rho G^A_{\rm G}$ (7.16)
QKBA	$G^<_{\rm Q} = -G^R_{\rm Q}\rho + \rho G^A_{\rm Q}$ (7.17)
FKBA	$G^<_{\rm O} = -G^R_{\rm O}\rho + \rho G^A_{\rm O}$ (7.18)

Each Ansatz is specified by a particular choice for the form of the propagators. This is indicated by the label. Here $G^{R,A}_{\rm G}$ denotes the true, fully renormalized propagators, $G^{R,A}_{\rm Q}$ the quasiparticle GF and $G^{R,A}_{\rm O}$ the free particle propagators. When using the Ansatz, all participating GF have to be labeled. Thus, although the GKBA given by (7.16) is clearly identical with (6.25), we use the label "G", so that $G^R_{\rm G} \equiv G^R$, etc. It may be asked which one can be expected from approximating the true propagators by another choice. This goes beyond the present discussion, but reasons have been given for using the QKBA in particular, in which the propagators are represented by the unrenormalized pole part of the true propagators. FKBA has been used inadvertently in derivations of the Boltzmann equation or the master equation in the second order weak coupling theory equivalent with the use of the plain Fermi golden rule.

Returning to our main task, it is enough to approximate the exact generalized scattering terms in the precursor quantum transport equation (5.6) by a properly selected Ansatz approximate expression, and the GME for the true particle distribution ρ results:

$$\frac{\partial \rho}{\partial t} + i[H_0, \rho]_- = -(\Sigma^R_X G^<_X - G^<_X \Sigma^A_X) + (G^R_X \Sigma^<_X - \Sigma^<_X G^A_X)\,. \tag{7.19}$$

We can clearly see that the quality with which the above GME describes the dynamics of the considered systems depends on the construction of suitable approximations for propagators.

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