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Between Green's Functions and Transport Equations: Reconstruction Theorems and the Role of Initial Conditions

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Abstract. Construction of the electron quantum transport equations from Non-Equilibrium Green's Functions is presently based on Reconstruction Theorems, reducing full description of a non-equilibrium system to a dynamic theory in terms of one-particle quantities. This approach, stemming from the original Kadanoff-Baym Ansatz, and based on a suitably renormalized NGF formalism, can be brought to a close parallel with the Time Dependent Density Functional Theory. This concerns, in particular, the role of correlations at a finite initial time. A universal treatment of these initial conditions is possible for the switch-on states, while more general initial states have so far to be treated individually.

1. Introduction

This contribution touches the theme of the Non-equilibrium Green's Functions as a tool for constructing quantum transport equations. This approach and its applications has been a flourishing and successful research field over the past nearly 20 years. There are, however, at least three reasons why to address the current state of this problem right now.

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, our 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 40 years ago [1]. Yet the procedure is still not quite routine, as witnessed by the continuing research activity, and the question Why? is fully justified.

The third reason is specific for electrons in atomic systems [1] (... solids). Just as it happened before for systems in equilibrium and the Kohn -Sham Density Functional Theory [2], the systematic quantum field treatment of many body systems out of equilibrium seems to face an emerging competitor in the Time Dependent Density Functional Theory [3].

These three topics will be discussed below. There is another current development concerning electronic systems. Originally, the NGF based transport theory has been formulated for extended

[1] we will have in mind the electrons as a specific example, as corresponds to our research orientation

systems [1, 4, 5, 6, 7, 8, 9, 10, 11]. The attention is presently shifting more and more towards 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 on a general level.

To define the "transport theory", we may start from the more general non-equilibrium quantum dynamics of a system described by the statistical operator (many-body density matrix) $\mathcal{P}(t)$. The dynamics is driven by the full Hamiltonian $\mathcal{H} + \mathcal{U}(t)$ consisting of the system Hamiltonian $\mathcal{H}$ and an additive external disturbance $\mathcal{U}(t)$. An initial state $\mathcal{P}_0$ at $t = t_0$ 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 $\langle \mathcal{X} \rangle_t = \mathrm{Tr} \mathcal{X} \mathcal{P}(t)$.

The transport theory obtains, 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. One, generalizing the Landau theory of Fermi liquids makes use of the quasiparticle distribution $f(\vec{r}, \vec{k}, t)$. To obtain a closed theory, a time-local Quantum Boltzmann equation [1, 4, 5, 10] for f is usually constructed. We will not follow this direction, suited for "slow" processes, like a stationary transport. [2] The other possibility is to work with the single-particle density matrix defined by the correspondence

$$\begin{array}{lcl} \langle \mathcal{X} \rangle_t = \mathrm{Tr} \mathcal{X} \mathcal{P}(t) & \overset{\text{additive}\mathcal{X}}{\longrightarrow} & \langle \mathcal{X} \rangle_t \equiv \overline{X}(t) = \mathrm{Tr} X \rho(t) \\ \mathcal{P}(t) & \overset{\text{REDUCTION}}{\longrightarrow} & \rho(t) \end{array} \tag{1}$$

A closed Quantum Transport Equation for ρ has the general form

$$\frac{\partial \rho}{\partial t} - \text{drift} = \Phi_t[\rho(\tau); \tau < t] \tag{2}$$

where "drift" means the bare one-particle dynamics and the effect of all interactions is contained in the generalized collision term on the r.h.s. 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/Ansatz approach are very close to those which were formulated by the founders of non-equilibrium statistical physics. The issues remain, the understanding and attitudes change. It will be important to recall several of these fundamental ideas pervading the development of transport theory [12, 13, 14, 15, 16, 5, 9, 10, 11].
I One of the central ideas of the transport theory, already invoked here, has always been the **reduced description** of the system. The relevant information about a gas of particles was contained in the one-particle distribution function $f(\vec{r}, \vec{k}, t)$. A closed equation for f was only conceivable, if, say, binary collisions in the gas were described in terms of f. Recall the Boltzmann's Stosszahlansatz for the binary distribution: $f_{12} \sim f_1 \times f_2$, Chapman and Enskog, BBGKY, ... Also the Kadanoff-Baym Ansatz[1] and all its suite are of this nature. All this points to the **reconstruction problem**: under which conditions the full description of a many-body interacting system can be built up from its single-particle characteristics? In Sec. 3, we will discuss possible answers to this question.

[2] A more comprehensive discussion of the transport problem has been presented in papers [9, 10, 11].

II The second crucial notion is the **hierarchy of characteristic times**. According to Bogolyubov [13, 14, 15, 5], 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* τ_c, the *collision time* τ_r and the *hydrodynamic time* τ_h. 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 relaxation of spatial inhomogeneities. In "normal" situations, the three times obey the inequality

$$\tau_c \ll \tau_r \ll \tau_h \tag{3}$$

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 that for times later than the chaotization time τ_c a many-body system becomes chaotized, and all higher particle correlation functions become a functional of the distribution function (**decay of initial correlations**). Thus, throughout the kinetic and the hydrodynamic stage, the reconstruction problem is expected to have a positive answer. A well defined time hierarchy (3) was found by a direct simulation for a number of model systems confirming the bold Bogolyubov's conjecture.

To complete the picture, it is important to consider also the time range of the order of τ_c, in other words the transition period between the decay of correlations and the onset of the kinetic stage. This is necessary to respect the correlated initial conditions. This regime of the initial transient is particularly interesting, if the time scales defined by τ_c and τ_r are not sharply separated. Another such case will be the dynamical transient induced by an external field whose characteristic times are sufficiently short. For example, an optical pulse is characterized by its duration, the ground period of the signal and the Rabi period measuring the pulse strength. These times should be compared with the intrinsic times of the system. This specifies the situation and the necessary version of transport theory used.

III The last basic concept we want to mention is that of the **quasi-particles**. Following the original Landau's conception, these are weakly excited states of a correlated system, whose properties resemble that of the gas of weakly interacting particles. Quasiparticles are known to exist in Fermion systems, like electron liquid or nuclear matter. A well known quasiparticle is a polaron, an electron surrounded by its polarization cloud of virtual phonons. The effect of correlation is reflected in the self-energy describing both the renormalization and life-time effects. Quasiparticles have typically a finite life-time τ. A bare particle turns into the dressed quasi-particle over the "formation time" τ_Q. If $\tau_Q \simeq \tau$, the quasiparticle 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. We thus arrive at the Landau-Peierls criterion $\tau_Q \ll \tau$ [12, 9] for the presence of the kinetic stage as a formalized expression of the notion that the "true" transport is carried by quasiparticles. This is, basically, true. However, the quasi-particles are vulnerable and elusive objects and cease to exist beyond the regime quasi-classical in time, in particular for strong and/or transient disturbances with short characteristic times. Just how short – that requires a detailed analysis, see Sec. 3.3.

2. Non-equilibrium Green's Functions

The Non-equilibrium Green's Function is defined in the usual manner [4, 5],

$$G(1,2) = -\mathrm{iTr}\left(\mathcal{P}_0\, \mathcal{T}_{\mathsf{c}}\{\psi(1)\psi^\dagger(2)\}\right) \tag{4}$$

with the field operators ψ, $\psi^\dagger$ in the Heisenberg picture with respect to t_0 and the time-ordering operator $\mathcal{T}_{\mathsf{c}}$ acting along the closed time path $\mathbb{C}$ (Schwinger contour, Keldysh contour) extending from t_0 to $+\infty$ and back.

To evaluate G by a perturbation expansion, the $\mathbb{C}$ contour has to be augmented by a Matsubara-like imaginary time interval; the task may be difficult for a general initial state, but, in principle, the NGF can be computed[17, 18, 19].

2.1. NGF and QuantumTransport
It is convenient to represent the contour-ordered NGF by the matrix real-time GF, $\|G^{\pm\pm}(1,2)\|$ with + and − labeling the branches of $\mathbb{C}$ Only two of the four components are independent. Kadanoff and Baym [1]used $G^{+-} \equiv G^{<}$ and $G^{-+} \equiv G^{>}$. A linear transformation of $\|G\|$ leads to the popular Keldysh matrix [21, 16], or to the Langreth-Wilkins matrix [22, 23, 4] we use here. The latter choice works with three components, the *less*-correlation function and two propagators,

$$G^{<} = G^{-+},\ G^{R} = (G^{--} - G^{-+}),\ G^{A} = (G^{--} - G^{+-}),\ G^{A}(1,2) = [G^{R}(2,1)]^{\dagger} \tag{5}$$

The link to the transport problem is given by the relation

$$\rho(x_1, x_2, t) = \mathrm{i}\, G^{<}(1,2)\big|_{t_{1,2}=t} \tag{6}$$

identifying the single-particle density matrix ρ with the time diagonal of the particle correlation function $G^{<}$.

This identity can be used in two ways. In the direct approach, the NGF is computed and the single particle density matrix is a corollary. As pointed out in the introduction, this may soon become a standard method with the present day powerful computers, once the NGF solvers will be perfected[24, 25]. In the indirect approach, a Quantum Transport Equation is derived from the equations of motion for the Non-equilibrium Green's Function. The task of solving this transport equation is much less demanding than the direct solution and it has been widely used over the past decade. A standard approach has gradually been established, and its basic features will be outlined in the next section.

2.2. Standard Way to QTE: Ansatz
The standard approach is characterized by three steps.
1st step It is assumed that

$$t_0 \to -\infty$$

and that we start from an uncorrelated equilibrium state. This so-called **Keldysh initial condition** [21, 4, 5] eliminates the problem of initial correlations and allows to introduce the Dyson equation and the self-energy in a simple way,

$$\|G\|^{-1} = \|G_0\|^{-1} - \|\Sigma\|, \quad G_0^{-1}(1,2) = [\mathrm{i}\partial_{t_1} - W - U(t_1)]\delta(t_1 - t_2) \tag{7}$$

The unperturbed GF is diagonal and its diagonal elements contain the "kinetic energy" and the external field.

The *less* component of (7) has the famous Keldysh integral form [4, 5]:

$$G^{<} = G^{R}\Sigma^{<}G^{A}, \tag{8}$$

while the Dyson equation for propagators reads simply

$$[G^{R,A}]^{-1} = [G_0]^{-1} - \Sigma^{R,A} \iff G^{R,A} = G_0 + G_0\Sigma^{R,A}G^{R,A},\ \text{etc.} \tag{9}$$

By computing the equal time limit of the expression $[G^{R}]^{-1}G^{<} - G^{<}[G^{A}]^{-1}$, the **Generalized Kadanoff-Baym Equation** is obtained [4, 5]:

$$\frac{\partial\rho}{\partial t} - \text{drift} = \Big[-G^{R}\Sigma^{<} + \Sigma^{<}G^{A} + \Sigma^{R}G^{<} - G^{<}\Sigma^{A}\Big]_{\text{equal times}} \tag{10}$$

2nd step The l.h.s. of (10) already has the desired form. The r.h.s. contains a number of double time quantities, which have to be step by step eliminated. First, a self-consistent **physical approximation** is selected, that is, the self-energy is expressed in terms of the GF,

$$\|\Sigma\| = \|\Sigma\left(\|G\|\right)\|.$$

A typical approximation will be RPA for interacting electrons, or the Migdal approximation for an electron-phonon system.

3rd step In the final step, use is made of an Ansatz to eliminate $G^<$. Widely used has been the Generalized Kadanoff-Baym Ansatz [26, 27, 4, 5]

$$G^<(t,t') = -\underset{t>t'}{G^R(t,t')\rho(t')} + \underset{t<t'}{\rho(t)G^A(t,t')} \tag{11}$$

This is a complement to (6): it is expressing the double-time function $G^<$ in terms of its single-time diagonal section ρ. When introduced into the GKBE (10), this leads finally to the Quantum Transport Equation

$$\frac{\partial\rho}{\partial t} - \text{drift} = \Phi[\rho(\tau);\tau<t\,|G^R,G^A] \tag{12}$$

having precisely the form (2), only here the functional dependence on the propagators is explicitly indicated. To summarize, a closed transport equation for ρ was derived in three steps. The memory kernel at the r.h.s. (generalized collision term) is formed by propagators, whose role is essential.

Basic considerations motivating and justifying the GKBA can be found in [9, 10, 11]. This Ansatz 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 non-interacting 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 [28]), and the response of electrons in semiconductors to sub-picosecond pulses (Quantum Optical Bloch Equations) [4]. 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[4, 5, 33].

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 quasi-particle 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 [9, 11]. Our goal in the next part of the paper will be to discuss the means of their systematic generation, comparison and assessment. This will be made possible by introducing the general concept of the reconstruction procedure.

3. Reconstruction Theorems

The general plan of generating quantum transport equations within the NGF scheme is to transform the GKBE (10)(... precursor transport equation) involving two-time GF's to a

closed transport equation for the single particle distribution function. For the purpose of this transformation, an Ansatz similar to (11) should be employed. The Ansatz serves to express the double-time function $G^<$ in terms of its single-time diagonal section $-\mathrm{i}\rho$.

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 as natural that virtually all of the relevant information about a non-equilibrium many body system can be unfolded from its reduced characteristics, namely a pair of double-point quantities, say $G^<$ and $G^>$. The Bogolyubov postulate, just as the Ansatzes, hint 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. [3]

It should be warned already here, however, that any Ansatz suffers from the following

DIFFICULTIES OF ANSATZES AS TOOLS FOR A RECONSTRUCTION SCHEME

D 1 An Ansatz plays the role of a physically well justified, but still approximate truncation of the NGF. That would make the reconstruction procedures approximate already by their nature.
D 2 The knowledge of the distribution function alone is not sufficient: propagators are also entering the equations, and their relationship to the distribution function is not obvious.
D 3 Last but not least, it is rather difficult to extend an Ansatz procedure so as to incorporate correlated finite-time initial conditions.

These problems of principle will be addressed below. In particular, we will sharpen up the reconstruction problem by searching for its exact solutions.

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

First, we recall once more the Bogoluybov postulate: In an autonomous system, the evolution is controlled by a hierarchy of times (3) and for times past the initial decay of correlations, a transport equation of the form (2) is valid. The related reconstruction has a rather symbolic form

$$\mathcal{P} = \widetilde{\Phi}[\rho], \qquad t > t_0 + \tau_c \tag{13}$$

We will return to this reconstruction loop when discussing the inversion schemes in Sec. 3.1. An explicit reconstruction along these lines is represented by the decouping technique of the BBGKY method [5]. While it has been successful in yielding a closed reduced description, the whole decoupling approach suffers from its approximate nature, lacking a firm basis equivalent to a reconstruction theorem.

Second, the density matrix projection method in the Liouville space leads to a partitioned expression for the projected (relevant) density matrix which is closed and exact. It can serve for generation of ever improving approximations in a systematic way and, in principle, to a reconstruction of the full statistical operator. This complex approach is technically rather remote from the NGF method, but has closely parallel goals. There are some very important developments aiming at a combined technique permitting to take advantage from both sides [29].

There is a third stream of research stemming from the fundamental paper by Schwinger on the use of the generating functional in non-equilibrium 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 first in equilibrium [2], then in the extension to the Time

[3] The TDDFT is even based on a single-point quantity, the local particle density, see the next section.

Dependent Density Functional Theory [3]. Some of the general results obtained in the context of this approach are about the closest to the fundamental formulation of the Reconstruction Problem. At the same time, TDDFT draws from an independent source of physical inspiration. In view of the interest of all this, we devote a separate paragraph to the inversion problem before discussing our main subject, the Ansatz approach.

3.1. Inversion Problem

Closely related to the reconstruction questions, although distinct in some respect, is the so-called Inversion Problem.

Schwinger [30] introduced as the first the closed time path $\mathbb{C}$ and the generating functional dependent on an external field $U^{\pm}(t)$ depending on the branch of the contour,

$$\mathrm{e}^{\mathrm{i}W(U^+,U^-)} = \mathrm{Tr}\ \mathcal{P}_0\, \tilde{\mathbf{T}}\, \mathrm{e}^{+\mathrm{i}\int_{t_0}^{\infty} \mathrm{d}\tau(\mathcal{H}-U^-(\tau)X)}\ \mathbf{T}\, \mathrm{e}^{-\mathrm{i}\int_{t_0}^{\infty} \mathrm{d}\tau(\mathcal{H}-U^+(\tau)X)} \tag{14}$$

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:

$$\overline{n}(x,t) = \left.\frac{\delta W}{\delta U^+(x,t)}\right|_{U^+=U^-=U} = -\left.\frac{\delta W}{\delta U^-(x,t)}\right|_{U^+=U^-=U} \tag{15}$$

It comes immediately to mind that the latter relations could be *inverted*, so that the field U would be expressed in terms of $\overline{n}$. Introducing this back into the time derivative of (15) 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 [31, 32].

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

$$U(t),\ \{t_0 \le t < \infty\} \rightleftharpoons \overline{n}(t),\ \{t_0 \le t < \infty\} \tag{16}$$

The importance of the inversion consists in the following: Starting from $\overline{n}$, an ultimately reduced data set, we may go, by (16), 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 (13).

The non-equilibrium Generating functional is, of course, close to the Non-equilibrium Green's Functions, which can be obtained as its non-local functional derivative. It is remarkable that it also provides a formal framework for the Time Dependent Density Functional Theory [3]. This theory has always been an alternative to the NGF theory and its most serious contender in the quest to become THE universal method of practical handling of non-equilibrium many-electron systems. This is similar to the known development for equilibrium systems, where the original Density Functional Theory, one of the most successful methods of description of many-electron systems, has won in the competion. Now the practical use of the Density Functional Theory is based on three pillars: the Kohn-Hohenberg theorem [2] stating that in equilibrium the bijection (16) is valid, the Kohn-Sham variational theorem permitting to introduce an equivalent system of effective non-interacting particles, and finally a specific approximation for the exchange& correlation potential. There is a basic difference between the first two steps, which are general and exact, and the actual description of the exchange and correlation in the system, which is by necessity approximate.

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** [3, 2]: Let $U(t)$ be a local potential smooth in time. Then, for a fixed initial state $|\Psi_0\rangle$, the functional relation $\overline{n}[U]$ 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 non-interacting particles moving in an effective potential local in space and time[3].

Given this progress, the present period is marked by a renewed search for an improved XC part of the time-dependent effective potential. Just like in the time independent case, this part of the task is going to be crucial for its prospective final success.

We will not follow the details of this developing field, making just several remarks. First, the importance of the Runge-Gross theorem extends beyond the density functional theory: it is an existence theorem putting the corresponding reconstruction on a sound footing regardless of the specific reconstruction procedure. Second, the dependence on the initial state enters both the RG theorem and the generating functional and all subsequent steps. So far, a tractable scheme has only been obtained for the switch-on states starting from equilibrium.

Comparing the RG theorem with the Bogolyubov postulate, we see immediately that there is no τ_c in the former, while it defines the period of the decay of correlations in the latter. This remains to be clarified, and, hopefully, reconciled, perhaps by investigating approximate time dependent density functionals for the early times $t_0 < t < t_0 + \tau_c$.

Third, the TDDFT is reliable only for the local electron density related quantities. Just like in the usual DFT, it is not straightforward to obtain the momentum dependent observables. For a complete treatment of the non-linear response, the inversion $\{\text{local } U(t)\} \rightleftharpoons \overline{n}(t)$ should be replaced by $\{\text{non}-\text{local } U(t)\} \rightleftharpoons \rho(t)$. Clearly, the Current Density Functional Theory, or similar extensions of the Density Functional Theory [2] are moving along this direction.

3.2. NGF Reconstruction Theorem

Let us return to the reconstruction task as defined at the beginning of Sec. 3. While a reconstruction based on, say, the GKBA, is but approximate, there exist relations we will call the **Reconstruction Equations, RE**, which lead to an exact reconstruction of $G^<$ from ρ:

$$
\begin{array}{c|c}
\boxed{t > t'} & \boxed{t < t'} \\
\multicolumn{2}{c}{G^<(t,t') =} \\
-G^R(t,t')\rho(t') & +\rho(t)G^A(t,t') \\
+\int_{t'}^{t} \mathrm{d}\bar{t} \int_{-\infty}^{t'} \mathrm{d}\bar{\bar{t}} G^R(t,\bar{t})\Sigma^<(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t') & +\int_{t}^{t'} \mathrm{d}\bar{\bar{t}} \int_{-\infty}^{t} \mathrm{d}\bar{t} G^R(t,\bar{t})\Sigma^<(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t') \\
+\int_{t'}^{t} \mathrm{d}\bar{t} \int_{-\infty}^{t'} \mathrm{d}\bar{\bar{t}} G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{\bar{t}})G^<(\bar{\bar{t}},t') & +\int_{t}^{t'} \mathrm{d}\bar{\bar{t}} \int_{-\infty}^{t} \mathrm{d}\bar{t} G^<(t,\bar{t})\Sigma^A(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t')
\end{array}
\tag{17}
$$

In fact, these equations were derived at the same time as the GKBA [26, 27]. If the Keldysh initial condition is assumed, they easily follow from the Dyson equations (8) and (9). The RE are inhomogeneous and their source terms correspond to the respective parts of the GKBA. Their exact solution can be obtained by iteration. 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. This important feature will be discussed shortly.

First, however, we have to warn that the Reconstruction Equations 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 un-physical, invalid results. In particular, this would impair the conservation laws.

The compatibility is provided by the GKBE (10). It has the meaning of a **precursor transport equation**, by which the density matrix ρ is obtained from the NGF as an input into the generalized scattering term. Recall now that also the GKBE is a consequence of the Dyson equation for $G^<$. In fact, RE and GKBE together are equivalent with the Dyson equation:

Dual Scheme I

Dyson equation for $G^<$ Eq. (8)	$\Longleftrightarrow$	$\begin{cases} \text{Reconstruction equations for } G^<, \text{ Eq. (17)} \\ \text{Precursor transport eq. for } \rho, \text{ Eq. (10)} \end{cases}$

This brings us to a novel understanding of the NGF treatment of quantum transport. 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. In one stream, the single-particle distribution ρ is obtained from a closed quantum transport equation. In the other stream, the NGF is reconstructed from known ρ. Then, it is introduced into the GKBE. This completes the path back to the transport equation. The two streams are mutually coupled:

NGF Reconstruction Scheme

ρ	$\longrightarrow$	$G^<$ RE
QTE	$\longleftarrow$	$G^{R,A}$ DE

(18)

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 non-equilibrium 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,

$$\{G^<, G^R, G^A\} \rightleftharpoons \rho \tag{19}$$

This theorem resolves on the fundamental level the **D 1** problem in our list of difficulties of Ansatzes. It should be compared with the alternative schemes listed in the preceding section. Let us start with the Runge-Gross theorem. Firstly, on one side of our dual relation stands the full ρ rather than its space diagonal $\overline{n}$. This may appear as a weaker result, but, in fact, the Legendre duality behind the NGF theorem extends to arbitrary non-local fields U and thus covers a class of physical situations much wider than those limited to the local external fields. Secondly, 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. Thirdly, the dual relation (19) links ρ with the NGF rather than with the external field U in the vein of Eq. (16). It may be said that, in this sense, the NGF reconstruction theorem makes true the Bogolyubov conjecture (13), albeit in a realistically restricted form.

The important question remains about the feasibility of the reconstruction scheme (18). 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[24, 25]. With all equations cast in the differential form, the solution proceeds in steps incremental in time. This may appear as abandoning the transport equation approach, but, in fact, this solver would permit to implement a new concept: an auto-adaptive scheme NGF/QTE, 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 Transport Equation when possible, like over the long periods of autonomous relaxation. So far, no progress along these specific lines has been reported.

2. Interaction strength as small parameter

Iteration of the reconstruction equations is less promising for computations than a solver, but it has a more basic context. It permits various interpretations. For non-interacting particles, the self-energies vanish and, by Eqs. (17), the GKBA is exact. 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 QTE. The problem with this expansion is that it mixes two levels: it tackles the many-particle correlations and the kinetic behavior simultaneously.

3. Collision duration time as small parameter

This approach is preferable in the present context, as it clearly distinguishes between the many-body level and the transport level. The theory is then fully renormalized, as it works with dressed GF. It may be objected that the collision duration time is not well defined. It has always been our position that, in fact, the Reconstruction Equations serve to offer an operational definition of the collision duration time in the course of their solution. This definition employs the special feature of the RE (17), namely their off-diagonal integration range. It also reflects the time/spectral structure of the self-energies. This is sketched in an idealized representation in Fig. 1. 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 width of the strip is identified with τ_Q for Σ^R and τ_c for $\Sigma^<$. They 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 non-equilibrium 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.

3.3. Role of Propagators

Up to now, our attention has been concentrated on the density matrix ρ. Now, we analyze in more detail the role of propagators in the whole scheme, thereby addressing the **D 2** problem. As a heuristic introduction, we begin with the Fluctuation-Dissipation Theorem. In equilibrium, it reduces the number of independent Green's function to one:

$$G^<(k,E) = f(E)\{G^A(k,E) - G^R(k,E)\} \tag{20}$$

The statistical factor f is universal, independent of the system. Because $G^A = (G^R)^\dagger$, there remains only one independent GF. We note in passing that this relation served as an heuristic origin of the Kadanoff-Baym Ansatz[1, 4].

Let us compare this with the GKBA (11) out of equilibrium,

$$G^<(t,t') = -G^R(t,t')\rho(t') + \rho(t)G^A(t,t')$$

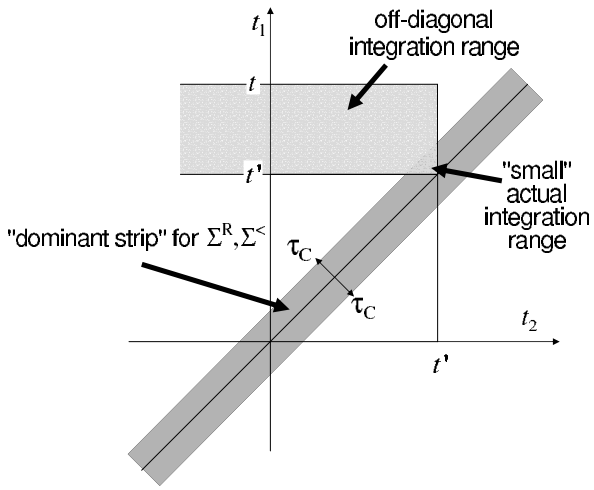

Figure 1. Integration range for the Reconstruction equations (retarded part)

The time representation is necessary; the essential change is that the universal statistical factor is replaced by the actual particle distribution. We may say that the Ansatz, and also the exact RE, reduce the number of independent GF from 2 to "$1\frac{1}{2}$". The transport theory thus rests on two constitutive parts, the one particle distribution and the propagators.

The Kadanoff-Baym transport theory employs the pair of correlation functions, $G^<$ and $G^>$. Which are then the properties of propagators favoring their use in the transport theory? We quote several of them without giving any details. Propagators control quantum coherence and memory in the QTE. Propagators are simpler than the particle correlation function: they

◇ describe propagation of one-particle excitations,
◇ correspond to the generalized spectral density,
◇ are weakly dependent on the particle distribution,
◇ obey Dyson eqs. with a strict causal structure.

Propagators are the proper tool for introducing the quasi-particle picture. General properties of propagators facilitate their modelling without detailed solution of the Dyson equations[4, 5, 33].

GKBA AND THE "SEMI-GROUP PROPERTY" OF PROPAGATORS

There is an old idea that these two concepts are closely related. Semigroup property (*composition rule for propagators*) is exact for free particles, even in an external field U(t):

$$G_0^R(t_1,t_2) = \mathrm{i}G_0^R(t_1,t_3)G_0^R(t_3,t_2) \qquad \boxed{t_1 \geq t_3 \geq t_2} \tag{21}$$

For fully dressed propagators, a vertex correction appears:

$$\begin{aligned} G^R(t_1,t_2) &= \mathrm{i}G^R(t_1,t_3)G^R(t_3,t_2) \qquad \boxed{t_1 \geq t_3 \geq t_2} \\ &\quad + \int_{t_3}^{t_1} \mathrm{d}t_4 \int_{t_2}^{t_3} \mathrm{d}t_5 G^R(t_1,t_4)\Sigma^R(t_4,t_5)G^R(t_5,t_2) \end{aligned} \tag{22}$$

A similar relation holds for G^A. The integration range is off-diagonal again, the time arguments of Σ^R straddling the splitting time t_3.

The last equation can be called the **Corrected** or Dressed **Semi-Group Rule**. Its universal structure is no accident: it follows from the gauge invariance of the 1st kind for the GF (... energy origin arbitrarily varying in time).

The Corrected Semi-Group Rule has a number of important applications. We mention only two, without entering into any details:

1. The Reconstruction Equations (17) can be derived by inserting the Rule (22) into the Dyson Equation (8). Thus, a purely kinematic factorization of the propagator permits to separate the kinematic/spectral features from the statistical ingredients of the correlation function.
2. The simple semi-group property leads to the GKBA (... ignoring the vertex corrections). This can be extended in a phenomenological way to the so-called quasi-particle rule and this again serves for the "derivation" of the Quasi- Particle KBA mentioned in Sec. 2.2. The exact CSG Rule is the source of a systematic generalization of these results.

4. Initial Conditions

We were able to resolve the problems **D 1** and **D 2** of Ansatzes as a basis for developing QTE; it remains to analyze the last problem labeled in Sec. 3 as **D 3**. It concerns the influence of an arbitrary initial state $\mathcal{P}(t_0) = \mathcal{P}_0$ on the NGF defined in (4). There is an extensive literature devoted to this problem [17, 18, 19, 20]; much less can be found about the relationship to the Quantum Transport Equation[19, 20]. Here, we restrict ourselves to quoting the most salient results concerning $G^<$.

The form of the Dyson equation for $G^<$ appears as unchanged. Compare

$$G^< = G^R \Sigma^< G^A \quad \text{for Keldysh limit } t_0 \to \infty \tag{8}$$

$$G^< = G^R \Xi^< G^A \quad \text{for an arbitrary } t_0 \tag{23}$$

There are two hidden differences. The integration limits in (23) extend now from t_0 rather than from $-\infty$. The new self-energy depends on the initial state,

$$\Xi^< = \quad \Xi^<_{t_0}\,[U\,|\mathcal{P}_0], \tag{24}$$

and it reflects the initial conditions by having a number of singular terms:

$$\Xi^< = {}_\circ\Sigma^<_\circ + {}_\circ\Sigma^<_\bullet + {}_\bullet\Sigma^<_\circ + {}_\bullet\Sigma^<_\bullet \tag{25}$$

The black dots denote a continuous time integration variable ranging from t_0 to ∞, the open circles the time variable fixed at t_0. The two "mixed" terms correspond to the quantities Σ^{c} and Σ_{c} of the famous paper[17]. Separating out the δ-factors, we may introduce continuous functions defining $\Xi^<$:

$$\begin{gathered} {}_\circ\Sigma^<_\circ(t,t') = \mathrm{i}\rho(t_0)\delta(t-t_0)\delta(t'-t_0) \\ {}_\bullet\Sigma^<_\circ(t,t') = \Lambda^<_\circ(t,t_0)\delta(t'-t_0), \qquad {}_\circ\Sigma^<_\bullet(t,t') = {}_\circ\Lambda^<(t_0,t')\delta(t-t_0) \end{gathered} \tag{26}$$

The fourth term, ${}_\bullet\Sigma^<_\bullet$, is a continuous function, just like $\Sigma^<$. The dots warn that its form reflects the initial correlations at t_0. The resulting explicit form of (23) is

$$\begin{aligned} G^<(t,t') &= \mathrm{i}G^R(t,t_0)\rho(t_0)G^A(t_0,t') \qquad\qquad t>t_0,\, t'>t_0 \\ &+G^R(t,t_0)\times\int_{t_0}^{t'}\mathrm{d}u\,{}_\circ\Lambda^<(t_0,\,u)G^A(u,t') + \int_{t_0}^{t}\mathrm{d}v G^R(t,v)\,\Lambda^<_\circ(v,\,t_0)\times G^A(t_0,t') \\ &+\int_{t_0}^{t}\mathrm{d}v\int_{t_0}^{t'}\mathrm{d}u\,G^R(t,v)\,{}_\bullet\Sigma^<_\bullet(v,u)G^A(u,t') \end{aligned} \tag{27}$$

If a well defined τ_c exists, the regions, where various parts of the self-energy are essentially non-zero, are sketched in Fig. 2. They all lie in the 1st quadrant $\{t_1 \geq t_0,\, t_2 \geq t_0\}$. The singular components are concentrated to intervals or even a single point. The figure corresponds to the switch-on states, for which ${}_\bullet\Sigma^<_\bullet = \Sigma^< + \widehat{\Sigma}^<$ and $\widehat{\Sigma}^<$ describes the distortion of ${}_\bullet\Sigma^<_\bullet$ around t_0.

4.1. Reconstruction for NGF with General Initial Conditions

So far, we just quoted important results on the NGF level. Now, an attempt will be made to repeat the transformation which has led to the NGF Reconstruction Theorem in Sec. 3.2. The formal analogy between the DE (23) and (8) permits to obtain the analogue to the Dual scheme I immediately:

DUAL SCHEME II

Dyson equation for $G^<$ Eq. (23)	$\Longleftrightarrow$	$\left\{\begin{array}{c}\text{Precursor transport eq. for } \rho, \text{ Eq. (28)}\\ \text{Reconstruction equations for } G^<, \text{ Eq. (29)}\end{array}\right.$

Also the new equations have a similar structure as the old ones. Only a few new terms appear, marked by arrows:

$$\frac{\partial\rho}{\partial t} - \text{drift} = \left[-G^R\Sigma^< + \Sigma^<G^A + \Sigma^RG^< - G^<\Sigma^A - G^R\overset{\uparrow}{\Sigma^{\mathsf{c}}} + \Sigma_{\mathsf{c}}\overset{\uparrow}{G^A}\right]_{\text{equal times}} \tag{28}$$

We show only the retarded part of the Reconstruction Equations.

$$\begin{aligned} G^<(t,t') &= -\,G^R(t,t')\rho(t') \qquad\qquad \boxed{t>t'\geq t_0}\\ &+\int_{t'}^{t}\mathrm{d}\bar{t}\int_{t_0}^{t'}\mathrm{d}\bar{\bar{t}}\,G^R(t,\bar{t})\overset{\uparrow}{\Xi^<}(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t') + \int_{t'}^{t}\mathrm{d}\bar{t}\int_{t_0}^{t'}\mathrm{d}\bar{\bar{t}}\,G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{\bar{t}})G^<(\bar{\bar{t}},t') \end{aligned} \tag{29}$$

Unfortunately, these equations cannot readily be used to start the dual process turning around ρ because of the influence of the initial state, which requires additional formal means going beyond a closed transport theory [20]. It is expected that the initial correlations will die out after the time period of roughly τ_c will have elapsed. In the interpretation given above and summarized in Fig. 2, the modified equation (28) reduces to the standard (10) for $t\gtrsim t_0+\tau_c$. This does not mean that its solution at later times does not depend on the initial correlation. On a scale much larger than τ_c, the early evolution will lead to an effective initial condition different from the simple one-particle $\rho_0=\rho(t_0)$. Something similar can be seen also in the RE (29). Only two of the four components of $\Xi^<$ really enter the integrals, namely ${}_\bullet\Sigma^<_\bullet$ and ${}_\bullet\Sigma^<_\circ$. If $t'-t_0\approx\tau_c$, while t is arbitrary, the integral does not vanish, but its decay time is the comparatively long τ of the propagator.

The situation is different, however, on the Ansatz level of approximation. If all corrections to GKBA are neglected, this also includes the initial correlations. The Ansatz is insensitive to the initial correlations. Combined with the GKBE, it yields a closed transport theory free of the problems with initial correlations. This is more a comment on the Ansatz than on the initial correlations, of course.

4.2. Switch-on states and their restart

The set of all "arbitrary" initial states is too broad and most of the states it includes are unphysical, being overcorrelated, undercorrelated, etc. Is is then justified to restrict the consideration to those initial states, which can be achieved by a physical process. One such class of states of particular interest may be termed the switch-on states. Their definition starts from the Keldysh initial condition: $\diamond$ start the evolution from an equilibrium state $\diamond$ shift their initial time $t_{-\infty}$ back to $-\infty$ $\diamond$ apply an arbitrary external field.

The system evolves in time through a continuous sequence of non-equilibrium states. The NGF for these states can be found by the simple Keldysh or Kadanoff-Baym technique and may be

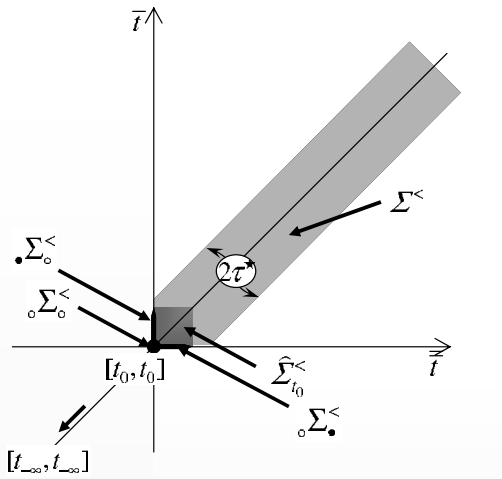

Figure 2. Structure of the self-energy $\Xi^<$

taken as "known". They are exceptional also in that they could be fully reconstructed from the given function $\rho(t)$ alone.

For any time $t_0 > t_{-\infty}$, the state generated in this way may serve as initial for a "restart" of the evolution at this newly selected initial time. Both processes, the original switch-on and the restart, describe the same evolution. This correspondence permits to relate the self-energy of the original switch-on state evolution with the self-energy for the restart evolution singular at the privileged t_0. For propagators, both self-energies coincide and need not be distinguished.

On the contrary, there are important modifications of the switch-on self-energy $\Sigma^<$ to the *less* quantities entering the DE (27). The correspondence relations read

$$ {}_\circ\Lambda^<(t_0,u) = \mathrm{i}\int\limits_{-\infty}^{t_0} \mathrm{d}\bar{t}\,\{G^R(t_0,\bar{t})\Sigma^<(\bar{t},u) + G^<(t_0,\bar{t})\Sigma^A(\bar{t},u)\} \tag{30} $$

and similarly for $\Lambda^<_\circ$. The regular part of the self-energy has two parts: the self-energy for the switch-on state, and the restart transient ($\widehat{\Sigma}^<$ in Fig. 2):

$$ {}_\bullet\Sigma^<_\bullet = \Sigma^<(v,u) + \int\limits_{-\infty}^{t_0} \mathrm{d}\bar{t} \int\limits_{-\infty}^{t_0} \mathrm{d}\bar{\bar{t}}\{\Sigma^R G^R \Sigma^< + \Sigma^R G^< \Sigma^A + \Sigma^< G^A \Sigma^A\} \tag{31} $$

In all these expressions, the self-energies straddle the initial time, in analogy to the mixed GF in [19]. The correlated initial behavior is concentrated just to terms of (27) with ${}_\circ\Lambda^<$, $\Lambda^<_\circ$, and $\widehat{\Sigma}^<$. The remaining terms, containing ρ_0 and $\Sigma^<$, persist also for a non-correlated initial condition.

Now we may return to Fig. 2. The assertion that the strips of non-zero values for the components of $\Xi^<$ are controlled by τ_c are obvious from the equations (30) and (31). Thus, for the restart processes, we have an analytic form for testing and deriving the Bogolyubov conjecture.

These results for the restart processes have bearing to the transport equations on two levels. First, we note that for $t' \to t_0$, the expression (27) reduces precisely to the reconstruction equation (17) (retarded part). This is not surprising, because of the nearly identical underlying physics, based on the Corrected Semi-Group Rule. The main distinction between both is a fixed initial condition for the restart, as contrasted to the floating initial condition for the Ansatz. Interestingly enough, the correction integrals in the reconstruction equations coincide with ${}_\circ\Lambda^<$

and $\Lambda^<_o$ for the restart self-energy. It is seen once more that the Ansatz level is too coarse to include the effect of initial correlations.

The second, more fundamental, link is to the finite time reconstruction equations (29). With the expressions (30), (31), basically results of a partitioning (folding down) technique, the finite time reconstruction becomes possible, based on a correspondingly renormalized perturbation scheme.

5. Conclusion

This paper did not aim at a balanced and exhaustive review of the landscape between the Non-equilibrium Green's Functions and the Quantum Transport Equations. We wanted to convey and motivate our belief that a substantial progress has been achieved in resolving a number of physical questions behind the effort to develop reliable and efficient methods and algorithms for solving the ever more complex and difficult problems of quantum transport.

◇ The Reconstruction Theorem and the related technique offer an exact framework for constructing Quantum Transport Equations.

◇ In fact, this approach is a new reformulation of the NGF method. The QTE problem is simply one aspect of the general approach, which can be cast into a suitable hybrid form.

◇ The single-particle density matrix is identified as a central physical quantity, which is uniquely related to the correlated behavior of the full non-equilibrium many-body system.

◇ The propagators are an important constituent of the theory and they are essential for a proper capturing of the extended quasiparticle behavior and for a systematic approach to the Causal Ansatz family.

◇ An extension of these considerations to finite time correlated initial conditions appears as feasible for the restart processes derived from switch-on states.

◇ The gap between the pure field techniques and the Time Dependent Density Functional Theory seems to be gradually closing.

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