Long and short time quantum dynamics: III. Transients

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Abstract

The quantum transport equations for fast transients have the structure of a Generalized Master Equations for the single-particle distribution, with causal memory terms. Nonequilibrium Green’s functions are reduced to GME if the Generalized Kadanoff–Baym Ansatz is applied. This Ansatz has been used with success both to non-linear transport and to optical transients in semi-conductors; further progress is linked with its extension to a family of the Causal Ansatzes, differing primarily in renormalization of the propagators. For the switch-on non-equilibrium states, generated by a perturbation from equilibrium, the renormalization to the dark dressed Green’s function followed by calculation of the induced self-energies is a productive direction. It also circumvents the problem of correlated initial conditions, far from a general solution otherwise. Such initial conditions appear as incompatible with a Causal Ansatz in general. The presently available formalism permits to study a transient process in the whole time range using the complete NGF, but making a flexible Ansatz-based reduction appropriate to the stage of dynamic evolution.

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1. Introduction

In this paper, the third in a small series ([1], hereafter called Paper I, [2], hereafter called Paper II) we embark on the route leading directly to equations for the quantum distribution of particles. In contrast to Paper II we will not start from the quasi-particle distribution, leaving the possibilities of invoking the quasi-particle concept to a later stage. The first step towards an equation for the one-particle density matrix, or the equivalent Wigner distribution, is the Generalized Kadanoff–Baym Equation (I.74) obtained as the equal-time element of the commutator differential equation for $G^\xi$, called the precursor transport equation (I.44) \{this numbering refers to Eqs. (74),
(44), etc. of Paper I):

\[ \frac{\partial \rho}{\partial t} + i[H_0, \rho(t)] = \text{interaction term}, \]

\[ \frac{\partial \rho}{\partial t} + i[H_0, \rho(t)]_\gamma = \int_{t_0}^{t_1} d\tilde{t} F[\rho(\tilde{t})]. \tag{2} \]

Let us recapitulate the reduction procedure following Section I.8.4. First, the self-energies are expressed as

\[ \Sigma^{R,A} = \Sigma^{R,A}[G^{R,A}, G^\prec], \quad \Sigma^\prec = \Sigma^\prec[G^{R,A}, G^\prec], \tag{3} \]

using a specific physical approximation. Then, the Reconstruction Theorem is applied to express \( G^\prec \) in terms of its time diagonal—that is, of the density matrix \( \rho \)—and propagators. The integral equations serving this purpose are (I.72) and (I.73), reproduced here: one equation for \( G^\prec \) valid in the \( t_1 > t_2 > t_0 \) wedge reads

\[ G^\prec(t_1, t_2) = -G^R(t_1, t_2) \rho(t_2) \]

\[ + \int_{t_2}^{t_1} d\tilde{t} \int_{t_0}^{t_1} d\tilde{t} G^R(t_1, \tilde{t}) \Sigma^\prec(\tilde{t}, \tilde{t}) G^A(\tilde{t}, t_2) \]

\[ + \int_{t_2}^{t_1} d\tilde{t} \int_{t_0}^{t_1} d\tilde{t} G^R(t_1, \tilde{t}) \Sigma^R(t, \tilde{t}) G^\prec(\tilde{t}, t_2). \tag{4} \]

The other equation, for \( t_0 < t_1 < t_2 \), is a conjugate to (4), as \( G^\prec(t_1, t_2) = -[G^\prec(t_2, t_1)]^\dagger \). It starts as

\[ G^\prec(t_1, t_2) = +\rho(t_1) G^A(t_1, t_2) + \cdots \tag{5} \]

All this is introduced into Eq. (1). A “GME” results, so far, however, strictly equivalent with the complete NGF treatment. That would mean an excessively subtle and complex structure of the interaction functional \( F[\rho] \) in Eq. (2).

The underlying exact reconstruction cannot be achieved in practice, and an approximate procedure must be introduced. If we do not consider some recent explorative work attempting to employ the TDDFT [3], the only method in use is one or another factorization Ansatz for \( G^\prec \), the Generalized Kadanoff–Baym Ansatz being a standard choice [4–8]. Quality of these factorizations and of the resulting equations of the GME type will be the main concern of this paper.

The outlined approach involves a transition from NGF to a transport equation. More recently, the tendency has been to directly solve the Dyson equations for the NGF, whether for the high-field transport, or for an optical excitation [9,10]. Special program packages, the NGF solvers, are being developed at several laboratories [11], etc. Details of this development are outside the scope of this paper [12]. On the other hand, there are some important general problems appearing in any approach, and we will introduce two basic issues now.

In a formulation close to the transport equation technique, the particle correlation function \( G^\prec \) is obtained from the Dyson–Keldysh equation, which we quote both in its explicit form, cf. (I.42),

\[ G^\prec(t_1, t_2) = iG^R(t_1, t_0) \rho_{\text{ini}} G^A(t_0, t_2) \]

\[ + \int_{t_0}^{t_1} dt_3 \int_{t_0}^{t_1} dt_4 G^R(t_1, t_3) \Sigma^\prec(t_3, t_4) G^A(t_4, t_2) \tag{6} \]

and in the symbolic one, (I.40),

\[ G^\prec = G^R \varphi^\text{ini} G^A + G^R \Sigma^\prec G^A. \tag{7} \]

Compared with the transport equation problem, the Dyson–Keldysh equation (6) is, on the level of exact treatment, equivalent with the coupled set of
the reconstruction Eqs. (1), (4), and (5). The difference is in the process of finding $G^\prec$: the reconstruction takes place in a cycle between the time diagonal and the rest of $G^\prec$:

$$t_1 = t_2, \quad (1) \nRightarrow t_1 \neq t_2, \quad (4, 5),$$

as discussed around Eq. (I.78) in Paper I. The approximations leading to the GME are made possible precisely by this structure of the theory.

In either form of the Dyson–Keldysh equation ((6) or (7)), we explicitly meet the basic issue of the initial conditions. It is implicit in $(1), (4)$ and $(5)$ as well. Here, they appear very simply, as the initial one-particle distribution:

$$\rho(t_0) = \rho_{\text{init}}.$$  (8)

or

$$\varrho^<_{\text{init}}(1, 2) = i\delta(t_1 - t_0)\delta(t_2 - t_0)\rho_{\text{init}}.$$  (9)

This type of the so-called uncorrelated initial conditions, traditionally used following Keldysh [13] has been discussed in Paper I (Sections I.7.4 and I.8.1), and will be the subject of a more thorough discussion below. Such an initial condition is natural for the GME (2).

An entirely arbitrary initial condition cannot be uniquely characterized by its one-particle reduced characteristics. We encounter then the correlated initial condition for the NGF. There may be singled out three special classes of simple initial conditions: the finite $t_0$ initial condition uncorrelated by assumption (Keldysh IC) as introduced here, the uncorrelated initial condition at $t_0 \to -\infty$ (the Bogolyubov decay of initial correlations), and the switch-on states. The last case is particularly appealing: the initial state at $t_0$ is generated by a perturbation of a “dark” (i.e., no field) state, which was created in a distant past. If this dark state is a state of equilibrium, it can be linked with the Bogolyubov case.

In the rest of the paper we will concentrate on these special initial conditions, although the general case will be characterized at the end of the paper, too. It is always safe to let the initial conditions disappear from sight by the limit $t_0 \to -\infty$.

The other basic feature common to the Dyson–Keldysh equation (6) and the equivalent reconstruction equations (1), (4) and (5) is the appearance of the full propagators $G^{R,A}$ and their self-energies $\Sigma^{R,A}$. It is natural that the propagators have to be known, as they form an inseparable part of the complete NGF matrix $G$. The propagators are defined by the Dyson equations

$$G^R = G_0^R + G_0^R \Sigma^R G^R,$$

$$G^A = G_0^A + G_0^A \Sigma^A G^A.$$  (10)

which visualize their role to link the problem with the non-interacting particles and to incorporate the effective external field as a boundary condition. The propagators can be generated in an entirely separate process but exceptionally (…for a purely elastic scattering). In general, they depend in their turn on the particle distribution through the physical approximation for the retarded and advanced self-energies, as is symbolically shown in Eq. (3). The whole notion of obtaining a GME might appear as hopeless, but fortunately this is not the case.

The propagators have a truly special position in the GME transport equation (2). The r.h.s. interaction integral contains the functional $F_\rho$, which results from replacing $G^\prec$ and $\Sigma^\prec$ in (1) by their “reconstruction” expressions which are based, in the final count, only on $\rho$ and the propagators. Thus, the functional structure of $F$ is built only upon the propagators. All basic physical features of the system, like its memory, quantum coherence, decay of correlations, etc., are determined by the properties of the propagators. One of the crucial point of the analysis made in this paper concerns the options of an approximate determination of the propagators and the proper way of their invoking in the transport problems.

2. GKB Ansatz

In order to construct the complete two-time correlation function $G^{\prec}(t_1, t_2)$ from its time diagonal $\rho(t) = -iG^{\prec}(r, t)$, we view Eq. (4), and its conjugate (5), as giving rise to an iterative scheme. As shown in detail in part I.8 of Paper I, or in Refs. [4,6], the first iteration

$$G^{\prec}(t_1, t_2) = -G^R(t_1, t_2)\rho(t_2) + \rho(t_1)G^A(t_1, t_2)$$  (11)
coincides with the approximate functional $G^\infty[\rho]$ called the Generalized Kadanoff and Baym Ansatz (GKBA). The small parameter of the iteration and of the resulting (asymptotic) expansion is the collision duration time $\tau_c$. This is an effective quantity which can best, although loosely, be defined inside Eqs. (4) and (5) as the time spread of $\Sigma^<$: if the self-energy is appreciably non-zero in a narrow strip (see Fig. 1), iteration of the lowest order GKBA term will nearly preserve its time-local factorization. This is a relative statement, of course. The GKBA is a good approximation in the limit $\tau_c \to 0$; this means that $\tau_c$ is small in comparison with other characteristic times in the system, as, e.g., the quasi-particle lifetime $\tau_e$.

2.1. Properties of the GKBA

Let us begin an analysis of the GKBA by stressing that the underlying iterative procedure cannot be directly linked with a perturbative expansion in terms of the particle–particle interaction. In this sense, the GKBA is non-perturbative, although it may be expected that weak interaction will be favorable for its applicability (cf. Section 6.3 below).

The structure of the GKB Ansatz is such that the time argument of the reduced density matrix $\rho$ is, in both terms, always the smaller of the two time arguments $(t_1, t_2)$ of the correlation function $G^\infty$. In this sense, the reduced density matrix $\rho$ represents a floating initial condition, while the propagators $G^{R,A}$ describe evolution of the system from the initial condition to a later time. The GKB Ansatz automatically keeps also the causal order of the factors $\rho, G^R$ and $G^A$ in conformity with the GKB Equation.

We will not dwell on comparison of the GKBA with the original Kadanoff–Baym Ansatz [14]. For this, we refer the reader to (I.8) and to Paper II. One general feature they have in common: they represent the utmost extension of the Fluctuation Dissipation formula to non-equilibrium. This statement has the following meaning: starting from the reduced information contained in $\rho$ and the propagators, either Ansatz permits to reconstruct an approximation to the whole particle correlation function as their product. There is also a basic difference between them. While the GKBA has the causal structure, in the KB Ansatz the density matrix appears as $\rho(1/2(t_1 + t_2))$ and this violates the causal ordering of times. The origin of this difference can be found in both the physical motivation and the applicability range of the Ansatizes in question. The KBA was devised for quasi-equilibrium situations and has been mostly built upon thermophysical considerations, the GKBA intended for fast processes far from equilibrium is predominantly dynamic and conforming with the dynamical structure of the NGF.

On the whole, the GKBA has a number of further important properties which make it consistent with the general NGF scheme. 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 non-interacting particles, it is exact for excitations arbitrarily far from equilibrium (cf. Section 4.1). Thus, it emerges as an interpolation scheme between two crucial exact limits. As 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 quasi-classical expansion in space, and, in fact, it is not associated with any specific representation for the GF.

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 such approximation a Causal Ansatz. As will be discussed below, a wide family of Causal Ansatzes already exists. The GKB, 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. As the first insight, we will take a glance at the two topics which have been attacked with success by an application of the GKBA: the hot electron transport and the response of electrons in semi-conductors to sub-picosecond pulses.
2.2. GME: Levinson equation

As the simplest example of the use of the GKBA, we may introduce Eq. (11) into the differential GKB equation (1) and derive in this way without effort a closed GME for $r$:

$$
\frac{\partial \rho}{\partial t} + i[H_0, \rho] = -i \int_{t_0}^{t} \mathrm{d}\bar{t}(G^R(t, \bar{t})\Sigma^<(\bar{t}, t) - \Sigma^<(t, \bar{t})G^A(\bar{t}, t))
$$

$$
+ i \int_{t_0}^{t} \mathrm{d}\bar{t}(\Sigma^R(t, \bar{t})\rho(\bar{t})G^A(\bar{t}, t)
$$

$$
+ G^R(t, \bar{t})\rho(\bar{t})\Sigma^A(\bar{t}, t)).
$$

This result 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 [15,16], has originally been derived by the density matrix techniques. Its derivation from the NGF has been the first success of the GKBA [4]. In fact, it re-established the Green functions as a serious contender in the everlasting competition with the more direct density matrix approach [6]. Namely, the GME obtained previously with the help of the KB Ansatz failed to describe correctly even the AC linear response in the weak scattering limit, as it predicted spurious sub-harmonic 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.

2.2.1. Levinson GME and the quantum BE compared

The Levinson GME is analyzed in I.6; it resembles the BE since it has the drift term on the left-hand side and interaction terms 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 quasi-classical limit, and it is not conditional on the quasi-particle 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 quasi-particle 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 r.h.s. integral describes the back scattering of electrons. In Eq. (12), 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, see, however, the discussion in Section 6.2. The second, forward scattering integral, on the other hand, has a sufficiently explicit structure to be compared with the BE.

2.2.2. Comparison continued: long-time dynamics (Paper II)

We want to contrast the two approaches, KBA --- BE linked with the quasiclassical expansion, and GKBA --- Levinson GME suited to describe dynamics beyond the quasiclassical limit. We ask, how the two approaches are related, if both the quasiclassical conditions and the quasi-particle picture may, in fact, be assumed. We make an assessment of that on the forward scattering term of Eq. (12). First, it is easy to verify that in the true Boltzmann limit, the integration can be completed by hand. There result two components. One is basically the commutator $i[\mathrm{Re} \Sigma, \rho]$ which should be transferred to the l.h.s. as the band structure renormalization, the other one yields the particle relaxation time as $\tau \sim 2 |\mathrm{Im} \Sigma|^{-1}$. Thus, this limit is fully recovered. A similar identification is not obvious once the quantum corrections are taken into account. The reason is the difference between the causal structure of the GME and the acausal nature of the quantum BE discussed in the preceding parts of this review series. The physical issues appearing in both approaches are identical (intra-collisional field effects, renormalization constants, off-shell propagation), but their formal representation is slightly different. It is an open conjecture that the two approaches are not entirely equivalent beyond the strict Boltzmann Equation asymptotics. The issue is the transition from short
times after the onset of a transient to the long-time asymptotics. For long times, the Wigner representation using mid-times for the quasi-particle distribution is optimized for the quasi-classical expansion purposes. A general proof is missing that by reconstructing the true distribution $\rho$ also the causal structure of the theory will be recovered. Moreover, an interpolation for the intermediate time region is not known.

2.3. Quantum optical Bloch equations

It would not be an excessive oversimplification to say that the high-field transport and the optical time-resolved spectroscopy, as two important areas treated within the $\text{NGF} \rightarrow \text{Quantum Transport Equation}$ approach, have been developing for a decade along two parallel, but almost independent lines. This is reflected, for example, in the corresponding structure of the basic monograph [6]. The former line of study typically seeks a transport equation for the quasi-particle distribution supplemented by a reconstruction functional for the observable values (the Levinson equation being a notable exception). The latter one, on the opposite, attempts to develop and use an inter-band version of the GME, the so-called Quantum optical Bloch equations.

2.3.1. GKBA and subpicosecond optical transients in semiconductors

Soon after introduction of the GKBA, this Ansatz was used to systematically develop the Quantum optical Bloch equations for semiconductors under the illumination by a short strong optical pulse. The e–e interaction has been treated within the RPA, the electron–phonon interactions to the second-order perturbation. The results obtained were spectacular, and the corpus of the related papers represents the most extensive verification of the wide practical applicability of the GKBA. The early period of this development is summarized in Ref. [6], where all technical details and the basic results are clearly presented. A somewhat more recent, excellent overview can be found in Ref. [7], for recent work, see Refs. [8,12].

Below, we will discuss some serious caveats and limitations concerning the GKBA. It would thus be extremely important to trace down the reasons why there were no serious obstacles hindering the use of the GKBA for treating the time resolved spectroscopy in semiconductors. Without going into details, we may suggest the following list. The many-body interactions were not very strong. The pulses used were not extremely short. The Ansatz was used to simplify the collision integrals in Eq. (1) involving summation over many states in the Brillouin zone. The computed time dependent results often concern global (integral) observables. As will be shown, all these special circumstances are favorable for the GKBA.

2.3.2. Optical transients in semiconductor alloys as a testing ground for GKBA

A parallel stream of papers on optical transients in semiconductors concerned disordered semiconductor alloys [10,17–21]. This case has an importance in itself, but it also extends the scope of the theory because of the presence of random internal potentials which lead to the violation of the $k$-selection rule, etc. The thrust of this work has been rather to develop methods for solving the Dyson equations for the NGF. On the way, however, also the questions of validity, meaning and generalizations of the GKBA have been explored and these results will be used in the following to discuss and document the general analysis of the whole concept of the GKBA.

2.3.3. Physical lesson: importance of the propagators

The implementation of the Quantum optical Bloch equations based on the GKBA for computing photoexcited transients in semiconductors was an immediate success. This success was the more remarkable since the propagators inserted into the interaction integrals were at the beginning taken as very simple time exponentials. The overall structure of the equations possessing the key physical properties listed above was sufficient to guarantee the qualitative consistency and the gross quantitative features of the computed responses [6]. Step by step the initial elation has somewhat receded, and it turned out that, actually, the properly
established propagators are decisive for any more delicate problems and for a detailed agreement with the experimental results. A complete determination of the dressed field-dependent propagators has been out of question, of course, except for the purposes of a direct test [22–24], because that would mean in the truth to more or less solve the complete NGF problem and the Quantum optical Bloch equations would loose their meaning.

A number of crucial requirements on the propagators have been established over the time; as the basic approximation level, the true propagators were replaced by model expressions, typically by the bare, unperturbed ones. The importance of this concept goes beyond the context of the GKBA and we devote to it the next section.

3. Dark state renormalization for the switch-on states

As pointed out already in the Introduction, presently our primary concern are transients, that is the switch-on states. Throughout the initial interval \((t_0 \rightarrow -\infty, t_U)\), the system remains in the equilibrium state. The equilibrium “dark” NGF triplet \(G^R_D, G^<_D, G^A_D\) (a single correlation function, in fact, because of the propagator conjugation and the Fluctuation–Dissipation Theorem for \(G^D_D\)) can be studied by equilibrium techniques much easier than the true NGF and can be found and stored beforehand. Then, at an instant \(t_U\), the external disturbance \(U\) hits the system. The GF are changed to \(G^R, G^<, G^A\). Causality demands that no observable change occurs prior to \(t_U\), the limitations on the quantum subdynamics are less strict, however. They are conveniently formulated in terms of correlation times, which in turn are made quantitative as the effective widths of the self-energies with respect to the internal time \(t = t_1 - t_2\). There are two of them, the chaotization time \(\tau_c\) for \(\Sigma^<\) and the quasi-particle formation time \(\tau_Q\) for \(\Sigma^{RA}A\). They may vary with the Wigner time \(\frac{1}{2}(t_1 + t_2)\) along the diagonal, but before and around \(t_U\), they assume the dark values, see Fig. 1. A time \(\tau^* = O(\max[\tau_c, \tau_Q])\) can then be defined such that all three self-energies can only differ from their dark counterparts, if both times are larger than \(t_{\text{init}} = t_U - \tau^*\), slightly preceding \(t_U\), that is, in the (++) quadrant with respect to \(t_{\text{init}}\).

We split the self-energies into their dark and induced parts:

\[
\Sigma^{RA} = \Sigma^{RA}_D + \Sigma^{RA}_I, \quad \Sigma^< = \Sigma^<_D + \Sigma^<_I.
\]

(13)

The induced parts are zero everywhere except in the (++) quadrant. We will employ this property and demonstrate that closed effective Dyson equations can be written for the full NGF matrix while keeping all time variables, external and internal alike, in the (++) quadrant.

3.1. Dark renormalization for the propagators

For propagators, their rearrangement is straightforward. Using the Dyson equation in the form
The overbrace unperturbed GF is labeled by $Q$ for quasi-particles, namely dark polarons excited and reshuffled by the effective external field as whole rigid entities. In the second rearrangement, the unperturbed GF corresponds to the dark polarons alone, while the quantity $W_{1}^{RA}$ includes the external field, the related instantaneous contribution to the mean field and the induced part of the self-energy. It is nothing but the induced part of the optical potential of the electrons. We will use this ‘underbraced’ form in the next sub-section.

### 3.2. Dark renormalization for the particle function

The Dyson–Keldysh equation (7) for the particle correlation function of a switch-on state is written simply with $t_{0} \to \infty$ initial condition as

$$G^{<} = G^{R} \Sigma^{<} G^{A}. \quad (16)$$

It only involves fully dressed quantities. For the dark state, we have

$$G_{D}^{<} = G_{D}^{R} \Sigma^{<}_{D} G_{D}^{A}. \quad (17)$$

In the first equation (16), we split the self-energy according to Eq. (13) and use the Dyson equations for both propagators in the second form of Eq. (15). The equation can be transformed to

$$G^{<} = G_{D}^{<} + G^{R} \Sigma^{<}_{D} G^{A}$$

$$+ G^{R} W_{1}^{R} G_{D}^{<} + G_{0}^{R} W_{1}^{A} G^{A}$$

$$+ G^{R} W_{1}^{R} G_{D}^{<} W_{1}^{A} G^{A}. \quad (18)$$

On the first line, there appear two basic ingredients: the dark correlation function and the ‘Bethe-Salpeter’ term involving the vertex renormalization. The rest of the equation are terms gradually dressing one terminal propagator of $G_{D}^{<}$, the other one, and both, cf. (17).

All internal times in the last equation are clearly larger than $t_{\text{init}}$, because one of the factors is always an induced optical potential. If the external times are also taken from the interval $(t_{\text{init}}, \infty)$, we obtain a closed equation involving only double-time quantities with times lying in the $(++)$ quadrant of the time plane in Fig. 1.

The renormalized Dyson equation (18) thus resolves the problem of arbitrarily correlated

\[ t_2 \]
\[ t_U \]
\[ t_{\text{init}} \]
\[ t_0 \sim - \infty \]
\[ t_{\text{init}} \]
\[ t_U \]
\[ \rightarrow t_1 \]
initial conditions for the switch-on states. These initial conditions are absorbed in the dark correlation function. As said already, the dark GF can be analyzed and obtained in advance by equilibrium techniques. In other words, in the non-equilibrium context, they play the role of known input quantities. This is an important exact result, which is also essential for the construction of transport equations for transients.

4. Meaning of the GKB Ansatz

In this section the GKBA will be approached from a different angle, following Ref. [18]. In this approach, its predominantly dynamic nature is stressed and linked with the so-called semi-group character of the single-particle propagation.

4.1. Non-interacting particles

To this end, we will first consider independent particles for which the following equation is valid:

$$G^<(t_1, t_2) = i G^R(t_1, t_0) \rho(t_0) G^A(t_0, t_2).$$

(19)

Here, $G^R$ describes a unitary evolution which, for times $t_1 > t_2 > t_0$, obeys the multiplication rule ("semi-group property")

$$G^R(t_1, t_0) = i G^R(t_1, t_2) G^R(t_2, t_0).$$

(20)

Using this semi-group property in Eq. (19) we obtain for $t_1 > t_2 > t_0$

$$G^<(t_1, t_2) = - G^R(t_1, t_2) G^R(t_2, t_0) \rho(t_0) G^A(t_0, t_2)$$

$$= - G^R(t_1, t_2) \rho(t_2),$$

(21)

which is just the retarded half of the GKB Ansatz. For the converse order of times, the advanced part of the GKBA is obtained. The GKB Ansatz appears here as an exact identity based on the semi-group property of free particle propagators.

4.2. Interacting particles

In the case of interacting particles we follow the heuristic argument of Ref. [18] and start from the GKB transport (6):

$$G^<(t_1, t_2) = i G^R(t_1, t_0) \rho(t_0) G^A(t_0, t_2)$$

$$+ \int_{t_0}^{t_1} dt_3 \int_{t_0}^{t_2} dt_4 G^R(t_1, t_3) \Sigma^<(t_3, t_4) G^A(t_4, t_2).$$

(6)

Let again $t_1 > t_2 > t_0$. The formal integration region shown in Fig. 2 is a rectangle with corners at $t_0, t_1, t_2$. This figure extends the times shown in Fig. 1 to times much beyond $t_{\text{init}}$ merging now with $t_0$: $t_{1,2} - t_0 \gg \tau_c$. It will be assumed that the actual integration involves only a strip of the width $2 \tau_c$.
along the time diagonal \( t_1 = t_2 \), where the self-energy \( \Sigma^< \) is significantly different from zero. If
the “small” area \( C \) is neglected, the integral extends only over the square \( t_1 < t_2, t_4 < t_2 \).

Due to collisions, the semi-group condition (20) for the propagators cannot be valid exactly. Let
us, nevertheless, assume its approximate validity. Then Eq. (6) is reduced to the form of the GKB
Ansatz
\[
G^<(t_1, t_2) = -G^R(t_1, t_2) \rho(t_2), \quad t_1 > t_2, \tag{22}
\]
where
\[
\rho(t_2) = -iG^<(t_2, t_2) = G^R(t_2, t_0) \rho(t_0) G^A(t_0, t_2)
- i \int_0^{t_2} dt_3 \int_0^{t_2} dt_4 G^R(t_2, t_3) \times \Sigma^<(t_3, t_4) G^A(t_4, t_2) \tag{23}
\]
in agreement with (6).

In deriving the Generalized Kadanoff–Baym Ansatz, three assumptions were invoked. Two
have a general character: an uncorrelated initial condition, and a uniformly small particle correlation

time. The third one, the semi-group rule, is specific for this argument. The conclusion is that,
instead of checking directly the Ansatz for \( G^< \), it is possible to study the multiplicative semi-group
rule for the propagators \( G^{RA} \).

### 4.3 Quasi-particle GKB Ansatz

We have seen the link between the GKB Ansatz 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.

#### 4.3.1 Quasi-particle multiplication rule for \( G^R \)

Consider first an equilibrium quasi-particle. The propagator \( G^R(t_1, t_2) \) is characterized by three
quantities: the pole energy \( E_W = E - i\tau_{\text{r}}^{-1} \), the renormalization constant \( z \) and the time of
formation \( \tau_0 \), which corresponds to the time spread of the kernel of the retarded self-energy
\( \Sigma^R \), just like \( \tau_{\text{r}} \) is related to \( \Sigma^< \). In order to achieve the correct hierarchy of the characteristic times,
the so-called quasi-particle condition, \( \tau_0 \ll \tau_{\text{r}} \), is required according to Section 1.3 of Paper I. Here,
\( \tau_{\text{r}} \) is the transport relaxation time which is comparable with the quasi-particle life-time \( \tau \).

Then
\[
G^R(t_1, t_2) = \begin{cases} 
\text{QP formation process} & t_1 < t_2 + \tau_0, \\
G^R_w(t_1, t_2) & t_1 > t_2 + \tau_0,
\end{cases}
\]
with \( G^R_w \) the Weisskopf–Wigner propagator. This propagator obeys, as a defining property, the exact
multiplication rule
\[
G^R_w(t_1, t_2) = i G^R_w(t_1, \tilde{t}) G^R_w(\tilde{t}, t_2). \tag{25}
\]

For the following hierarchy of times,
\[
t_1 \gg \tilde{t} \gg t_2 + \tau_0 \gg t_0, \tag{26}
\]
the modified multiplication rule for \( G^R \) is obvious:
\[
G^R(t_1, t_2) = i G^R_w(t_1, \tilde{t}) G^R(\tilde{t}, t_2). \tag{27}
\]

In contrast, the original semigroup factorization (20) is not satisfactory: at \( t_1 = \tilde{t} \), a spurious kink
appears because of a repeated quasi-particle formation \([18,20,10]\). For times \( t_1 > \tilde{t} + \tau_0 \), the
factorized expression has the value \( z^2 G^R_w(t_1, t_2) \) rather than the correct one as given in Eq. (24).

The rule now may be generalized to non-equilibrium by postulating that, to the true propagator
\( G^R \), a time of formation \( \tau_0 \) and a construct called \( G^R_w(t_1, t_2) \) characterized in Eq. (25) exists
such that for times satisfying (26) the modified composition rule (27) holds. The conditions for
validity of this rule, presently just postulated, will be discussed later.

#### 4.3.2 Quasi-particle Ansatz for \( G^< \)

On the way to the new Ansatz we continue as above in Section 4.2. We start from the exact
relation (6) and substitute everywhere \( G^R \) by its factorized form. Only now we use Eq. (27) instead
of Eq. (20). Integration regions are again sketched in Fig. 2. The newly invoked feature is the dashed
horizontal line at \( t_1 = t_2 - \tau_0 \). Below this line, the rule (27) is exact. The quasi-diagonal 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 Eq. (27). Ignoring this, we obtain

\[
G^<(t_1, t_2) = -G^R_W(t_1, t_2)\rho(t_2), \quad t_1 > t_2,
\]

where \( \rho \) is given by the exact expression (23), just as before.

4.4. Generalizations

Clearly, neither the GKBA (22), nor the QKBA (28) have been proven, but firstly, both have been linked with the related multiplication rule for propagators. Secondly, 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 quasi-particle behavior of the system can be assumed. Thirdly, the two Ansatzes appear as two instances of a general factorization \( G^c = G^R \rho \) with the subscript \( \bullet \) 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 in Section 2. This sheds a new light on the empirically introduced modified ansatz-type decouplings discussed in Section 2.3.3: they are specific instances of a Causal Ansatz. 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.

5. Short-time dynamics and initial condition

It is natural to expect that a transport theory based on an evolution GME-like equation for the density matrix, such as Eq. (12) or Eq. (32) will be associated with an initial condition at an initial time \( t_0 \) of the form

\[
\rho(t_0) = \rho\text{\textsubscript{init}} \quad \text{(prescribed)}.
\]

The initial condition may be very important at early times of the non-equilibrium evolution of the system. In the simplest case, \( \rho\text{\textsubscript{init}} \) will be the equilibrium state before the start of a transient process, but in general, an arbitrary non-equilibrium situation may come into play.

In line with this simple reasoning, we have limited ourselves to the case that also the initial condition for the NGF is specified by \( \rho\text{\textsubscript{init}} \) and have written the particle correlation function \( G^c \) as Eq. (6). This is the original formulation associated with the work of Keldysh [13,6]. In the early formulation of the NGF formalism by Keldysh, and Kadanoff and Baym [14], the question of the initial condition was resolved by letting \( t_0 \rightarrow -\infty \) in conjunction with the assumption of decay of the initial correlations. That was fully justified, if the interest was paid to the long-time transport behavior. With the attention turning to the short-time quantum dynamics, the necessity of completing the NGF formalism by a proper treatment of the so-called correlated initial condition. It should be stressed that this problem is not limited to the theory, but has a direct bearing on the growing area of various short-time experimental techniques.

The classical work on correlated initial conditions is given in papers by Fujita [28], Hall [29], Danielewicz [30], Kukharenko and Tikhodeev [31] and Wagner [32]. They tried to reformulate the NGF perturbation scheme using a modified time contour to include the initial condition. In particular, Wagner and Danielewicz considered the Wick theorem extended to the situation when the initial condition is included. In last years there are several new papers on this theme [33–37] (see also Refs. [38–40]), but we are still far from solving the problem of the initial condition satisfactorily. Two qualitative points have to be quoted in connection with the present discussion of the Ansatzes. First, the Ref. [33] introduces an important notion of mutual consistence between the initial condition and the physical approximation for the self-energy. Second, in Ref. [34], the authors discuss the relationship between the correlated initial condition and the GKBA.

Most of these questions fall, in fact, outside the scope of this study. We will confine ourselves to a few comments. First, we write down the general form of \( G^c \) with the correlated initial condition...
included [30,34]:

\[
G^< (t_1, t_2) = iG^R(t_1, t_0)\rho(t_0)G^A(t_0, t_2) \\
+ G^R(t_1, t_0) \int_{t_0}^{t_2} dt_4 A^<_\text{left}(t_0, t_4)G^A(t_4, t_2) \\
+ \int_{t_0}^{t_1} dt_3 G^R(t_1, t_3)A^<_\text{right}(t_3, t_0)G^A(t_0, t_2) \\
+ \int_{t_0}^{t_1} dt_3 \int_{t_0}^{t_2} dt_4 G^R(t_1, t_3)\Sigma^< (t_3, t_4)G^A(t_4, t_2).
\]

(30)

In comparison with Eq. (6), two additional terms including the functions \(A\) appear. They are “semi-singular” with one of the time arguments fixed at \(t_0\). The initial correlations are contained just in these “less” quantities. Not so conspicuous, but important is the appearance of the self-energy \(\Sigma^<\) built directly for the restricted time region \([t_0, \infty) \otimes [t_0, \infty)\), rather than a simple clipping of the \((++)\) quadrant, even if a full \(\Sigma^<\) existed in the whole time plane.

It might appear that there would be no big change in attempting to derive the GKBA from Eq. (30) rather than from Eq. (6). However, we would need an additional Ansatz for the \(A\)s, as stressed in Ref. [34]. An extended formalism would be necessary, based on additional physical assumptions.

In the second comment, we amplify on the preceding one and return to the fact that a true GME is consistent with the simple “uncorrelated” initial condition (29). We would like to formulate the conjecture that validity of the GKBA excludes the possibility of correlated initial conditions, in other words that the Ansatz will turn the additional \(A\) functions to zero. Such is certainly the case of electrons in a random medium considered in Section 6, as may easily be demonstrated, see Section 6.4.

The last comment refers to Section 3.2, where we have derived an expression (18) for \(G^<\) in the \((++)\) quadrant, in which all initial correlations at a time before the start of a non-equilibrium process were condensed in the dark component \(G^<_{\text{D}}\). As a simple application linking this result with the initial conditions in general, let us assume an uncorrelated case by writing the dark particle function as

\[
G_D^< = G_D^R \rho^<_{\text{init}} G_D^A + G_D^R \Sigma^<_{\text{D}} G_D^A.
\]

The \(A\)’s of Eq. (30) thus should vanish, and we use basically Eq. (7) for the dark state, being just more careful about distinguishing between the self-energies relevant to the time intervals \((-\infty, +\infty)\) and \((t_{\text{init}}, +\infty)\). Introducing this into (18), we get

\[
G^< = G^R \rho^<_{\text{init}} G^A + G^R \left(\Sigma^<_{\text{D}} + \Sigma^<\right) G^A.
\]

The uncorrelated initial condition is transferred from the dark GF on the full NGF.

6. Electron dynamics in disordered alloys

This section is concerned with electrons in disordered alloys. As mentioned in Section 2.3.2, the alloy case provides an ideal opportunity to discuss and document our general analysis of the whole concept of the GKBA. Selected references are listed there, too. We have to introduce a few concepts and symbols peculiar to the disordered systems. No background knowledge will be needed, but it can be found, for example in Ref. [41].

For simplicity, we assume no interactions, so that in a given disordered sample, called configuration, the propagator \(G^\varepsilon_C\) corresponds to independent particles moving in a prescribed static random potential \(V_C\) (the label ‘\(C\)’ denotes random—configuration dependent—quantities), and similarly for \(G^\varepsilon\) and \(\rho_C\). Instead of working with a given configuration, a configuration average \(\langle \ldots \rangle_C\) is introduced. For example, the condition \(\langle V_C \rangle_C = 0\) means that the potential fluctuates around its mean value. These fluctuations play the role of “frozen” quantum fields and the averaged GF have to be treated by means of the field theory. Thus, with the averages \(G^\varepsilon = \langle G^\varepsilon_C \rangle_C,\ G^\varepsilon^\varepsilon = \langle G^\varepsilon_C \rangle_C\) genuine self-energies \(\Sigma^\varepsilon, \Sigma^\varepsilon^\varepsilon\) are associated. In the self-consistent Born approximation, the self-energies are given by

\[
\Sigma^\varepsilon = \langle V_C G^\varepsilon V_C \rangle_C.
\]
This is the lowest order non-trivial conserving approximation. For one configuration, we are dealing with independent electrons, so that $G^R_C$, $G^<_C$ and $\rho_C$ satisfy the general factorization rules (20), (21). A configuration average of these identities leads to doubts about the semigroup property and the GKBA for the averaged GF:

$$G^R = i(G^R_C G^R_C/C) = i(G^R_C) = iG^R G^R,$$

$$G^< = -(G^<_C \rho_C/C) = -(G^<_C) = -G^R \rho$$

because the random factors originate from the same disordered environment and are statistically correlated. For calculating the corresponding vertex corrections, systematic procedures, specific for disorder, are available.

6.1. Propagators [18,20,10]

The specific situation considered is a two band semiconductor model illuminated by a light pulse. Even without illumination the electron and hole propagators are affected by the disorder (an instance of the “dark polarons” of Section 3.1). For a typical moderate disorder it was verified [10] that in the dark the quasi-particle notion works well. The time of formation $\tau_{Q_{\text{dark}}}$ was shown to be rather short and dependent on the excitation energy with respect to the band edge ... an explicit manifestation of the Landau–Peierls criterion, see [42] and Section I.3 of Paper I.

A steady intense illumination leads to the so-called light induced band hybridization [17]. Well-defined quasi-particles incorporating both this band mixing due to the light and the disorder related band smearing can be defined [18]. The two agents act in a coherent fashion. As a result, the time of formation is influenced by the presence of the hybridization gap. Around the gap, the semigroup rule (20) is violated, while the quasi-particle rule (27) works well.

A direct numerical study of propagators in the presence of light pulses is made easy for disorder, as in this case, the propagators do not depend on the particle distribution and can be found independently of $G^<$. Their analysis [20,10] corroborates the results for a steady illumination and leads to the following picture: there is a pronounced anisotropy of the quasi-particle behavior in the Brillouin zone. Far from the resonance, the quasi-particle picture is reasonably precise. For regions close to the resonance, where a transient hybridization gap affects the behavior of the carriers, the quasi-particle factorization works reasonably well at times outside of the core of the pulse. For times overlapped by the pulse, the outcome depends on its intensity. For strong fast pulses, the quasi-particle picture fails and the direct full quantum treatment becomes unavoidable. As a criterion of adiabaticity of the pulse guaranteeing the quasi-particle regime, the simple rule that the relative change of the external field over the time of formation should be small, was formulated in Ref. [19].

If the full field-dependent self-energy is split according to the definition (13) repeated here:

$$\Sigma^R = \Sigma^R_{\text{dark}} + \Sigma^R_{\text{induced}},$$

it turns out that the two parts behave in a very different manner [10]. The dark component, as said already, is almost local in time and gives rise to a nearly perfect Weisskopf–Wigner quasi-particle behavior. The induced component will typically be weaker, but it is always spread over the pulse duration leading to the coherence effects mentioned. It appears as convenient to use the dark quasi-particles as a reference system and incorporate the light-induced effect as their rearrangement [10], as in the upper line of Eq. (15). This renormalization is the point of departure for calculating $\Sigma^R_{\text{induced}}$.

6.2. Particle correlation function, density matrix

In Ref. [10], the main result was a direct solution of the Dyson equations for electrons in the alloy under the action of the light pulse. In the self-consistent Born approximation (31), all components of double time quantities $\Sigma^R, A, <, G^R, A, <(k)$ and of a single time observable $\rho(k)$ were obtained. This opened up the path to a direct numerical test
of the GKBA. The test was based on the solution of the “precursor” equation (1) for \( \rho \) in two ways. First, the scattering integrals on the r.h.s. were taken as a given input, with the values of the self-energies and Green’s functions as obtained from the direct solution. This was really just a check on the integration procedure. The values of \( \rho(k) \) were faithfully reproduced. In the second step, the r.h.s. was converted to a true GME using the GKBA, very much like in the case of the Levinson equation (12). Only now the Ansatz was inserted into the explicit SCBA expressions for \( \Sigma \)'s and the reduction of the back scattering integrals was completed:

\[
\frac{\partial \rho}{\partial t} + i[H_0, \rho]_-
= -i \int_{-\infty}^t d\bar{t} \left( G^R \rho G^A + V_C G^R \rho V_C G^A \right)_C
+ i \int_{-\infty}^t d\bar{t} \left( V_C G^R \rho G^A + G^R V_C G^A \right)_C
+ [G^R(t, \bar{t}) \mapsto G^R, \, \rho(\bar{t}) \mapsto \rho, \, G^A(t, \bar{t}) \mapsto G^A].
\]

(32)

The propagators were known, and the equation was solved for \( \rho \). For the \( k \)-points near the resonance, the solutions exhibited marked quantitative deviations from exact results. For the \( k \)-integrated photoexcitation \( \text{Tr}_k \rho \), the overall agreement was much better. The time profile of all components of the full band-to-band excitation had the same general character for both solutions and their difference was on the order of 10\%.

Before the onset of the pulse, both the exact and the GKBA solutions were nearly identical, then they started deviating from each other. The difference saturated to maximum and kept constant after the pulse. These results support our general observations. Firstly, the Ansatz fails during the pulse because of the violation of the quasi-particle representation caused by \( \Sigma^R_{\text{induced}} \), cf. Eq. (13). Secondly, as already speculated is Section 2.3.1, the Ansatz works better for total, \( k \)-integrated quantities.

An important requirement concerning any transport equation is the particle number conservation. Quite generally, this is equivalent with the condition \( \text{Tr}(\text{r.h.s. of (1)}) = 0 \). It can be shown that the Self-Consistent Born Approximation (31) is conserving the particle number [10]. Presently, it is important to note that this conserving property is not lost by the additional GKBA approximation, as is apparent from the GME (32).

Similar tests have not been performed for QKBA, the quasi-particle Ansatz modification (28). However, this Ansatz was checked by explicitly constructing the exact and approximate \( \Sigma^R \) for a model with a sharp step-like onset of a strong constant illumination. Differences between the two sets of data were indiscernible [18].

6.3. GKBA vs. Born approximation

Here, we return to the key remark made in Section 2, with reference to part I.8 of Paper I, or to Refs. [4,6], namely that the GKBA is logically independent of the strength of the particle interactions. This was made explicit in deriving the optical Bloch equation for alloys, Eq. (32) in two steps: first the Born approximation for the random interactions, then the GKBA. In the literature, however, often an alternative opinion has been expressed, considering the factorization of propagators and of the density matrix a part of the perturbative expansion of the reduced Liouville equation of motion for the density matrix. While these views have their justification, there are reasons to distinguish between the two small parameters: the interaction strength on the one hand, the short formation times on the other hand.

Returning to the alloy case once more, the Liouville equation for one configuration reads

\[
\frac{\partial \rho_C}{\partial t} + i[H_0, \rho_C]_- = -i[V_C, \rho_C].
\]

Taking \( V_C \) as the perturbation and starting from \( \rho_C \approx \rho \), we get, in the lowest non-vanishing approximation,

\[
\frac{\partial \rho}{\partial t} + i[H_0, \rho]_-
= -i \int_{-\infty}^t d\bar{t} \left( G^R \rho G^A + V_C G^R \rho V_C G^A \right)_C
+ i \int_{-\infty}^t d\bar{t} \left( V_C G^R \rho G^A + G^R V_C G^A \right)_C,
\]

as the perturbation and starting from
an equation almost identical with Eq. (32), but
with all propagators in the scattering integral
replaced by their non-self-consistent counterparts.
This result is “typical”, that is, a similar
outcome is obtained also for the electron–phonon
interactions and for the single-particle channel of
the RPA for electron–electron interactions. This
agreement is not surprising, considering the
similarity of the corresponding lowest order Feyn-
man diagrams of the general form

\[ \text{Importantly more recent developments in the}
\text{density matrix method admittedly lead to im-
proved perturbation expansions and to renor-
malized transport equations. Still, we believe}
\text{that the NGF/Ansatz methodology follows in a}
\text{natural and ideally straightforward manner}
\text{the basic physical line of capturing the hierar-
chy of characteristic times in non-equilibrium}
\text{processes.}

6.4. Proof of the Conjecture of Section 5 in the case
of disordered alloys

Finally, we return to the Conjecture that validity
of the GKBA excludes the possibility of correlated
initial conditions, as formulated at the end of
Section 5. For one configuration, we have Eq. (19).
Using Eq. (29) and writing

\[ G_C^A = G + \rho_\text{reg} (G_C^A - G^A), \]
\[ G_C^A = G^A + \rho_\text{reg} (G_C^A - G^A), \]
\[ G_C^A = G^A(t_1, t_0), G_C^A = G^A(t_0, t_2), \]

e. we split \( G^< \) into four terms:

\[ \begin{align*}
-i G^< & = (G_C^R \rho_\text{reg} G_C^A)_C \\
& = G^R \rho_0 G^A + G^R (\rho_0 G_C^A - G^A)_C \\
& + (G_C^R - G^R) \rho_0 G_C^A G^A \\
& + (G_C^R - G^R) \rho_0 (G_C^A - G^A)_C.
\end{align*} \] (33)

These four contributions correspond one by one to
the four terms of Eq. (30), and could be identified
in detail using Dyson equations for both propa-
gators, yielding formal, but explicit expressions for
both \( A \) functions. This may be skipped here. Our
assertion is proved easily as follows. Take the first
term on the second line:

\[ \begin{align*}
\langle \rho_0 [G_C^A - G^A] \rangle_C & = \langle \rho_0 G_C^A - \rho_0 G^A \rangle_
\text{GKBA} \\
& \Rightarrow \rho_0 G^A - \rho_0 G^A = 0 \\
& \Rightarrow A^< = 0, \quad q.e.d
\end{align*} \] (34)

and similarly for the second term.

7. Summary of results and open questions

There are two essential, not mutually unrelated,
notions governing the area of non-equilibrium
transients in quantum systems, the time hierarchy
in the non-equilibrium processes, and the role of
quantum coherence which have precedence over
any specific approximation scheme and are com-
mon to all approaches to the problem of quantum
transport equations. We hope to have shown that
the NGF/Causal Ansatz methodology yields the
most direct materialization of the concept of the
hierarchy of characteristic times, while providing
ample space for a proper self-consistent treatment
of the internal coherence phenomena. This is not
to dismiss the alternative of direct density matrix
techniques; the book [7] by Bonitz offers both
alternatives in parallel, and in the paper series [43],
the authors earnestly try to reconcile the two
languages and obtain a synthetic picture.

7.1. Status of the Causal Ansatz approach

The GKBA itself and its clones provide a
systematic and, to certain degree, controlled
transition from the NGF dynamics to a simplified
GME like description of the system evolution.
This has two advantages. Primarily, the GMEs are
much easier to solve by numerical means. On top,
however, the GMEs provide a language of the
transport equations important for interpreting the
internal processes and the observable results in
relationship to experiment. They also form a
bridge between NGF and the density matrix
methods. There are, thus, enough reasons not to
dismiss the Ansatz approach even in the present
times of enthusiasm about the direct NGF
approach.
7.2. Limits of the Causal Ansatz approach

A Causal Ansatz, literally taken, is suitable for processes which may bring the system far from equilibrium, but should, at the same time, be properly “moderate”. This broad requirement includes, as we have seen, two main conditions. On the one hand, the initial state, to which the system will have been prepared at the start of the process, has to be uncorrelated, that is, specified by the initial distribution \( \rho(t_0) \) alone. On the other hand, the two formation times \( \tau_Q, \tau_c \) should be very short in comparison with all other characteristic times. This implies firstly that the characteristic times of the external fields cannot be very short, secondly that a (non-stationary) quasi-particle picture, expressed by the quasi-particle multiplication rule, has to be a good approximation. Coherence effects beyond the quasi-particle behavior and persisting over long periods of time will, consequently, not be properly described. This does not concern the coherent quasi-particle propagation, off-shell processes and time-energy uncertainty considerations: all these physical ingredients are correctly captured by the GKBA or a GKB-like Ansatz.

7.3. Choice of the Ansatz

Last, but not least, the question of selecting a suitable Ansatz should be touched upon. It should be of the form \( G^A = \rho G^R + G^0 \rho \), as discussed in Section 4.3.2. There is a choice, in the first place, from two formally motivated Ansatzes, the GKBA and the QKBA employing the \( G^R, G^0 \) propagators, respectively. In addition, several model choices, including the free propagator \( G^R \), the RPA propagator, and the dark polaron propagator, were tested in practice, sometimes as they stood, sometimes augmented by an adjustable damping parameter. These models should be understood as model simplifications of the QKBA. The reported results were good to excellent; as pointed out above, if it comes to observables of an integral character, the Ansatz is bound to be at least semi-quantitative. These encouraging results have, of course, their back side: certain insensitivity of the results to the detailed form of the Ansatz.

7.4. Towards the future

The NGF/Causal Ansatz technique employs as the primary step the factorization reflecting the characteristic time hierarchy in non-equilibrium processes. Only in the second step, a specific physical approximation (based on a decoupling, or a perturbation method) is implemented.

The advantages of the full NGF \( \rightarrow \) GME procedure are then twofold: it provides a natural framework for physically consistent, systematically built approximations, and a natural extension of the technique to advanced approximations, like the CPA for disorder, \( T \)-matrix for e–e interactions, vertex corrections (recoils, ...) for phonons, etc.

There is no unique form of the “Ansatz” factorization; in fact, at our disposal, there are at least two methods of developing improved Ansatzes. One, strictly formal, is based on the exact integral equations of I.8.3, repeated in the Introduction. The other one, introduced in Section 4, has a more heuristic character. It is important that both methods are open, that is, the boundary between an already existing Ansatz and the underlying NGF basis remains and is fluid, subject to shifts. This is particularly well suited for the difficult tasks combining widely differing time domains. To each of the domains, another basic approximation may be appropriate, and it is essential to join these disjunct formalisms into one more complex procedure without apparent seams.

This relates, first of all, to more subtle manifestations of quantum coherence in the short time dynamics matched to the intermediate time interval, when the short time evolution undergoes the transition to the long time quantum transport. Clearly, an intermediate theory improving the plain GKBA like factorization differently in both time domains, but not invoking the full NGF internal quantum sub-dynamics would be the immediate goal, but so far has not been developed. It is easier to visualize a theory working directly with the NGF, but being dynamically reduced by
an appropriate Causal Ansatz in dependence on the time range involved.

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