Correlated initial condition for an embedded process by time partitioning

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Study of transients in the electron quantum transport by nonequilibrium Green's function often requires an explicit inclusion of correlations at a finite initial time. For processes embedded in a host process, a universal treatment of the correlated initial conditions based on the formalism of partitioning in time allows to express their self-energy including the "irregular" correlation part in terms of the known properties of the host process. This unified formalism also yields the renormalized semigroup property for propagators and the reconstruction equations for the particle correlation function. The Bogolyubov principle of the decay of correlations then permits to buildup a theory of quantum transport equations with finite-time initial conditions.

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I. INTRODUCTION

This paper is devoted to closely related topics in the nonequilibrium Green's function (NGF) theory[1–8] of nonequilibrium quantum dynamics, all stemming from the task of describing the short time transient processes in quantum transport. The first question addressed here concerns the influence of the many-body initial state on the NGF.[9–16] This problem has been present in the NGF theory from the outset and we outline the history of its resolution below. Our contribution to these efforts is to employ the notion that a physically admissible initial state is an outcome of previous history (preparation), and from this to find its role for the future evolution.

Such description of a process with prescribed initial conditions (ICs) at a finite time appears as a specific instance of a general question, the second one posed in this paper: how to formalize the notion of the past and the future with respect to a selected instant (≡the present) in the structure of NGF formalism.

For this purpose, we introduce a technique we call the partitioning in time, or time partitioning for brevity. This name refers to the similarities with the usual partitioning in the Hilbert space, also known as the downfolding method:[17] the full NGF is expressed in terms of its time partitions, like the future-future diagonal block, the past-future off-diagonal block, etc., all defined with respect to the "present" as the dividing time for partitioning.

The dividing time need not have a privileged position; the case of the initial time is an exception. In the transport theory, every instant of the running time separates the instantaneous future from the instantaneous past; the latter plays the role of a gliding initial condition for the evolution of the carrier distribution. The time partitioning equations can in this case be identified with the so-called reconstruction equations which form a rigorous basis for developing the quantum transport equations from the NGF point of view. This will be the third topic discussed in the present paper. In the case of finite-time transients considered here, however, both types of dividing times (initial time and running time) enter simultaneously and the theory is bound to take account of this.

The initial time of a physical process distinguishes itself among all possible dividing times not because it has been subjectively chosen but because it typically represents a true divide between the past—a completed preparatory stage—and a commencing qualitatively different process in question. This may correspond to the onset of an external field, the case we consider in this paper. For theoretical investigations, an important, although artificial, case might be the starting state of uncorrelated particles, with the interactions suddenly turned on at the initial time. Yet another situation, of a great generality and importance, corresponds to a sudden change in the environment of the system at the initial time. In general, an open system is treated by NGF as being a constituent part of a broader system which incorporates also the environment consisting of baths, galvanic contacts, particle reservoirs, etc.[18] A sudden activation of, say, a thermal contact to a bath, clearly is a severe disturbance of the system, with fundamental changes in its boundary conditions, conserving properties, and relaxation characteristics. A paradigmatic model of a bath, the Caldeira-Leggett model,[19,20] has been used to study the dynamics of a system suddenly joined with a bath in the seminal paper.[21] The research along these lines has continued ever since.[20,22,23] So far, the problem has defied the NGF treatment, however. The situation is different with attaching leads to a small (mesoscopic) electron system. Here, the NGF are technique of choice and we have outlined in some detail the solution of the transient behavior of a molecular bridge between two infinite leads which are alternately connected and/or disconnected in a sudden fashion.[24] This is an adaptation of the famous model of Jauho *et al.*[25] to include the switching effects. In our work,[24] we have used already the basic concept of the time partitioning in anticipation of the present paper. A sequel containing a detailed numerical study is under preparation.

At this place, we confine ourselves to these comments. A related more extended discussion will be deferred to the final part of the whole paper, where we will profitably link our present results with an outlook to their future generalization. Let us now concentrate on a characterization of the two physical areas we study in this paper using the time partitioning: the finite-time correlated initial conditions and the quantum transport picture of the short-time transients.

To appreciate the problem of *correlated initial conditions*, a brief historical remark may be useful. As shown in Eq. (1), the NGF may be defined in an usual manner for an arbitrary

many body initial state involving all kinds of correlations. Already the founders of the NGF method were aware, however, of the problem that for correlated initial conditions no Wick theorem holds for the closed time path $\mathbb{C}$. They circumvented it by letting the initial time tend to $-\infty$ with the motivation that for the transport equations, the initial conditions are not essential after elapse of an opening period. Early attempts dealing with the finite-time initial conditions for NGF include the work of Hall, Fujita, Nozières' group and, in particular, of Craig. These references are given in the key paper by Danielewicz,[9] who developed a comprehensive treatment of the initial conditions coming back to the basic concepts by Kadanoff and Baym. Starting from his work, a technique has gradually been developed[9,10,12] in which the real time $\mathbb{C}$ loop is extended by a Matsubara-type imaginary time period during which the correlated state is formed from an auxiliary noncorrelated one. The perturbation expansion of G is then performed along this augmented open time "loop." A fully general treatment extending the ideas of Danielewicz is due to Wagner. He showed, in particular, that the original notion of an analytical continuation between the real and imaginary time axis is not needed.

In the Danielewicz-Wagner treatment, the initial time appears in the middle of the extended time contour, joining the preparatory imaginary time interval with the "physical" real-time domain. Our approach, as sketched above, employs a similar idea. The initial time serves now to join together two parts of a global "host" process, both taking place on the real time axis: the preparation in the "past," and the physical process proper in the "future." The underlying perturbation scheme would now be the Keldysh expansion. We have proposed[24,26] to join both methods under the name of *diachronous techniques*.

This allows to distinguish them from the alternative approaches—beyond the scope of this paper—which should be described as *synchronous*. They are represented by several more recent studies made by people around the Rostock group.[11–16] The difficult average over a correlated initial many-particle state is transformed to an expansion of the NGF equations of motion in terms of a Bogoliubov-Born-Green-Kirkwood-Yvon-type chain of equal-time correlation functions for particle complexes. With a suitable termination capturing the relevant reduced information about the correlations, the NGF can be obtained.

The NGF describes adequately *quantum transport* arbitrarily *far from equilibrium* and driven by arbitrary external fields. In particular, incorporating properly the initial conditions at a finite initial time into the NGF, we fully capture the desired characteristics of the ensuing transient processes in terms of two-time correlation functions. We intend to discuss the conditions for and the ways of reducing the theory to equations for an electron distribution function of a single time, akin to the quantum Boltzmann equations for the extended systems, or the generalized master equations for the spatially restricted systems. The entire field of such quantum transport equations is vast, of course, and the problem of fast transients stands somewhat off its traditional mainstream. Recently, it gains at importance, however.

We may contrast it with the case of quantum Boltzmann equation. This equation is suited for an extended system under the influence of fields smooth both in space and in time. Regardless of the technique of deriving it, it is formally characterized by use of Wigner variables and of a quasiclassical expansion both in space and time. Most importantly, it is an equation for the *quasiparticle distribution* function and the properties of physical particles are obtained from a reconstruction functional which is a part of the complete theory. This approach started from the seminal work of Landau[27] and its school[2,28,29] and it continues flourishing.[30–36] As a link to the NGF approach followed here, we may cite the early classics by Kadanoff and Baym.[1] A reduction in the NGF equations of motion to the Boltzmann equation has been achieved there by a specific approximate factorization of the particle correlation function, the so-called Kadanoff-Baym Ansatz (KBA). In this Ansatz, one of the factors is just the sought for quasiparticle distribution.

Transients cannot be treated in the quasiclassical limit, at least early after their onset and they generically fall into one category with processes driven by fields which are not extremely slow in time, by rf waves or optical pulses, for example. For the reduction NGF$\rightarrow$quantum transport equation in this case, the original KB Ansatz has been modified to the so-called generalized KBA (GKBA).[4,37,38] This Ansatz has a strictly causal structure and consists in factoring out of the particle correlation function its "time diagonal," the one-particle density matrix. Thus it deals with the *distribution of bare particles*, as does also the resulting quantum transport equation. We have to ask about the validity of the Ansatz for processes starting at a finite initial time. Bogolyubov has postulated, as a corollary of his more general principle of the decay of correlations, that the initial correlations die out within a finite characteristic time, after which the system enters its kinetic stage of evolution controlled by a quantum transport equation for the single-particle distribution. This conjecture has been verified in a number of particular cases. Here, it is closely bound with the Ansatz validity and we will discuss all these questions jointly. As pointed out above, the formal tool for this is provided by the time partitioning equations. They can be cast into the form of reconstruction equations introduced in a different way already in Ref. 37 as an exact counterpart of the approximate GKBA expression for the particle correlation function. Presently, they will be generalized to processes with a finite initial time and this will permit to formulate general criteria for the use of a quantum transport equation in a transient regime.

The paper has the following structure. In Sec. II we give basic definitions and notation, contrast the correlated and uncorrelated IC and identify the latter with the Keldysh initial conditions.[39] In Sec. III, we first interpret the finite-time process in question with a process embedded in a host process an preceded by a preparation stage. The related Schwinger-Keldysh contours are defined. In Sec. III B, a proof is given of the invariance of the NGF with respect to the choice if the initial time. Sec. IV is the core part of the paper. The invariance of the NGF is used to express the self-energy of the embedded process including the initial condition terms in terms of the self-energy of the host process. To this end, the formalism of the partitioning in time is built up, in which any function of time is split into two parts, a projection onto the past (P) and onto the future (F). This is first done for the

propagator components of the NGF in Sec. IV A. The double-time quantities have four partitions. Both diagonal partitions obey the Dyson equation without modification while the *FP* and *PF* partitions lead to equations which can be identified with the renormalized composition rule for propagators.[40–42] By contrast, the correlation functions like $G^<$ have a self-energy sensitive to initial conditions. The partitioned form of $G^<$ is derived in Sec. IV B. It is the used to obtain the self-energy of the embedded process, which is compared with the results of Ref. 9. The remaining sections are concerned with the physical consequences of the developed formalism. First, Sec. V invokes the Bogolyubov principle of the decay of correlations. For the self-energy, it means that all its components are negligible outside a strip along the time diagonal in the double-time plane. Its width $\tau^\star$ is comparable with the Bogolyubov correlation time. In Sec. V A, it is shown that for the IC terms of the self-energy this implies that they are concentrated to a finite area of the $\tau^\star$ adjoining the point of initial time. This, in turn, allows to show in Sec. V A that the NGF itself contains IC-dependent terms attenuated at the rate of the GF relaxation time and superseded by a term with a floating initial condition. Section VI is concerned with the quantum transport theory for processes starting at a finite initial time. For these processes, Bogolyubov conjecture states that later than $\tau^\star$ after the process started, the process is governed by a closed transport equation for the single-particle distribution. We use our results for the NGF to corroborate this conjecture. In the first step, Sec. VI A, we show that for the precursor transport equation, which is the point of departure for the NGF approach to quantum transport equations. The proof is completed in Sec. VI B devoted to deriving the reconstruction equations of the quantum transport theory in the case of a finite initial time and demonstrating that the IC-dependent terms die out within the $\tau^\star$ time after the start of the embedded process. The reconstruction equations form together with the precursor transport equation a closed system allowing to formulate an exact approach to quantum transport and also to obtain approximate transport equation in a systematic manner. We discuss from this angle the generalized Kadanoff-Baym Ansatz and show that it is too coarse to capture the effect of initial conditions, being suited rather for the steady asymptotic transport regime. In Sec. VI C, we take a broader look on the transient transport and the NGF as an option for its description, with emphasis on open systems.

II. NGF AND QUANTUM DYNAMICS

The dynamics of the system is defined by the full Hamiltonian $\mathcal{H}+\mathcal{U}(t)$ consisting of the system Hamiltonian $\mathcal{H}$ and an additive external disturbance $\mathcal{U}(t)$. A dynamical process is described by the statistical operator $\mathcal{P}(t)$ which is fully specified by its initial state $\mathcal{P}_\mathrm{I}$ at $t=t_\mathrm{I}$ (an arbitrary equilibrium or out-of-equilibrium state).

The nonequilibrium Green's function is defined in the usual manner,[4–6]

$$G(1,2) = -i\,\mathrm{Tr}(\mathcal{P}_\mathrm{I}\boldsymbol{T}_\mathrm{c}\{\psi(1|t_\mathrm{I})\psi^\dagger(1'|t_\mathrm{I})\}) \tag{1}$$

with the Heisenberg field operators ψ, $\psi^\dagger$ anchored at t_I, and the time-ordering operator $\boldsymbol{T}_\mathrm{c}$ acting along the closed time path $\mathbb{C}$ extending from t_I to $+\infty$ and back. To indicate the initial time, we occasionally write $G_{t_\mathrm{I}}(1,1')$ instead of $G(1,1')$. We will use this convention when working with two initial times at once.

We represent the contour-ordered NGF, following Keldysh,[2,39] by a 2×2 matrix GF of real time, employing the Langreth-Wilkins (LW) matrix[4,43,44] having three components, the less-correlation function $G^<$ and two (equivalent) propagators, $G^A(1,1')=[G^R(1',1)]^\dagger$. The Dyson equations for the propagators have the form

$$G^{R,A} = G_0^{R,A} + G_0^{R,A}\Sigma^{R,A}G^{R,A}, \quad \text{etc.} \tag{2}$$

The less component of the Dyson equation can be quite generally cast into the form[9]

$$G^< = G^R\Xi^<G^A,$$

$$\Xi^< = {}_\circ\Sigma_\circ^< + {}_\circ\Sigma_\bullet^< + {}_\bullet\Sigma_\circ^< + {}_\bullet\Sigma_\bullet^<. \tag{3}$$

For later convenience, we use the more systematic notation of Ref. 40 for the self-energy $\Xi^<$: The integrations in Eq. (3) start at t_I. The four terms have a varying degree of singularity at the initial time, as indicated by circles. The open circles indicate a time variable fixed at t_I, the filled ones a time variable continuous in (t_I,∞). The regular term ${}_\bullet\Sigma_\bullet^<$ (called $\check{\Sigma}^<$ in Ref. 12) corresponds to the Dyson equation as it is usually written for $t_\mathrm{I}\to-\infty$, namely, $G^<=G^R\Sigma^<G^A$. The other terms have the form

$$\begin{aligned}
&{}_\circ\Sigma_\circ^<(t,t') = i\rho(t_\mathrm{I})\delta(t-t_\mathrm{I}^-)\delta(t'-t_\mathrm{I}^-), \quad \rho(t) = -iG^<(t,t),\\
&{}_\bullet\Sigma_\circ^<(t,t') = \Lambda_\circ^<(t,t_\mathrm{I})\delta(t'-t_\mathrm{I}^-),\\
&{}_\circ\Sigma_\bullet^<(t,t') = {}_\circ\Lambda^<(t_\mathrm{I},t')\delta(t-t_\mathrm{I}^-) \qquad \boxed{t_\mathrm{I}^- = t_\mathrm{I}-0}.
\end{aligned} \tag{4}$$

Two terms, ${}_\circ\Sigma_\circ^<$ and ${}_\bullet\Sigma_\bullet^<$, correspond roughly to the self-energy for uncorrelated initial conditions. The remaining two singular terms (famous Σ^c, Σ_c of Ref. 9) originate from the initial correlations. They are equivalent to single-time continuous functions $\Lambda_\circ^<(t,t_\mathrm{I})$, ${}_\circ\Lambda^<(t_\mathrm{I},t')$ dependent on t_I as on a parameter. For the correlated initial conditions, these two functions must be determined in addition to the regular *less* self-energy. To verify the uncorrelated IC limit of Eq. (3), let us write $\Sigma^<$ for ${}_\bullet\Sigma_\bullet^<$ and use the uncorrelated, that is unperturbed, $\rho(t_\mathrm{I})\to\rho_0(t_\mathrm{I})=iG_0^<(t_\mathrm{I},t_\mathrm{I})$ to transform

$$\begin{aligned}
G^R{}_\circ\Sigma_\circ^<G^A &\to G^R[i\rho_0(t_\mathrm{I})]G^A\\
&= G^R[G_0^R]^{-1}G_0^R[i\rho_0(t_\mathrm{I})]G_0^A[G_0^A]^{-1}G^A\\
&\equiv f^<
\end{aligned}$$

and finally set ${}_\circ\Sigma_\bullet^<$ and ${}_\bullet\Sigma_\circ^<$ to zero. Equation (3) becomes

$$G^< = f^< + G^R\Sigma^<G^A,$$

$$f^< = (1+G^R\Sigma^R)G_0^<(1+G^A\Sigma^A). \tag{5}$$

This is identical with the famous form of the Dyson equation with uncorrelated initial conditions for the correlation function given by Keldysh.[3,4,39]

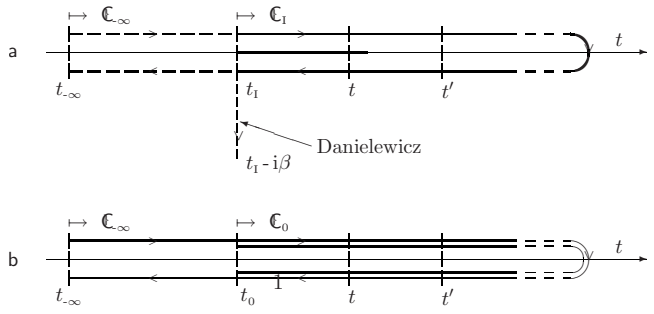

FIG. 1. The NGF time contour and its extensions. The process under study evolves along the Schwinger-Keldysh trajectory $\mathbb{C}_{\mathrm{I}}$ starting and ending at t_{I}. (a) It is augmented by a preparation stage running between $t_{-\infty}$ and t_{I}. The joint process has the $\mathbb{C}_{-\infty}$ trajectory. For comparison, the well-known extension (Refs. 9 and 10) by an imaginary stretch ending at the formal "temperature" β is shown and labeled "Danielewicz." (b) Within any host process extending over $\mathbb{C}_{-\infty}$, an arbitrary dividing time t_0 defines an embedded process along $\mathbb{C}_0$. (a) shows one special case with a particular physical interpretation: t_0 is identified with the initial time t_{I}.

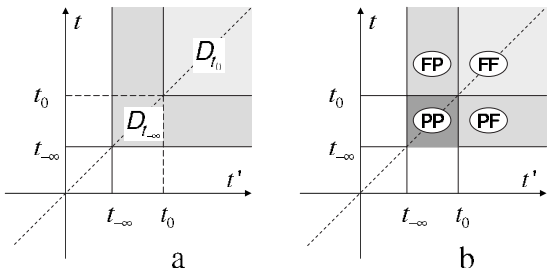

FIG. 2. (a) Definition ranges $D_{t_{-\infty}}$ of the full process and D_{t_0} of the restarted process are the first quadrants with the initial times specifying their lower left corners, see Eq. (6). (b) In the partitioning language the whole $D_{t_{-\infty}}$ range is cut into four partitions at the crossing point $[t_0,t_0]$. The future-future partition coincides with the restart process time range D_{t_0}.

III. PROBLEM OF INITIAL CONDITIONS FOR NGF

As discussed in Sec. I, various methods have been developed, how to circumvent the difficult average in Eq. (1). The point of departure in our approach characterized as *real-time diachronous* is the notion that any physically admissible initial state $\mathcal{P}_{\mathrm{I}}$ is an outcome of previous history (preparation). In order to employ this feature for determining future evolution of the system, we have to formalize the notion of the past and the future with respect to a selected instant (≡the present) in the structure of NGF formalism. Then we will continue the Green's function from the time block of the preparation stage to the "relevant" time block of the future evolution described by Eq. (1).

A. Start of a finite-time transient as a restart of the host process

We turn to our basic task of determining explicit expressions for the NGF with an initial time t_{I}, at which the correlated initial state is $\mathcal{P}_{\mathrm{I}}$. As stated already, we restrict our study to processes whose initial state coincides with the intermediate state at which an antecedent (preparation) process has arrived at the selected initial time. Beyond that time, the evolution continues as the dynamical process in question ("measurement" or "observation"). The two processes follow *coherently* one after another and, consequently, form together a united process. This is sketched in Fig. 1(a). In particular, if the preparation stage starts from an uncorrelated state at an indefinitely remote past, $t_{-\infty}\to-\infty$, the united process can be viewed as one of the Keldysh switch-on processes. Also shown in Fig. 1(a) is the Danielewicz-Wagner contour, along which the finite-time process in question is augmented by an artificial process taking place on an imaginary time interval, and again, the two partial processes have to be viewed as coherent segments of a unique whole.

From a more abstract point of view, the interpretation of the two stages as preparation and the physical (or measurement) process is entirely subjective and depends on the special importance ascribed to the given initial time. It is more productive to think in terms of two processes differing only in their time definition range. One is the long host process, starting at some instant $t_{-\infty}$ from $\mathcal{P}_{-\infty}$, the other is a shorter "embedded" process, which starts at an arbitrarily chosen initial time. This alternative interpretation is presented in Fig. 1(b). To stress the fluid nature of the "initial" time, we change the notation to t_0. This instant is elected to be the present. The host process encompasses both the past and the future with respect to t_0 while the embedded process takes place wholly in the future. Both processes describe the same evolution beyond t_0. This coincidence permits to buildup the NGF of the short process as the future "partition" of the long process. Once this is done, the embedded process may be viewed as an independent "restart" process, which is being restarted from a frozen initial state $\mathcal{P}_0=\mathcal{P}_{-\infty}(t_0)$ at t_0. The influence of this initial state is incorporated through the construction of the NGF for the embedded process; the many-body state itself does not enter the formalism explicitly anywhere.

B. Invariance of the NGF with respect to the restart time

Now we will demonstrate that the NGF is invariant with respect to the choice of the initial time. To this end, we compare two nonequilibrium Green's function differing by their initial times and, hence, by their definition ranges D_{t_0}, $D_{t_{-\infty}}$ [Fig. 2(a)]. We consider the less correlation function; $G^{>}$ would be treated similarly and the R,A components are their combinations. We have

$$G^{<}_{t_{-\infty}}(1,1') = -i\,\mathrm{Tr}[\mathcal{P}_{t_{-\infty}}\psi^{\dagger}(1'|t_{-\infty})\psi(1|t_{-\infty})],$$

$$G^{<}_{t_0}(1,1') = -i\,\mathrm{Tr}[\mathcal{P}_{t_0}\psi^{\dagger}(1'|t_0)\psi(1|t_0)] \qquad (6)$$

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

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

$$\psi(1|t_{-\infty}) = \mathcal{K}(t_{-\infty},t)\psi(x)\mathcal{K}(t,t_{-\infty}), \quad \psi^\dagger(1'|t_{-\infty}) = \cdots,$$

$$\psi(1|t_0) = \mathcal{K}(t_0,t)\psi(x)\mathcal{K}(t,t_0), \quad \psi^\dagger(1'|t_0) = \cdots \tag{7}$$

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

$$\mathcal{P}_{t_0} = \mathcal{K}(t_0,t_{-\infty})\mathcal{P}_{t_{-\infty}}\mathcal{K}(t_{-\infty},t_0). \tag{8}$$

Introducing all these relations into the definition (6), we find that, in fact, the values of the two GF's are identical over the common definition range D_{t_0} and can be denoted by $G^<$ without the time label,

$$G^<(1,1') \equiv G^<_{t_{-\infty}}(1,1'), \quad t,t' \geq t_{-\infty},$$

$$G^<(1,1') \equiv G^<_{t_0}(1,1'), \quad t,t' \geq t_0. \tag{9}$$

The restart time may be an arbitrary time later than $t_{-\infty}$ and the result (9) thus proves that the definition of the GF for an embedded process is invariant with respect to shifting its initial (restart) time t_0.

IV. TIME PARTITIONING

Next, we employ the invariance, Eq. (9), of the NGF to relate the self-energies of the two processes. To achieve this goal, we split the whole time domain of the host process at t_0 into the past, the preparation period, and the future, the observation period. The latter coincides with the time domain of the embedded process. The host NGF gets partitioned into four blocks, as represented in Fig. 2(b). The future-future partition coincides with the time domain D_{t_0} of the embedded NGF. We will make use of this to obtain explicit expressions for the embedded NGF from the Dyson equation for the host NGF by a technique we call time partitioning. This technique will be made clear in the course of the derivations. In other words, we develop in parallel the formal means suited for resolving the second main question of the paper.

Consider a process starting at $t_{-\infty}$. Let $t_0 > t_{-\infty}$ be the dividing time between the past and the future. The whole time domain $[t_{-\infty},\infty)$ is divided into two parts, $[t_{-\infty},t_0]$ and $[t_0,\infty)$. Any function of time can be split or *partitioned* into the corresponding two components by means of projection operators P,F: with ϑ being the unit step function, I the unit operator in the space of single-particle states, we get

$$P(t,t') = \vartheta(t_0-t)\vartheta(t-t_{-\infty})\delta(t-t')I,$$

$$F(t,t') = \vartheta(t-t_0)\delta(t-t')I,$$

$$P + F = \delta(t-t')I \equiv 1. \tag{10}$$

Similarly, a regular double-time quantity X can be partitioned to four quadrants of the two-time plane,

$$X = PXP + PXF + FXP + FXF.$$

Our aim will now be to obtain explicit expressions for the partitioned NGF with help of the Dyson equation. This would mean repeating the standard partitioning procedure (see, for example, Ref. 17) for the matrix NGF. This systematic formal way will be described elsewhere. Here, we will proceed by components, which are more transparent and lead directly to relations having physical interpretation.

A. Time partitioning for propagators

The retarded quantities are nonzero only for $t > t'$ and we get $PG^RF = P\Sigma^RF = 0$. The time diagonal blocks of the Dyson Eq. (2) for G^R then preserve its unpartitioned form,

$$PG^RP = PG_0^RP + PG_0^RP \cdot \Sigma^R \cdot PG^RP, \tag{11}$$

$$FG^RF = FG_0^RF + FG_0^RF \cdot \Sigma^R \cdot FG^RF. \tag{12}$$

This means that propagation starting and ending in the past/in the future is closed in itself and is not influenced by the complementary time domain. In particular, the retarded self-energy for the embedded process coincides with that of the host process within the embedded time domain D_{t_0}.

The remaining FP block of the Dyson equation for G^R has the structure

$$FG^RP = FG_0^RP + FG_0^RF \cdot \Sigma^R \cdot FG^RP + FG_0^RF \cdot \Sigma^R \cdot PG^RP + FG_0^RP \cdot \Sigma^R \cdot PG^RP. \tag{13}$$

By definition, the free propagator corresponds to a unitary evolution. It thus satisfies the multiplicative composition law (the "semigroup rule")

$$G_0^R(t,t') = iG_0^R(t,t_0)G_0^R(t_0,t') \quad \text{for } t \geq t_0 \geq t'. \tag{14}$$

This may be rewritten as

$$FG_0^RP = FG_0^RF \cdot L^R \cdot PG_0^RP,$$

$$L^R(t,t') = i\delta(t-t_0^+)\delta(t_0^- - t')I \tag{15}$$

on defining a time-local operator L whose time arguments must be infinitesimally shifted, as indicated.

Introducing Eq. (15) into Eq. (13) and making use of Eqs. (11) and (12), we finally obtain

$$FG^RP = FG^RF \cdot (L^R + F\Sigma^RP) \cdot PG^RP. \tag{16}$$

With the time arguments written out explicitly, the equation reads

$$G^R(t,t') = iG^R(t,t_0)G^R(t_0,t') \qquad \boxed{t \geq t_0 \geq t'}$$
$$+ \int_{t_0}^{t} d\bar{t} \int_{t'}^{t_0} d\bar{\bar{t}} G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{\bar{t}})G^R(\bar{\bar{t}},t'). \tag{17}$$

Similar relations are obtained for G^A. In the symbolic form,

$$PG^AF = PG^AP \cdot (L^A + P\Sigma^AF) \cdot FG^AF, \tag{18}$$

where $L^A = [L^R]^\dagger$.

This completes the time partitioning for propagators.

The resulting Eqs. (16) and (17) for G^R may be compared with their counterparts, Eqs. (14) and (15) for G_0^R. The latter represent a factorization of the GF commonly called the semigroup property. It was necessary to invoke the factorized

form, Eq. (15), for the free propagator in order to derive the Eq. (16) for the full propagator in which the semigroup factorization is renormalized. The renormalization consists in a nonlocal vertex correction to the time-local bare factorizing vertex L^R. This result for G^R coincides with the renormalized semigroup property previously reported in Refs. 40–42 in connection with the reconstruction theorem and the nonequilibrium Ward identity for NGF.

Here, it is linked with the partitioning and gives the formalism some physical content. The past and the future cannot be cleaved apart at a sharp instant, except in the mean-field approximation incorporating strictly the "singular," that is time-local components of the self-energy. The regular double-time self-energy leads to blurring of the sharp time borderline. The partitioning consists, in fact, of expressing the whole propagator in terms of its two diagonal blocks, past-past and future-future. These blocks are joined by the diagonal, or off-diagonal blocks of the self-energy, as needed. In explicit terms, the off-diagonal blocks mean that the integration range is off-diagonal with the time arguments of Σ^R or Σ^A mutually separated by the partition time t_0.

B. Time partitioning for $G^<$

The partitioning of $G^<$ is obtained from the four blocks of the Dyson equation $G^<=G^R\Xi^<G^A$, Eq. (3) for the host GF. We take advantage of the possibility of suppressing the label $t_{-\infty}$. The off-diagonal blocks of the propagators are substituted for by the partitioning expressions, Eq. (16) for G^R and the analog for G^A, with the result,

$$PG^<P = PG^RP \cdot \Xi^< \cdot PG^AP, \tag{19}$$

$$PG^<F = PG^RP \cdot \Xi^< \cdot FG^AF + PG^<P \cdot (L^A + \Sigma^A) \cdot FG^AF, \tag{20}$$

$$FG^<P = FG^RF \cdot \Xi^< \cdot PG^AP + FG^RF \cdot (L^R + \Sigma^R) \cdot PG^<P, \tag{21}$$

$$\begin{aligned} FG^<F = {} & FG^RF \cdot \Xi^< \cdot FG^AF \\ & + FG^RF \cdot \Xi^< \cdot PG^AP \cdot (L^A + \Sigma^A) \cdot FG^AF \\ & + FG^RF \cdot (L^R + \Sigma^R) \cdot PG^RP \cdot \Xi^< \cdot FG^AF \\ & + FG^RF \cdot (L^R + \Sigma^R) \cdot PG^<P \cdot (L^A + \Sigma^A) \cdot FG^AF. \end{aligned} \tag{22}$$

In agreement with the general "causal" structure, an advantage of the LW representation,[4,43,44] each term contains just one less factor surrounded by retarded factors from the left and advanced factors from the right. This causal structure is further underlined by the propagation from past to present limiting the order of the P and F projectors. Just like for the propagators, only the time diagonal blocks $FG^<F$, $FG^RF,\ldots,PG^AP$ enter the partitioning Eqs. (19)–(22), while the coupling of the two time domains is provided by the off-diagonal blocks of the self-energy.

The unidirectional nature of the propagators leads to a very different role of the past and of the future in the resulting partitioned expressions. Looking first at Eq. (19), we see that the correlation function restricted to the past does not feel the future for an obvious causality reason. The same is true for the propagators, Eq. (11), and, hence, for the whole NGF. Considering next the two off-diagonal blocks of the NGF, we find that always just two of its three components are nonzero. For the future-past block, these are FG^RP [Eq. (16)] and $FG^<P$ [Eq. (21)] while $FG^AP=0$. Note that Eq. (16) and the second term of Eq. (21) have an identical structure with the PP block of the GF in question linked with the FF block of the propagator by means of the renormalized vertex $L^R+F\Sigma^RP$. An essential additional term enters Eq. (21), however. As will be discussed below, Eq. (21) is intimately related to the reconstruction equations known from the NGF theory of quantum transport equations. The same remarks hold for the PG^AF, $PG^<F$ pair with necessary modifications.

The host process and the embedded process each satisfy their own Dyson equations, which define the respective self-energies $\Sigma^{R,A}_{t_{-\infty}}$, $\Xi^<_{t_{-\infty}}$ and $\Sigma^{R,A}_{t_0}$, $\Xi^<_{t_0}$. Our task will be to use the invariance condition (9) to mutually relate the two sets of self-energies, or, more specifically, to construct the restart self-energies reflecting the initial conditions for the embedded NGF at t_0. First, as concerns the propagator self-energies, we have already seen in Eq. (12) that they are invariant with respect to the choice of the restart time in the sense of Eq. (9). For the embedded particle correlation function, the Dyson equation

$$G^<_{t_0} = G^R_{t_0}\Xi^<_{t_0}G^A_{t_0} \tag{23}$$

is identified with $FG^<F=FG^RF\Xi^<_{t_0}FG^AF$, see Fig. 2(b), and the self-energy is extracted from Eq. (22) as

$$\begin{array}{cccc} \Xi^<_{t_0} = F\Xi^<F & \vdots & \vdots & \vdots \\ + F\Xi^< \cdot PG^AP \cdot \Sigma^AF & + F\Xi^< \cdot PG^AP \cdot L^A & \vdots & \vdots \\ + F\Sigma^R \cdot PG^RP \cdot \Xi^<F & \vdots & + L^R \cdot PG^RP \cdot \Xi^<F & \vdots \\ + F\Sigma^R \cdot PG^<P \cdot \Sigma^AF & + F\Sigma^R \cdot PG^<P \cdot L^A & + L^R \cdot PG^<P \cdot \Sigma^AF & + L^R \cdot PG^<P \cdot L^A \\ \Xi^<_{t_0} = \left[\bullet\Sigma^<_\bullet\right]_{t_0} & + \left[\bullet\Sigma^<_\circ\right]_{t_0} & + \left[\circ\Sigma^<_\bullet\right]_{t_0} & + \left[\circ\Sigma^<_\circ\right]_{t_0} \end{array}. \tag{24}$$

The nine terms of $\Xi^<_{t_0}$ correspond to the block decomposition $(F\Xi^<F,\ldots,P\Xi^<P)$ of the host $\Xi^<$ by lines and to the Danielewicz four parts of the self-energy in the Dyson Eq. (23) by columns.

V. INITIAL CONDITIONS AND THE DECAY OF CORRELATIONS

The outcome of the preceding formal section can be summarized in two equivalent ways. As an answer to the general question posed in this paper about separation of the past and future within the NGF formalism, we have the partitioning equations expressing the complete NGF for a host process in terms of its *PP* and *FF* partitions, that is of the NGF for the preparation stage and the observation stage, which are coupled by the off-diagonal *FP* and *PF* partitions of the NE self-energy. For the NGF propagator components, the equations are Eqs. (11), (12), (16), and (18). The four equations for the particle correlation function are (19)–(22).

The second, narrower, but physically central question concerning the NGF of an embedded process, is answered for the propagators by Eq. (12), or, which is the same, by the plain Dyson Eq. (2) with the understanding that the external time domain is D_{t_0}. For the correlation function of the embedded process, the Dyson equation is given by Eq. (23) with the self-energy listed in Eq. (24).

This last result, crowning in some sense our effort, does not look very simple. It may be profitably used, however, in conjunction with the assumption about a short-time range of correlations—Bogolyubov principle of the decay of correlations. We devote this and the next sections to analyzing this conception and to indicating some areas of its use. In particular, we address in the next section the quantum transport theory in the presence of correlated initial conditions.

A. Self-energy and the decay of correlations

For analyzing the initial conditions for the embedded NGF if will be convenient to rewrite the restart Dyson equation, Eq. (23), in the form[45]

$$G^<_{t_0}(t,t') = \int_{t_0}^{t} d\bar{t}\int_{t_0}^{t'} d\bar{\bar{t}}\, G^R \Xi^< G^A \qquad \boxed{t \geq t_0, t' \geq t_0}$$
$$+ \int_{t_0}^{t} d\bar{t}\int_{t_0}^{t'} d\bar{\bar{t}}\, G^R \underbrace{[\Xi^<_{t_0} - \Xi^<]}_{\Theta^<_{t_0}} G^A \tag{25}$$

with the *FF* block of the host self-energy $\Xi^<$ singled out in the first line. The difference $\Theta^<_{t_0}$ in the second line describes the effect of the initial conditions. The resulting $FG^<F$ must coincide with the expression following from the host Dyson equation, $G^<_{t_0} = FG^R\Xi^<G^AF$. In the latter, the integration extends over the whole $D_{t_{-\infty}}$, while the restart Dyson equation contains only the *FF* $(\ldots D_{t_0})$ part of the integral involving $\Xi^<$. The initial conditions at the restart time t_0 capture in a condensed form the contribution of the three remaining $\Xi^<$ blocks, i.e., the integral over $D_{t_{-\infty}} \backslash D_{t_0}$, to $G^<_{t_0}$.

The IC correction $\Theta^<_{t_0}$ is identical with the last three lines of Eq. (24), from which it is apparent, how the integral is folded down into the initial conditions. A substantial portion is taken up by the uncorrelated IC term ${}_\circ\Sigma^<_\circ$. This simplest possible contribution to the finite-time initial conditions results in the coherently propagated initial one-particle density matrix of the restart process, $G^R(t,t_0)\rho(t_0)G^A(t_0,t)$. It is in a perfect harmony with the framework for genuine quantum transport equations, that is, closed equations for the quantum distribution function $\rho(t)$. Of the other contributions to $\Theta^<_{t_0}$, two are the Danielewicz correlated IC terms ${}_\circ\Sigma^<_\bullet$ and ${}_\bullet\Sigma^<_\circ$. The remaining one, ${}_\bullet\Theta^<_\bullet \equiv {}_\bullet\Sigma^<_\bullet - \Xi^<$ specifies the initial correction to the host less self-energy. This last feature is natural for the restart interpretation of an embedded process while its meaning within the general NGF approach to initial conditions is less certain.[12] (In this reference, ${}_\bullet\Sigma^<_\bullet$ is called $\check{\Sigma}^<$).

The correlated IC terms of $\Xi^<_{t_0}$ are expressed in terms of the host process explicitly, as given by the expanded form of Eq. (24). All these expressions, seven altogether, have a common structure. Both external times belong to the future while the internal motion involves a virtual excursion of the system into the past.

For example, one of the ${}_\bullet\Theta^<_\bullet$ terms is

$$[F\Sigma^R P G^R P \Xi^< F](\bar{t},\bar{\bar{t}}) = \int_{t_{-\infty}}^{t_0} du \int_{t_{-\infty}}^{t_0} dv \Sigma^R(\bar{t},u) G^R(u,v) \Xi^<(v,\bar{\bar{t}}). \tag{26}$$

The virtual propagation takes place between u and v, entirely in the past time domain, while past and future are linked by the self-energy factors, whose time arguments are separated by the restart time t_0. The same is true of all other correlated IC contributions to $\Xi^<_{t_0}$, only in those containing a contact L factor the corresponding inner and outer times are t_0-0 and t_0+0, respectively. Thus $[{}_\bullet\Sigma^<_\circ]_{t_0}$ reads

$$\left[{}_\bullet\Sigma^<_\circ\right]_{t_0} = F\Xi^< \cdot PG^AP \cdot L^A + F\Sigma^R \cdot PG^<P \cdot L^A = -i\left[\int_{t_{-\infty}}^{t_0} du \Xi^<(t,u) G^A(u,t_0) + \int_{t_{-\infty}}^{t_0} du \Sigma^R(t,u) G^<(u,t_0)\right]. \tag{27}$$

It is decisive for the actual role of initial correlations that the off-diagonal coupling in all IC terms is mediated by the self-energy: it suggests itself to invoke the Bogolyubov principle stating that the temporal correlations in the system decay within a period with a characteristic time τ_c (often called the collision duration time in transport theory). This principle translates into the assumption[6] that the host less self-energy $\Xi^<(t,t')$ is negligible out of the strip $|t-t'| < \mathcal{O}(\tau_c)$ along the time diagonal, and also that a similar formation time τ_Q exists for Σ^R and Σ^A. All components of the self-energy should thus be concentrated to a strip

$$|t-t'| < \mathcal{O}(\tau^\star) \quad \tau^\star = \mathcal{O}(\tau_c, \tau_Q). \tag{28}$$

Then the following restrictions hold for the time variables in Eqs. (26) and (27), and, by the same token, in all correlated IC terms,

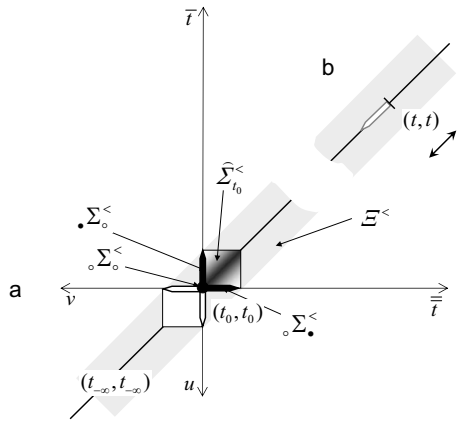

FIG. 3. Double time plane. The gray strip along the equal-time diagonal corresponds to the condition (28). Outside the strip all self-energy components should be practically zero. (a) The time axes crossing at $[t_0,t_0]$, cut the plane into partitions; the semiaxes rimming the time range of the embedded process (future-future quadrant) are labeled $\bar{t},\bar{\bar{t}}$, the opposite ones pointing into the past are labeled u,v—see Eqs. (26) and (27). By the condition (29), the IC corrections to $\Sigma^<$ are restricted to the shaded square anchored at $[t_0,t_0]$ or its edges, as shown by labels. The integration ranges in Eqs. (26) and (27) are similarly restricted to the white square and its boundaries. Details are given in the main text. (b) The running time for the one-particle density matrix is $t=t'$. If selected far enough from t_0, $t>t_0+2\tau^\star$, both propagators $G^R(t,\bar{t})$, $G^A(\bar{\bar{t}},t')$ in the IC term of Eq. (25) will already be, by Eq. (31), in the quasiparticle mode and decaying at the rate τ. The generalized collision terms in the precursor equation have a 1D integration range along the time diagonal between $[t,t]$ and $[t-\tau^\star,t-\tau^\star]$ as shown by a white arrow. The intersection of this stretch with the square of nonzero IC corrections to the self-energy is thus empty for $t>t_0+2\tau^\star$ and the IC terms in the precursor equation vanish in agreement with the Bogolyubov conjecture.

$$t_0+\tau^\star>\bar{t}>t_0>u>t_0-\tau^\star,$$

$$t_0-\tau^\star<v<t_0<\bar{\bar{t}}<t_0+\tau^\star. \tag{29}$$

These inequalities are important in two respects, as indicated schematically in Fig. 3(a).

First, the external times are restricted to an intersection of two strips of a $\tau^\star$ width flanking from the future side the lines $t=t_0$ and $t'=t_0$ in the double-time plane. Thus, all correlated IC corrections are negligible outside this squarelike region close to the intersection $(t,t')=(t_0,t_0)$. This is an explicit consequence of the Bogolyubov principle. The partitioning expressions for correlated initial conditions, like Eq. (26), are well suited for testing and analyzing the validity of this important hypothesis. The four IC terms are concentrated to the following regions: $_\bullet\Theta^<_\bullet$ to the square $[t_0,t_0+\tau^\star]\otimes[t_0,t_0+\tau^\star]$, $_\circ\Sigma^<_\bullet$ to its vertical side, $_\bullet\Sigma^<_\circ$ to its horizontal side, both crossing at (t_0,t_0), finally $_\circ\Sigma^<_\circ$ is concentrated to the single corner point (t_0,t_0).

Second, as also shown in Fig. 3(a), the inner (integration) time variables are also restricted to similar strips, but now on the side of the past. That means that the memory of the past required by the correlated initial conditions need not reach beyond $t_0-\tau^\star$. This is the gain of the restart formulation contained in Eqs. (23) and (24) as compared with the host Dyson equation: in $G^<_{t_0}=FG^R\Xi^<G^AF$, the integrations would reach down to $t_{-\infty}$.

B. Evolution of $G^<$

The IC contributions to the resulting $G^<_{t_0}$ should also vanish with increasing time. To assess the rate of their attenuation, we will consider the "typical" case governed by the hierarchy of characteristic times,

$$\tau^\star\ll\tau, \tag{30}$$

where τ has the meaning of a quasiparticle lifetime. Because $t_0+\tau^\star$ serves as an estimate of the upper limit of the integration range for the IC integral in the second line of Eq. (25), we see that

$$t-t_0\geq t-\bar{t}>t-t_0-\tau^\star,$$

$$t'-t_0-\tau^\star<t'-\bar{\bar{t}}<t'-t_0. \tag{31}$$

This shows that for times t,t' well beyond $t_0+\tau^\star$ both propagator factors in Eq. (25) have the lifetime τ as an estimator for their decay, cf. Fig. 3(b), for the equal time case $t=t'$. This holds for the uncorrelated part of the initial condition and also for all correlation contributions to Eq. (25). In general, there is no reason for the correlation part of the initial conditions to decay faster than the uncorrelated initial conditions. We mention that because of opposing views found in the literature.[38] In any case, long after the onset of the (restart) process, the initial conditions die out, and the Dyson equation becomes

$$G^<_{t_0}(t,t')=\int_{t_0}^{t}d\bar{t}\int_{t_0}^{t'}d\bar{\bar{t}}G^R\Xi^<G^A\quad t,t'\gg t_0+\tau. \tag{32}$$

This estimate is valid for a general double-time argument (t,t'), but also for the two times equal $t=t'$. This means that the decay time for the initial density matrix ρ_0 is $\frac{1}{2}\tau$. Thus, the host self-energy alone governs the long time asymptote of any embedded process, and the lower integration limits may be shifted up, from $t_{-\infty}$ to t_0.

VI. QUANTUM TRANSPORT WITH FINITE-TIME INITIAL CONDITIONS

The problem of quantum transport for a given system is completely solved, of course, once the particle correlation function has been constructed. Here, we have in mind a solution of the same problem in a narrower specific sense, namely, by means of a quantum transport equation. Even today, with the massive effort to master a direct solution of the Kadanoff-Baym or equivalent equations for the NGF, the possibility of using the simpler transport equations is appealing. On the one hand, both the construction and the solution of transport equations is usually physically more transparent and well controlled. On the other hand, a practical solution of the transport equations is incomparably easier than a direct attack at the NGF equations. The NGF formulation re-

mains, of course, as the rigorous reference framework, and, in our approach, also as the starting point, from which the transport equation is obtained by a sequence of approximate steps. We adhere to the Ansatz philosophy, according to which the transition NGF→quantum transport equation is separated from a specific physical approximation for the many-body aspects of the problem. The particular problem we will address is the transient quantum transport with finite-time initial conditions. As will emerge, our discussion will be based on the time-partitioning equations. It may be said that the following is a first nontrivial application of the formalism on a physical question.

We will not return to the general discussion presented in Sec. I. We only summarize that for the transient case, we build a transport equation for the one-particle density matrix that is the distribution of true bare particles. Instead of using the Wigner time variables, our formalism has a strictly causal structure. We will thus not use a quasiclassical expansion, although the decay time of correlations should be the shortest of all characteristic times. Finally, the initial condition terms fading away during the transient should be incorporated. In this connection, special attention will be paid in to the Bogolyubov conjecture which states that a process starting from a correlated nonequilibrium state at a finite time enters the kinetic stage of evolution immediately after the initial correlations decay, that is beyond the initial period lasting $\tau^\star$. In the kinetic regime, the evolution is governed by a closed quantum transport equation for the one-particle density matrix. In a broad outline, this follows from the general principle of the decay of correlations. One purpose of this section is to look into this relationship by formal means developed in the preceding sections and to modify and extend the standard procedure of deriving the quantum transport equations (called also transport equations for short) in order to incorporate the finite-time initial conditions. In particular, we demonstrate that for any initial state generated by a preparation process, the Bogolyubov conjecture can be proved provided a finite $\tau^\star$ time exists.

A. Precursor quantum transport equation and the Bogolyubov conjecture

Our analysis will proceed in two steps. First, precursor transport equation will be considered in this section. Section VI B will be devoted to its reduction to a quantum transport equation proper.

The precursor transport equation (known also as the generalized Kadanoff-Baym equation) is the starting point on the way from NGF to transport equations. It is a differential equation obtained from Eq. (23), and Eq. (2) written as $[G^{R,A}]^{-1}=[G_0^{R,A}]^{-1}-\Sigma^{R,A}$. It already has a structure closely related to transport equations,

$$G_0^{-1}G^< - G^<G_0^{-1} = \Sigma^R G^< - G^<\Sigma^A + - G^R\Xi^< + \Xi^<G^A + - G^R\Theta_{t_0}^< + \Theta_{t_0}^<G^A. \tag{33}$$

At equal external times, $t=t'$, the left-hand side (lhs) of the last equation represents an unrenormalized drift of the one-particle density matrix ρ,

$$\text{lhs of (33)} \overset{t=t'}{\to} \frac{\partial\rho}{\partial t} + i[H_0,\rho]_-. \tag{34}$$

This has the form proper for a quantum transport equation in which $H_0(t)$ is the mean-field one-particle Hamiltonian. The "generalized collision" terms on the right-hand side involve double-time less quantities even for $t=t'$, however. The related integrals extend only to the past because of the presence of the propagator factors. The one-dimensional (1D) integration range is restricted by $\tau^\star$ again, as sketched by a white arrow in Fig. 3(b). The last two generalized collision terms take the initial conditions into account explicitly and their integrand may be nonzero only in the square $\bar{t},\bar{\bar{t}}<t_0+\tau^\star$ of Fig. 3(a). The intersection of this square with the integration range thus becomes empty as the running time t exceeds $t_0+2\tau^\star$ and the initial conditions do not enter any more. This is a formal expression of the Bogolyubov conjecture for the precursor equation. The remaining terms depend on the initial conditions implicitly and their form becomes the same as in the case without initial conditions in the same time region. To achieve the quantum transport equation proper, another standard step is needed, in which all less quantities entering the generalized collision terms will be replaced by expressions involving only the single time distribution of particles ρ.

B. Reconstruction equations and the problem of quantum transport equation

In this section, we continue with the derivation of quantum transport equation from the NGF equations with finite initial time t_0.

We first summarize the method of generating a quantum transport equation from the precursor transport equation standard for the Keldysh initial conditions at $t_0\to-\infty$: (1) the double-time $G^<(t,t')$ is replaced by an expression involving only its time diagonal $\rho(t)=-iG^<(t,t)$ and propagators, (2) this expression is also introduced into the self-energy, for which a self-consistent approximation specifying the self-energy in terms of the Green's function is assumed. The resulting transport equation depends on the approximate replacement. The historically first one is the famous Kadanoff-Baym Ansatz,[1,4] schematically $G^<=\frac{1}{2}[\rho,G^A-G^R]_+$. We will concentrate on the generalized Kadanoff-Baym Ansatz,[4,37,38]

$$G^< = -G^R\rho + \rho G^A. \tag{35}$$

This approximation has a systematic place in an exact scheme for a quantum transport equation employing the reconstruction equations [4,6,37]

$$\begin{aligned} G^<(t,t') &= -G^R(t,t')\rho(t') \qquad \boxed{t\geq t'} \\ &+ \int_{t'}^{t} d\bar{t}\int_{-\infty}^{t'} d\bar{\bar{t}}\, G^R(t,\bar{t})\Sigma^R(\bar{t},\bar{\bar{t}})G^<(\bar{\bar{t}},t') \\ &+ \int_{t'}^{t} d\bar{t}\int_{-\infty}^{t'} d\bar{\bar{t}}\, G^R(t,\bar{t})\Xi^<(\bar{t},\bar{\bar{t}})G^A(\bar{\bar{t}},t') \\ G^<(t,t') &= \rho(t')G^A(t,t') + \cdots \qquad \boxed{t'\geq t}. \end{aligned} \tag{36}$$

The name symbolizes that the two halves of Eq. (36) together permit to reconstruct full $G^<$ from ρ, in other words, to reconstruct a full double-time function from the knowledge of its time diagonal. If the integrals were neglected, the reconstruction would be immediate, but approximate: Eq. (36) would become just the generalized Kadanoff-Baym Ansatz, Eq. (35).

For the present task, we need to extend the notion of reconstruction equations also to the case of finite-time initial conditions, specifically for the embedded (restart) process. The desired equations are in general a consequence of the Dyson equation, specifically of Eq. (25) here. The time partitioning leads to the result almost without effort. First, the partitioning equations for the off-diagonal blocks, Eqs. (20) and (21), are adapted by renaming $t_0 \mapsto t_{-\infty}$ and $t'' \mapsto t_0$. Second, consider, say, the *FP* block. The times involved are ordered as $t' < t'' < t$. The reconstruction equation is obtained by letting the lower two time variables coalesce while keeping their order: $t''-t' \to 0+0$. The partitioning time t'' becomes sliding together with t' but this poses no difficulty. We get

$$G^<_{t_0}(t,t') = -G^R(t,t')\rho(t') \qquad \boxed{t \geq t' \geq t_0}$$

$$+ \int_{t'}^{t} d\bar{t} \int_{t_0}^{t'} d\bar{t} G^R \Sigma^R G^<_{t_0}$$

$$+ \int_{t'}^{t} d\bar{t} \int_{t_0}^{t'} d\bar{t} G^R \Xi^< G^A$$

$$+ \int_{t'}^{t} d\bar{t} \int_{t_0}^{t'} d\bar{t} G^R [\Xi^<_{t_0} - \Xi^<] G^A . \tag{37}$$

The result for the complementary *PF* block is analogous, just as in Eq. (36). If we did not single out the IC terms in Eq. (37), it would look almost identical with Eq. (36), except for the integration limits. The point is, of course, that the IC terms compensate for the truncated integration limits of the host process.

It is interesting to compare the behavior of the full Dyson equation with the reconstruction equations. The last integral in Eq. (37) involving the initial conditions is similar to its analog in Eq. (25), the integration area is different, however. While it is a whole rectangle with the corners (t_0,t_0) and (t,t') in the Dyson equation, it only extends over its upper part with the lower left corner shifted to (t',t_0) for the reconstruction equation. As a consequence, as soon as $t' > t_0 + \tau^\star$, the IC term in the reconstruction Eq. (37) vanishes. We have seen before that the characteristic time for such vanishing in the full Dyson equation is rather τ. This can be understood as follows. The Dyson equation is actually an explicit formula for $G^<_{t_0}$ and the initial conditions are bound to enter it explicitly. By contrast, the reconstruction equations are true integral equations, involving the initial conditions in an oblique manner and imposing them on $G^<_{t_0}$ as on a solution in a successive manner.

This contrasting behavior illuminates the transport equation alternative for generating the full $G^<$ correlation function. In an exact version of this transport approach, reconstruction equations are not standalone equations, but one part of a linked twin process whose other constitutive part is a transport equation obtained in an iterative solution cycle from the precursor transport equation: $G^<_{t_0}$ is substituted from the reconstruction equations, the transport equation is solved for the density matrix $\rho(t)$ and this in turn enters the reconstruction equation as an input.

The initial conditions enter this process both in the reconstruction equations and in the precursor transport equation explicitly, but in both cases only within the early period of time, $t < t_0 + \tau^\star$. Altogether, a formalism for treating transient processes results, which is different for the short initial time interval $(t_0, t_0+\tau^\star)$, and for the rest of the process: all initial conditions are built in during the initial *formation* period, subsequently they are propagated by the dynamics of the process at later times. There are two consequences. First, the differing roles of the initial conditions in the Dyson equation and the quantum transport equation context become harmonized. Second, the outlined transport equation scheme fully corroborates the Bogolyubov conjecture described in Sec. V A.

Finally, we are in the position to discuss, how the finite-time initial conditions affect the possibilities of an approximate direct construction of a quantum transport equation based on the nonequilibrium Green's functions. In other words, of shortcutting the {reconstruction eq. $\rightleftharpoons$ precursor transport equation} cycle. A popular method has been based on the GKBA, Eq. (35). This is an approximation neglecting the integral terms in the reconstruction equation. If all corrections to GKBA are neglected, this also includes the initial correlations. The GKBA itself is insensitive to the initial correlations, that is, it is too coarse to take them into account. Combined with the precursor transport equation, it yields a closed transport theory which is still not free of the initial correlations inherent to the generalized scattering terms, and which is not really consistent in this sense. However, no quantum transport equation theory has the ambition to provide a detailed description of short-time correlations, as this is precluded by the use of the Bogolyubov principle and by an asymptotic long-time nature of the transport equation, which are at its basis.

C. Note on transport in open systems

We conclude the discussion of various approaches to electronic quantum transport by returning to the remarks on the time-variable environment of the electron subsystem. These general comments need not be repeated here; the important point is that, in addition to the internal nonequilibrium dynamics of electrons driven perhaps by external fields, there may be expected important effects of a *changing* environment. Consider a suddenly opened thermal link between the system and a phonon bath. This will have an immediate influence on the electron Green's function, which must adapt to the new decay channels which will cause a loss of coherence of the propagation, reduce the relaxation time, etc. This

process of adaptation will be gradual, having the character of a transient. It is clear that the time-partitioning formalism is ideally suited for such process: the preparation stage is without the thermal contact and it defines the initial state for the follow up, the process of relaxation of the electron subsystem induced by the suddenly attached thermal bath. We have thus at our disposal a Green's-function formalism parallel to the Nakajima-Zwanzig projection method[20] or to the path-integral formulation of Refs. 19 and 21, both developed within the density-matrix technique. We have treated in this manner a similar situation for a mesoscopic molecular bridge[24] with the electron leads suddenly switched on or off. In this case, the switching is accompanied by exchange of particles, in addition to the exchange of energy. The details are different for the two processes but the basic structure of the equations is the same. Namely, it turns out that it is possible to construct the transient Green's function from the two asymptotic steady-state Green's functions, ON and OFF, as from building blocks. The technique is reminiscent of the well-known matching of surface Green's function, only it takes place along the time coordinate rather than in space, in the direction perpendicular to the surface. Obviously, this straightforward approach is restricted to the case that the electron transient does not induce a back reaction in the reservoirs. A systematic treatment of this more general physical situation is a challenging theoretical task.

To conclude this brief discussion, there is a possibility of a uniform treatment of transient processes induced by external fields and by changes in the environment of the system. This is achieved by reformulating the complex initial conditions for the many-particle state in terms of the history of its single-particle Green's function, and a consistently constructed description of the subsequent transient evolution.

VII. CONCLUSIONS

The main results of this paper include: (1) the method of partitioning in time, which permits to relate the NGF and their Dyson equations for a host process and for its components projected onto the past and the future with respect to an arbitrarily selected dividing time. (2) The host process may be thought as composed by the preparation process in the past and by the measuring process in the future, so that measurement starts from an initial state created by the preparation process; it may be arbitrarily out of equilibrium and incorporate all correlations in the many-body system. The NGF then starts from a correlated initial condition prepared in a controlled manner. (3) The partitioning equations are intimately related to the renormalized composition rule for propagators, to the reconstruction equations for the particle correlation function and, by this, also to the nonequilibrium Ward identity,[41,42] although the latter aspect was not discussed here.

(4) The time partitioning is useful for systems, in which the decay time for correlations is short in accordance with the Bogolyubov principle: the past and the future of the host process are coupled only over the period on the order of the correlation time around the dividing instant (present, initial time for the measurement process). (5) These results on the NGF level permit an exact general formulation of the quantum transport equations with correlated initial conditions.

For the future work, we may see two broad directions: (1) to obtain a direct NGF method of treating transients with correlated initial states (NGF solver), the partitioning technique should be combined with suitable preparation processes, in particular, the switch-on processes generated from the Keldysh initial condition and yielding both equilibrium and nonequilibrium initial states for a transient. The partitioning method will serve to transform the general Keldysh method into a building-block scheme.

(2) There is a possibility of a uniform treatment of transient processes induced by external fields and by changes in the environment of the system, contributing to the NGF description of open systems. The progress along these lines will depend of developing the ways on incorporating the back reaction of the (imperfect) baths and reservoirs composing the environment.

(3) The present exact framework for transport equations can be used to develop approximate transport equations for transients starting from a correlated initial state in a controlled way. The only general requirement will be that the correlations decay at a rate faster than any other change in the system. A consistent transport scheme will then describe the transient in three stages: first, the decay of correlations ending with formation of an effective uncorrelated initial condition. The ensuing kinetic stage will be described in terms of a causal Ansatz, possibly improved over the GKBA. The whole kinetic stage will be further divided into the early period with the initial condition still acting and the true kinetic stage with no memory of the initial state.

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