PHYSICAL REVIEW B VOLUME 44, NUMBER 12 15 SEPTEMBER 1991-II

Expansions of nonequilibrium Green's functions

Mathias Wagner*
I. Institut für Theoretische Physik, Jungiusstrasse 9, D-2000 Hamburg 36, Federal Republic of Germany

(Received 9 March 1990)

We present a Green's-function formalism generalized to treat arbitrary time-dependent systems initially prepared with an arbitrary density matrix. On the basis of a simultaneous expansion of the usual real-time development operator and the density matrix, we define a Green's function ordered along an extended contour. In this way we are able to treat real-time many-particle Green's functions and initial correlations on the same footing. Both can be decomposed by Wick's theorem. Thus we may utilize familiar diagrammatic analysis for evaluating the Green's function, and finally arrive at a generalized Dyson's equation. The Green's function can be represented by a (3×3) matrix, which includes the Green's functions used in the Feynman, Matsubara, and Keldysh theories, if the corresponding statistical average is taken. From a matrix representation of Dyson's equation, a basic set of five coupled equations is derived, which explicitly shows the corrections to the Keldysh theory due to an arbitrary initial many-particle density matrix.

I. INTRODUCTION

Green's-function techniques usually rely on an expansion of the Green's function in question in an infinite series of higher Green's functions and a subsequent contraction into products of one-particle Green's functions. This decomposition is greatly simplified by the use of suggestive diagrammatic representations. The rigorous foundation of this procedure is known as Wick's theorem. Up to now several Green's-function formalisms are available (such as those of Feynman, Matsubara, and Keldysh) and their procedures of contraction and the corresponding diagrams seem to be very similar. However, the validity of these contractions depends on the physical properties of the system in question. This is due to the restricted range of validity of Wick's theorem. The most general proof of this theorem as given by Danielewicz[1] has clearly shown the strict necessity for the statistical average to be taken over a one-particle density matrix only. This property of the density matrix is assured differently in the Feynman, Matsubara, and Keldysh theories. Matsubara's approach is only valid for a thermal density matrix, whereas in the Feynman theory as well as in the Keldysh theory an adiabatic switching on of the many-particle interactions is assumed. As a result of the various restrictions imposed, none of these theories includes all the others. Fujita[2,3] was the first who suggested in his pioneering work important improvements. In essence, he used initial correlation functions χ_l to describe the many-particle contribution of the density matrix not accounted for in Wick's theorem. This led to a set of "generalized equations of Kadanoff and Baym." Later, Hall[4] simplified this theory by utilizing the concept of Keldysh Green's functions. However, these Green's functions and the initial correlation functions were still treated differently. It is the purpose of this paper to develop a coherent and systematic contraction theory, which treats these functions on an equal footing. The corresponding Green's-function formalism will be applicable to arbitrary nonequilibrium systems with arbitrary initial density matrices. The main advantages are a further simplification of the theory and the fact that the common theories of Feynman, Matsubara, and Keldysh may be shown to be special cases of the general theory presented here.

The paper is organized as follows: In Sec. II we develop the foundation of a Green's-function formalism valid for arbitrary nonequilibrium systems. It is based on a Green's function suitably defined on a contour c^*. The main result is an exact diagrammatic expansion of this Green's function and the corresponding generalized Dyson's equation. Then, in Sec. III, we present a (3×3)-matrix representation of the Green's function. Writing Dyson's equation in this representation, we derive a basic set of five coupled equations in Sec. IV. In particular this set contains the well-known equation for the spectral density and a transport equation modified by initial correlations of the density matrix. In Sec. V we conclude this paper by discussing our theory's connections with the other time-path theories of Feynman, Matsubara, and Keldysh.

II. THE CONTOUR-PATH FORMALISM

In order to work out the underlying concept we start by reviewing some basic facts. The formal description of an arbitrary experiment may be divided into two parts. In the first place, one has to specify the initial state of the system at a given time t_0. We will refer to this procedure as the "preparation of the system at t_0." However, the information usually given at this point is not sufficient to determine the exact state. Instead, the initial preparation has to be described with a probability distribution function ρ, which associates with each state $|n\rangle$ a certain weighting factor $\rho(n)$, where $0\le\rho(n)\le1$ and $\sum_n \rho(n)=1$. This leads to the well-known concept of the density matrix

$$\rho(t_0) \equiv \sum_n |n(t_0)\rangle \rho(n) \langle n(t_0)| \ . \tag{1}$$

The expectation value of an arbitrary observable O at t_0 is then given by

$$\begin{aligned}\langle O(t_0)\rangle &= \mathrm{Tr}[\rho(t_0)O(t_0)] \\ &= \sum_n \langle n(t_0)|\rho(n)O(t_0)|n(t_0)\rangle \ .\end{aligned} \tag{2}$$

We may therefore state that the preparation of the system at t_0 corresponds to a determination of $\rho(t_0)$. Since we will use the Heisenberg picture, where the density matrix is time independent, we will frequently drop the argument t_0.

The second part of the experiment is a monitoring of the response of the system, i.e., its development in time, which is governed by the Hamiltonian $\mathcal{H}(t)$. For its description we choose the Heisenberg picture. There the states are time independent and the observables obey the equation of motion

$$i\frac{d}{dt}O_{\mathcal{H}}(t) = [O_{\mathcal{H}}(t), \mathcal{H}(t)] + i\frac{\partial}{\partial t}O_{\mathcal{H}}(t) \ . \tag{3}$$

This picture is particularly useful, since it distinguishes the preparation of the system at t_0 and its following time development most clearly. The time-dependent expectation value is then given by

$$\langle O(t)\rangle = \sum_n \langle n(t_0)|\rho(n)O(t)|n(t_0)\rangle \ . \tag{4}$$

In this paper we will focus our interest on the evaluation of two-point functions

$$\langle O(t,t')\rangle = \langle O_1(t)O_2(t')\rangle \ , \tag{5}$$

such as the correlation functions

$$\begin{aligned} i\hat{G}^{12}(1,1') &= -\langle \Psi^{\dagger}_{\mathcal{H}}(1')\Psi_{\mathcal{H}}(1)\rangle \ , \\ i\hat{G}^{21}(1,1') &= \langle \Psi_{\mathcal{H}}(1)\Psi^{\dagger}_{\mathcal{H}}(1')\rangle \ , \end{aligned} \tag{6}$$

which are also known as $G^{<}$ and $G^{>}$. Here $1 \equiv (\mathbf{x}_1, t_1)$ and $\Psi^{\dagger}_{\mathcal{H}}, \Psi_{\mathcal{H}}$ denote creation and annihilation operators in the Heisenberg picture. From these functions every one-particle property may be derived. Unfortunately, we are faced with two serious problems when trying to calculate these two-point functions for an interacting system with an arbitrary initial preparation. The first crucial point is that in solid-state physics the system is usually an interacting many-particle system at time t_0. Hence the states $|n\rangle$ occurring in the definition (1) of the density matrix are many-particle states, i.e., $\rho(t_0)$ is a many-particle density matrix. This is an important difference to the ordinary scattering theory, where the system is generally assumed to be noninteracting at the time of preparation and the interaction is adiabatically switched on afterwards. Though this procedure is well established in scattering theory, its application to solid-state physics is doubtful. And secondly, the time-development operator corresponding to the equation of motion (3) involves many-particle contributions via the Hamiltonian $\mathcal{H}(t)$. A straightforward evaluation of the correlations (6) is only possible for a noninteracting system. This is a system initially prepared with a one-particle density matrix ρ_0, which, moreover, evolves in time according to a noninteracting Hamiltonian $\mathcal{H}(t) \equiv H_0$. In this very special case, however, we may even calculate higher (i.e., many-particle) correlation functions by using Wick's theorem. It states how such a many-particle correlation may exactly be decomposed into sums and products of one-particle correlations. The most general proof of Wick's theorem is due to Danielewicz.[1] He showed rigorously the equivalence of the two statements "Wick's theorem holds exactly" and "The operators to be averaged are noninteracting and the initial density matrix is a one-particle density matrix." These circumstances suggest to search for an appropriate expansion of the correlation functions which allows for the use of Wick's theorem. This will be our next task. To begin, we notice that the restriction of Wick's theorem necessitates a twofold expansion. We have to take care of the initial density matrix and the time-development operator. Formalisms suitable for some special initial density matrices have already been developed by Feynman, Matsubara, and Keldysh. However, we will allow for an *arbitrary* initial density matrix. The connection to the theories of Feynman, Matsubara, and Keldysh will be discussed in the last section.

Let us first consider the initial density matrix $\rho(t_0)$ and expectation values at t_0. We search for an expansion of the many-particle density matrix of Eq. (1) in terms of a one-particle density matrix ρ_0. To this end we will now develop a formalism very similar to that used in Matsubara theory.[5] The basic idea is that Matsubara's expansion procedure only relies on the fact that the thermal density matrix is an exponential function. However, since the density matrix is positive definite and Hermitian, it may always be written as an exponential function

$$\rho(t_0) = \frac{1}{Z}\exp[-\lambda\mathcal{B}(t_0)], \quad Z = \mathrm{Tr}\exp[-\lambda\mathcal{B}(t_0)] \tag{7}$$

with $\mathcal{B}$ as an arbitrary Hermitian, particle-conserving many-particle operator and λ as a real parameter. In particular, we notice that $\mathcal{B}$ is in general *not* equal to $\mathcal{H} - \mu\mathcal{N}$. In analogy to the Matsubara theory we then define for an arbitrary operator O a Heisenberg picture with respect to $\mathcal{B}$ as

$$O_{\mathcal{B}}(\tau) \equiv \exp[i\tau\mathcal{B}(t_0)]O_S(t_0)\exp[-i\tau\mathcal{B}(t_0)] \ . \tag{8}$$

Here the index S denotes as usual the Schrödinger picture and the argument τ is purely imaginary. We stress that the notion "Heisenberg picture" used here is only due to the formal analogy to that picture known in quantum mechanics. In the present context τ should not be confused with the time or viewed as an imaginary time; it is simply a parameter. Now we split off a one-particle density matrix from ρ. For that purpose we choose an arbitrary one-particle operator B_0. It is useful, but not mandatory, to do it in a way that the difference

$$B' = \mathcal{B} - B_0 \tag{9}$$

is small. The density matrix is then rewritten as

$$\rho=\frac{1}{Z}\exp(-\lambda B_0)\exp(\lambda B_0)\exp(-\lambda\mathcal{B})$$
$$=\frac{Z_0}{Z}\rho_0\exp(\lambda B_0)\exp(-\lambda\mathcal{B}) \ , \tag{10}$$

where

$$\rho_0\equiv\frac{1}{Z_0}\exp(-\lambda B_0), \quad Z_0=\mathrm{Tr}\exp(-\lambda B_0) \tag{11}$$

is a one-particle density matrix. The operator

$$S_{c'}(\tau,0)\equiv\exp(i\tau B_0)\exp(-i\tau\mathcal{B}) \tag{12}$$

satisfies the differential equation

$$i\frac{\partial}{\partial\tau}S_{c'}(\tau,0)=B'_{B_0}(\tau)S_{c'}(\tau,0) \ . \tag{13}$$

Here B'_{B_0} is given in the interaction picture with respect to B_0, which is defined for an arbitrary operator O as

$$O_{B_0}(\tau)\equiv\exp(i\tau B_0)O_S(t_0)\exp(-i\tau B_0) \ . \tag{14}$$

Equation (13) may formally be integrated as

$$S_{c'}(\tau,0)=T_{c'}\exp\left[-i\int_0^\tau d\tau' B'_{B_0}(\tau')\right] , \tag{15}$$

where the operator $T_{c'}$ orders along the contour $c'=[0,-i\lambda]$ (compare Fig. 1)

$$T_{c'}O_1(\tau_1)O_2(\tau_2)\equiv\begin{cases}O_1(\tau_1)O_2(\tau_2), & \tau_1>\tau_2 \text{ on } c' \\ -O_2(\tau_2)O_1(\tau_1), & \tau_1\le\tau_2 \text{ on } c' \ .\end{cases} \tag{16}$$

Inserting this into Eq. (10) we eventually get for the initial density matrix

$$\rho=\frac{Z_0}{Z}\rho_0 S_{c'}(-i\lambda,0)\equiv\frac{Z_0}{Z}\rho_0 S_{c'} \ . \tag{17}$$

With this expansion we have reached our first goal. We now may write an arbitrary expectation value at t_0 as

$$\langle O(t_0)\rangle=\frac{Z_0}{Z}\sum_{n_0}\langle n_0(t_0)|\rho_0 S_{c'}O(t_0)|n_0(t_0)\rangle \ . \tag{18}$$

This has the same form as Eq. (2), if we regard ρ_0 as the *initial* density matrix and the product $(Z_0/Z)S_{c'}O(t_0)$ as the operator to be averaged. The advantage is that ρ_0 is a one-particle density matrix and that $S_{c'}O(t_0)$ contains noninteracting operators (i.e., in the interaction picture) only. Hence Wick's theorem holds for each term in the expansion of the $S_{c'}$ matrix. Finally we notice that one recovers the Matsubara theory for the special choice of a thermal density matrix, where $\mathcal{B}=\mathcal{H}-\mu\mathcal{N}$ and $\lambda=\beta$.

Now we turn to the evaluation of two-point functions at times $t,t'\ge t_0$. There we have to deal, moreover, with the second restriction of Wick's theorem, which is that the time-development operator has to be a one-particle operator. However, the evolution in time is described by a time-dependent Hamiltonian $\mathcal{H}(t)$, which usually includes many-particle interactions. To utilize Wick's theorem, though, it is necessary to perform an expansion of the time-development operator similar to the treatment of the initial density matrix. An appropriate method has already been introduced by Keldysh.[6] Nevertheless, for the sake of completeness let us summarize its main features here. The formal expansion will be seen to be very similar to that used for the initial density matrix.

The two-point function (5) contains products of operators at two times. To simplify matters let us start by considering an operator $O(t)$ with a single time argument only. The generalization for products of operators with several times will be simple. We begin with the Heisenberg picture according to Eq. (3). It is easily verified that

$$O_{\mathcal{H}}(t)=\left[\tilde{T}\exp\left[i\int_{t_0}^t d\tau\mathcal{H}(\tau)\right]\right]O_S(t)$$
$$\times\left[T\exp\left[-i\int_{t_0}^t d\tau\mathcal{H}(\tau)\right]\right] \tag{19}$$

is a formal solution of Eq. (3). Here T and $\tilde{T}$ are the time- and antitime-ordering operators for real time

$$\begin{aligned}TO_1(t_1)O_2(t_2)&\equiv\begin{cases}O_1(t_1)O_2(t_2), & t_1>t_2 \\ -O_2(t_2)O_1(t_1), & t_1\le t_2 \ ,\end{cases}\\ \tilde{T}O_1(t_1)O_2(t_2)&\equiv\begin{cases}O_1(t_1)O_2(t_2), & t_1<t_2 \\ -O_2(t_2)O_1(t_1), & t_1\ge t_2 \ .\end{cases}\end{aligned} \tag{20}$$

However, in the long run it is not easy to deal simultaneously with ordering and antiordering operators. A convenient way to memorize the ordering is the use of the contour c shown in Fig. 2. This contour runs on the upper branch from $t_0^{\wedge}=t_0$ to t and on the lower branch back to $t_0^{\vee}=t_0$. Nevertheless, both branches are still lying on the real time. The vertical offset in Fig. 2 is only a

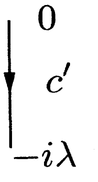

FIG. 1. Generalized contour c' of Matsubara.

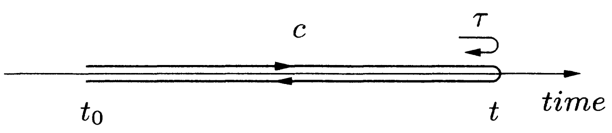

FIG. 2. Keldysh contour c.

graphical method to demonstrate the different sense of ordering. On the upper branch the ordering and the direction of time integration are chronological, whereas they are antichronological on the lower one. This perfectly suits the time development as given by Eq. (19). The upper branch corresponds to the exponential expression on the right-hand side, while the lower one matches the one on the left-hand side. Hence the procedure of ordering may be simplified if we use a contour integral along c and an operator T_c ordering along this contour. Then we may abbreviate Eq. (19) as

$$O_{\mathcal{H}}(t)=T_c \exp\left[-i\int_c d\tau\, \mathcal{H}(\tau)\right] O_S(t) . \tag{21}$$

To account for Wick's theorem we now start by expanding the time-development operator in terms of a development operator corresponding to a noninteracting system. To this end we decompose the total Hamiltonian into two parts

$$\mathcal{H}(t)=H_0+H'(t) , \tag{22}$$

where H_0 is a time-independent, noninteracting but otherwise arbitrary Hamiltonian. In the interaction picture with respect to H_0 the operators obey the differential equation

$$i\frac{d}{dt}O_{H_0}(t)=[O_{H_0}(t),H_0]+i\frac{\partial}{\partial t}O_{H_0}(t) . \tag{23}$$

The Heisenberg and the interaction picture are synchronized at the initial point t_0, where the system has been prepared

$$O_{\mathcal{H}}(t_0)=O_{H_0}(t_0) . \tag{24}$$

With that the operators evolve in time as

$$O_{H_0}(t)=\exp[i(t-t_0)H_0]O_S(t)\exp[-i(t-t_0)H_0] . \tag{25}$$

Combining this with Eq. (21) yields

$$O_{\mathcal{H}}(t)=S_c(t_0^{\vee},t)O_{H_0}(t)S_c(t,t_0^{\wedge}) , \tag{26}$$

where we have defined the S_c matrix on the contour c as

$$\begin{aligned} S_c(\tau_2,\tau_1)\equiv{} & \exp[i(\tau_2-t_0)H_0] \\ & \times T_c \exp\left[-i\int_{\tau_1}^{\tau_2} d\tau\, \mathcal{H}(\tau)\right] \\ & \times \exp[-i(\tau_1-t_0)H_0] . \end{aligned} \tag{27}$$

It obeys a differential equation similar to Eq. (13)

$$i\frac{\partial}{\partial \tau_2}S_c(\tau_2,\tau_1)=H'_{H_0}(\tau_2)S_c(\tau_2,\tau_1) , \tag{28}$$

which is readily integrated to

$$S_c(\tau_2,\tau_1)=T_c \exp\left[-i\int_{\tau_1}^{\tau_2} d\tau\, H'_{H_0}(\tau)\right] . \tag{29}$$

So, finally we have expressed the operator in the Heisenberg picture in terms of operators in the interaction picture

$$O_{\mathcal{H}}(t)=T_c S_c O_{H_0}(t) , \tag{30}$$

where the S_c matrix along the whole contour c is given by

$$S_c \equiv S_c(t_0^{\vee},t_0^{\wedge}) . \tag{31}$$

Up to now we have considered an operator $O(t)$ depending on a single time argument only. The result (30) is easily extended to the case of the two-point function (5). There we have

$$O_{\mathcal{H}}(t,t')=T_c S_c O_{H_0}(t,t') , \tag{32}$$

where the contour c has to go through t and t' in the ordering given by the operators $O_1(t)$ and $O_2(t')$.

Combining this with the corresponding expansion of the initial density matrix we may eventually write an expectation value of an operator $O(t,t')$ as

$$\langle O(t,t')\rangle=\frac{Z_0}{Z}\sum_{n_0}\langle n_0(t_0)|\rho_0 S_{c'} T_c S_c O_{H_0}(t,t')|n_0(t_0)\rangle . \tag{33}$$

The twofold expansion of the initial density matrix and the time-development operator may conveniently be combined to one single expansion. To this end we utilize the striking similarity between the treatment of the initial density matrix and the time-development operator, both of which are exponential functions. We link the two contours c' and c together, $c^*\equiv c'c$ (compare Fig. 3), and introduce a c^*-contour-ordering operator T_{c^*} as

$$T_{c^*}\equiv T_{c'}T_c , \tag{34}$$

which orders along c^*. Hence a point on c is always "earlier" than a point on c'. A similar contour has also been proposed by Mills.[7]

Furthermore, we define a Heisenberg picture with respect to

$$\mathcal{K}(\tau)\equiv\begin{cases}\mathcal{H}(\tau), & \tau \text{ on } c\\ \mathcal{B}(\tau), & \tau \text{ on } c'\end{cases} \tag{35}$$

which is a combination of the Heisenberg pictures defined in Eqs. (21) and (8). Similarly the transformation to the interaction picture is performed with respect to K_0, where

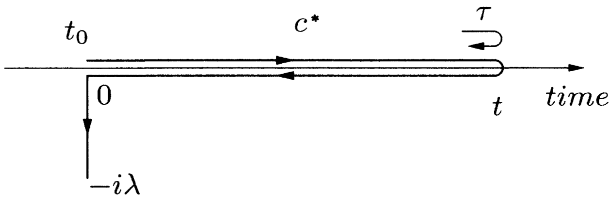

FIG. 3. The contour c^* starts at t_0 and ends at $-i\lambda$. However, note that the x-y plane used to illustrate this contour can in general not be viewed as a complex-time plane. This depicture is only a guide to the eye for better revealing the ordering and integration along the contour.

$$K_0(\tau)\equiv\begin{cases}H_0(\tau), & \tau \text{ on } c\\ B_0(\tau), & \tau \text{ on } c'\ .\end{cases} \tag{36}$$

We collect the expansions of the initial density matrix [Eq. (17)] and the time-development operator [Eq. (30)] in the S_{c^*} matrix

$$\begin{aligned}S_{c^*}\equiv S_{c^*}(-i\lambda,t_0^{\wedge})&=S_{c'}(-i\lambda,0)S_c(t_0^{\vee},t_0^{\wedge})\\&=T_{c^*}\exp\left[-i\int_{c^*}d\tau K'_{K_0}(\tau)\right]\ ,\end{aligned} \tag{37}$$

where

$$K'_{K_0}(\tau)\equiv\begin{cases}H'_{H_0}(\tau), & \tau \text{ on } c\\ B'_{B_0}(\tau), & \tau \text{ on } c'\ .\end{cases} \tag{38}$$

With these definitions we may write Eq. (33) as

$$\langle O(t,t')\rangle=\frac{Z_0}{Z}\,{}_0\langle T_{c^*}S_{c^*}O_{H_0}(t,t')\rangle_0\ , \tag{39}$$

where ${}_0\langle\ \rangle_0$ denotes an average with respect to ρ_0

$${}_0\langle O\rangle_0\equiv\mathrm{Tr}(\rho_0 O)\ . \tag{40}$$

The crucial point about the representations (33) or (39) is that they meet all requirements for the validity of Wick's theorem: Firstly, the average is taken over a one-particle density matrix ρ_0 and secondly, all operators are given in an interaction picture corresponding to a noninteracting system. So Wick's theorem holds for each term in the expansion of the S_{c^*} matrix. Unfortunately, the application of this theorem immediately reveals that such an expansion will contain other functions than the real-time correlations (6) as well. That means that for the real-time functions the system of equations is not closed. The reason is that the S_{c^*} matrix is defined on c^*, whereas the operator $O_{H_0}(t,t')$ is defined for real time only. However, by performing the contraction procedure we encounter averages of all possible pairings of two operators defined on the whole contour c^*, and therefore we have to continue $O_{H_0}(t,t')$ to c^*. A convenient way of handling this problem is to inspect *one* single function, which comprises all the functions occurring in the expansion, since then no distinction of different cases is necessary. This basic function is the c^*-contour-ordered Green's function, which is for fermions defined as

$$\begin{aligned}iG(1,1')&\equiv\langle T_{c^*}\Psi_{\mathcal{H}}(1)\Psi^\dagger_{\mathcal{H}}(1')\rangle\\&=\begin{cases}\langle\Psi_{\mathcal{H}}(1)\Psi^\dagger_{\mathcal{H}}(1')\rangle, & \tau_1>\tau_{1'} \text{ on } c^*\\ -\langle\Psi^\dagger_{\mathcal{H}}(1')\Psi_{\mathcal{H}}(1)\rangle, & \tau_1\le\tau_{1'} \text{ on } c^*\ .\end{cases}\end{aligned} \tag{41}$$

Here both arguments $\tau_1,\tau_{1'}$ lie on the whole contour c^* and the field operators are defined in the Heisenberg picture with respect to $\mathcal{H}$. Obviously this function covers all possible pairings of a creation and an annihilation operator defined on c^*. For example G is equal to the real-time correlations (6) for one argument lying on the upper branch of c and the other one on the lower one. We also notice that the field operators are continuous functions of their contour arguments, since we have the synchronization

$$O_{\mathcal{H}}(t_0)=O_{\mathcal{B}}(0)\ . \tag{42}$$

However, at the connection between c and c' their derivatives are in general not continuous.

By using the representation (39), we have for the c^*-contour-ordered Green's function

$$iG(1,1')=\frac{Z_0}{Z}\,{}_0\langle T_{c^*}S_{c^*}\Psi_{K_0}(1)\Psi^\dagger_{K_0}(1')\rangle_0\ . \tag{43}$$

The expansion of the S_{c^*} matrix yields for the first terms

$$\begin{aligned}iG(1,1')=\frac{Z_0}{Z}\Bigg[&{}_0\langle T_{c^*}\Psi_{K_0}(1)\Psi^\dagger_{K_0}(1')\rangle_0-\frac{i}{1!}\int_{c^*}d\tau_2\,{}_0\langle T_{c^*}K'_{K_0}(\tau_2)\Psi_{K_0}(1)\Psi^\dagger_{K_0}(1')\rangle_0\\&-\frac{1}{2!}\int_{c^*}d\tau_2\int_{c^*}d\tau_3\,{}_0\langle T_{c^*}K'_{K_0}(\tau_2)K'_{K_0}(\tau_3)\Psi_{K_0}(1)\Psi^\dagger_{K_0}(1')\rangle_0+\cdots\Bigg]\ .\end{aligned} \tag{44}$$

The very first term is called the free c^*-contour-ordered Green's function

$$iG_0(1,1')\equiv{}_0\langle T_{c^*}\Psi_{K_0}(1)\Psi^\dagger_{K_0}(1')\rangle_0\ . \tag{45}$$

To determine the higher terms we now specify the interaction operator K'_{K_0}. According to (38) we have to distinguish its behavior on c and c'. On c it describes physical many-particle interactions of the considered particles. On c', however, the "development" operator $\mathcal{B}$ is determined by the initial density matrix and is in general not given by the Hamiltonian $\mathcal{H}$. Hence B'_{B_0} does not necessarily describe physical many-particle interactions. Nevertheless it has formally the same structure as a many-particle operator. Therefore we may write K'_{K_0} as a sum over generalized one-, two-, etc., particle interactions $V_1,(1/2!)V_2,\ldots$

$$\begin{aligned}K'_{K_0}(\tau_1)=&\frac{1}{1!}\int d\mathbf{x}_1\Psi^\dagger_{K_0}(1)V_1(1)\Psi_{K_0}(1)\\&+\frac{1}{2!}\int d\mathbf{x}_1\int_{c^*}d\tau_2 d\mathbf{x}_2\Psi^\dagger_{K_0}(2)\Psi^\dagger_{K_0}(1)V_2(1,2)\\&\times\Psi_{K_0}(1)\Psi_{K_0}(2)+\cdots\ ,\end{aligned} \tag{46}$$

where $V_1, V_2, \ldots$ are arbitrary functions defined on the contour c^* (and in $\mathbf{x}$ space), which are assumed to be symmetric with respect to an interchange of their arguments. We do not need to know their exact specification, which depends on the considered interactions and on the initial density matrix $\rho(t_0)$. We point out, however, that these functions are in general not continuous at the connection between c and c'. Since K'_{K_0} contains at least two field operators, the terms in the expansion (44) involve c^*-contour-ordered many-particle Green's functions of arbitrary order. Now Wick's theorem states that each c^*-contour-ordered n-particle Green's function may exactly be decomposed into products of n one-particle Green's functions as

$$\begin{aligned} G_{n_0}(1,2,\ldots,n,1',2',\ldots,n') &\equiv (-i)^n {}_0\langle T_{c^*}\Psi_{K_0}(1)\Psi^\dagger_{K_0}(1')\Psi_{K_0}(2)\Psi^\dagger_{K_0}(2')\cdots\Psi_{K_0}(n)\Psi^\dagger_{K_0}(n')\rangle_0 \\ &= \sum_{p,p'} \frac{(-1)^{|p|+|p'|}}{n!} G_0(p(1),p'(1'))G_0(p(2),p'(2'))\cdots G_0(p(n),p'(n')) \; , \end{aligned} \tag{47}$$

where $p(i), p'(i')$ are permutation functions. For example, the two-particle Green's function can be contracted to

$$\begin{aligned} G_{2_0}(1,2,1',2') &= -{}_0\langle T_{c^*}\Psi_{K_0}(1)\Psi^\dagger_{K_0}(1')\Psi_{K_0}(2)\Psi^\dagger_{K_0}(2')\rangle_0 \\ &= G_0(1,1')G_0(2,2') - G_0(1,2')G_0(2,1') \; . \end{aligned} \tag{48}$$

With that each term of the expansion (44) is equal to a sum over products of one-particle Green's functions. The resulting vast number of terms in each order in the interaction may conveniently be described by diagrammatic methods. We show in the Appendix that the diagrams are identical with those introduced by Feynman. Moreover, the notations of connected and disconnected, topologically distinct, etc. diagrams are the same and they are used in the same way. This is not surprising, since it reflects the basic mathematical structure of the expansion (44), which is the same in the Feynman, Matsubara, and Keldysh theories, and the fact that Wick's theorem holds. The "only" difference lies in the fact that the diagrams are evaluated differently in each theory. Here we use c^*-contour-ordered Green's functions and integrate each vertex over the contour c^*.

Next we notice that this infinite series of diagrams has the same self-similar structure as in the Feynman theory. This is the graphical correspondence to the fact that the c^*-contour-ordered Green's function obeys a Dyson's equation

$$\begin{aligned} G(1,1') &= G_0(1,1') \\ &\quad + \int_{c^*} d\tau_2 d\mathbf{x}_2 d\tau_3 d\mathbf{x}_3 G_0(1,2)\Sigma(2,3)G(3,1') \; , \end{aligned} \tag{49}$$

where the self-energy Σ is as usual defined as a sum over all topologically distinct proper self-energy diagrams.

With that we have obtained an exact set of equations, namely Dyson's equation (49), and the exact (diagrammatic) representation of the self-energy. It is closed for the c^*-contour-ordered one-particle Green's function G in the sense that no higher Green's function occurs. The price to be paid is the infinite number of diagrams defining the self-energy. The set of equations is valid for arbitrary initial density matrices $\rho(t_0)$ and arbitrary Hamiltonians $\mathcal{H}(t)$. Once the one-particle Green's function is determined, we may extract from it the real-time correlation functions (6) and the physical information contained in them. Equations similar to Eq. (49) have been derived by several authors (Fujita,[2,3] Hall[4]), who have used other definitions for the Green's functions and self-energies, as well as another contour of "time" integration. We will compare their approach with our theory in Sec. V.

In this paper we will not discuss schemes for deriving approximate solutions for the c^*-contour-ordered Green's function G, since they are formally very similar to those used in the Feynman, Matsubara, and Keldysh theories. In essence they rely on a suitable choice of a subset of diagrams for the self-energy. And finally we remark that the expansion procedure developed here is not restricted to the treatment of one-particle Green's functions. We may treat higher Green's functions in the same manner.

III. A MATRIX REPRESENTATION

For practical calculations it is more convenient to use a matrix representation for the c^*-contour-ordered Green's function, which we will now introduce. For this purpose we decompose the contour into three parts (compare Fig. 3). The first one consists of the upper branch of c, which runs from t_0 in positive time direction, the second one is given by the lower branch leading back to t_0 and the third one is the hook c'. The c^*-contour-ordered Green's function has two parameters, τ_1 and $\tau_{1'}$ on the contour c^*. Thus there are nine different possibilities to distribute these two parameters over the three branches, which can naturally be grouped in a (3×3) matrix

$$\hat{G}(1,1') = \begin{bmatrix} \hat{G}^{11}(1,1') & \hat{G}^{12}(1,1') & \hat{G}^{13}(1,1') \\ \hat{G}^{21}(1,1') & \hat{G}^{22}(1,1') & \hat{G}^{23}(1,1') \\ \hat{G}^{31}(1,1') & \hat{G}^{32}(1,1') & \hat{G}^{33}(1,1') \end{bmatrix} . \tag{50}$$

The row index denotes the position of τ_1 on the three branches, whereas the column index refers to the position of $\tau_{1'}$. The matrix elements are evaluated by determining the effect of the contour-ordering operator T_{c^*} on the product $\Psi(1)\Psi^\dagger(1')$ for each configuration $\tau_1, \tau_{1'}$ on the contour c^*.

The first four possibilities with real-time arguments t_1, t_2 are well known in the Keldysh theory

$$
\begin{aligned}
i\hat{G}^{11}(1,1') &= \langle T\Psi(1)\Psi^{\dagger}(1')\rangle = \begin{cases} \langle \Psi(1)\Psi^{\dagger}(1')\rangle = i\hat{G}^{21}(1,1'), & t_1 > t_{1'} \\ -\langle \Psi^{\dagger}(1')\Psi(1)\rangle = i\hat{G}^{12}(1,1'), & t_1 \leq t_{1'} \end{cases} \\
i\hat{G}^{22}(1,1') &= \langle \tilde{T}\Psi(1)\Psi^{\dagger}(1')\rangle = \begin{cases} \langle \Psi(1)\Psi^{\dagger}(1')\rangle = i\hat{G}^{21}(1,1'), & t_1 < t_{1'} \\ -\langle \Psi^{\dagger}(1')\Psi(1)\rangle = i\hat{G}^{12}(1,1'), & t_1 \geq t_{1'} \end{cases} \\
i\hat{G}^{12}(1,1') &= -\langle \Psi^{\dagger}(1')\Psi(1)\rangle \;, \\
i\hat{G}^{21}(1,1') &= \langle \Psi(1)\Psi^{\dagger}(1')\rangle \;.
\end{aligned} \tag{51}
$$

The contour-ordering operator T_{c^*} works chronologically on the upper branch and antichronologically on the lower one. Therefore the diagonal elements $\hat{G}^{11}$ and $\hat{G}^{22}$ are, respectively, the time- and antitime-ordered Green's functions. In contrast to that, for the off-diagonal elements, the ordering of the field operators is fixed, since their arguments are lying on different branches of the contour. Therefore we have as off-diagonal elements the real-time correlation functions $\hat{G}^{12}$ and $\hat{G}^{21}$, which have already been introduced in Eq. (6).

The component $\hat{G}^{33}$ has both of its arguments $\nu_1 = \tau_1$, $\nu_{1'} = \tau_{1'}$ on the hook c' and is given by

$$
\begin{aligned}
i\hat{G}^{33}(1,1') &= \langle T_{c'}\Psi(1)\Psi^{\dagger}(1')\rangle \\
&= \begin{cases} \langle \Psi(1)\Psi^{\dagger}(1')\rangle, & \nu_1 > \nu_{1'} \text{ on } c' \\ -\langle \Psi^{\dagger}(1')\Psi(1)\rangle; & \nu_1 \leq \nu_{1'} \text{ on } c' \;. \end{cases}
\end{aligned} \tag{52}
$$

By using the properties of the trace it is easily verified that $\hat{G}^{33}$ obeys periodic boundary conditions

$$
\hat{G}^{33}(1,1') = -\hat{G}^{33}(1,2)\big|_{\mathbf{x}_2 = \mathbf{x}_{1'}, \nu_2 = \nu_{1'} - i\lambda} \tag{53}
$$

(the negative sign is for fermions) and depends on $\nu_1 - \nu_{1'}$ only

$$
\hat{G}^{33}(1,1') = \hat{G}^{33}(\mathbf{x}_1, \mathbf{x}_{1'}, \nu_1 - \nu_{1'}) \;. \tag{54}
$$

Last but not least there are some mixing matrix elements with one real-time argument and one on c'

$$
\begin{aligned}
i\hat{G}^{13}(1,1') &= i\hat{G}^{23}(1,1') \\
&= -\langle \Psi^{\dagger}(1')\Psi(1)\rangle, \quad \nu_{1'} \text{ on } c' \\
i\hat{G}^{31}(1,1') &= i\hat{G}^{32}(1,1') \\
&= \langle \Psi(1)\Psi^{\dagger}(1')\rangle, \quad \nu_1 \text{ on } c' \;.
\end{aligned} \tag{55}
$$

Since they have arguments on different branches of the contour, they are again correlation functions with a fixed ordering of the field operators.

The matrix representation of the self-energy is a little bit more complex. We will see in the following investigation that there are two main types with different representations, namely the regular and the irregular self-energy. This notation has been introduced in the Keldysh theory by Danielewicz.[1] A decomposition of the self-energy into two parts, however, was already used by Kadanoff and Baym[8] for the electron-electron interaction. They denoted them as Σ^{HF} and Σ^{C}, respectively.

The regular self-energy is, for example, due to the electron-phonon interaction. It has a representation similar to the c^*-contour-ordered Green's function

$$
\hat{\Sigma}^{\mathrm{reg}}(1,1') = \begin{bmatrix} \hat{\Sigma}^{11}(1,1') & \hat{\Sigma}^{12}(1,1') & \hat{\Sigma}^{13}(1,1') \\ \hat{\Sigma}^{21}(1,1') & \hat{\Sigma}^{22}(1,1') & \hat{\Sigma}^{23}(1,1') \\ \hat{\Sigma}^{31}(1,1') & \hat{\Sigma}^{32}(1,1') & \hat{\Sigma}^{33}(1,1') \end{bmatrix} . \tag{56}
$$

The matrix elements obey the relations

$$
\begin{aligned}
\hat{\Sigma}^{11}(1,1') &= \begin{cases} -\hat{\Sigma}^{21}(1,1'), & t_1 > t_{1'} \\ -\hat{\Sigma}^{12}(1,1'), & t_1 \leq t_{1'} \end{cases} \\
\hat{\Sigma}^{22}(1,1') &= \begin{cases} -\hat{\Sigma}^{21}(1,1'), & t_1 < t_{1'} \\ -\hat{\Sigma}^{12}(1,1'), & t_1 \geq t_{1'} \end{cases} \\
\hat{\Sigma}^{13}(1,1') &= -\hat{\Sigma}^{23}(1,1'), \quad \nu_{1'} \text{ on } c' \\
\hat{\Sigma}^{31}(1,1') &= -\hat{\Sigma}^{32}(1,1'), \quad \nu_1 \text{ on } c' \;.
\end{aligned} \tag{57}
$$

These relations are very similar to those obeyed by the c^*-contour-ordered Green's function. In fact, the relations of the matrix elements of the product $\hat{\tau}_3\hat{\Sigma}^{\mathrm{reg}}\hat{\tau}_3$, where

$$
\hat{\tau}_3 \equiv \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} , \tag{58}
$$

are identical with (51) and (55).

The irregular self-energy describes, for example, external potentials and effective one-particle potentials due to the electron-electron interaction. It does not have the properties of a c^*-contour-ordered Green's function, since it contains a δ function on the contour, i.e.,

$$
\hat{\delta}(\tau_1 - \tau_{1'}) = \begin{bmatrix} \delta(t_1 - t_{1'}) & 0 & 0 \\ 0 & -\delta(t_1 - t_{1'}) & 0 \\ 0 & 0 & \delta(\nu_1 - \nu_{1'}) \end{bmatrix} . \tag{59}
$$

Hence its matrix representation is diagonal and given by

$$
\hat{\Sigma}^{\mathrm{irreg}}(1,1') = \begin{bmatrix} \hat{\Sigma}^{11}(1,1') & 0 & 0 \\ 0 & \hat{\Sigma}^{22}(1,1') & 0 \\ 0 & 0 & \hat{\Sigma}^{33}(1,1') \end{bmatrix} , \tag{60}
$$

where

$$\begin{aligned}\hat{\Sigma}^{11}(1,1')&=\Sigma_1(1,1')\delta(t_1-t_{1'})\ ,\\ \hat{\Sigma}^{22}(1,1')&=-\Sigma_1(1,1')\delta(t_1-t_{1'})\ ,\\ \hat{\Sigma}^{33}(1,1')&=\Sigma_3(1,1')\delta(\nu_1-\nu_{1'})\ .\end{aligned} \tag{61}$$

In the following we will extend the notion "regular" and "irregular" to arbitrary matrices. A regular matrix has elements obeying the relations (57), whereas an irregular matrix is diagonal like (60) and (61). The reason for distinguishing them is their different transformational behavior.

The convenience of this matrix representation becomes evident when we inspect products of c^*-contour-ordered (Green's) functions. There are two different types of products to be investigated. Firstly, we have the so-called serial product or convolution

$$F(1,1')=\int_{c^*} d\tau_2 d\mathbf{x}_2 A(1,2)V(2)B(2,1')\ . \tag{62}$$

We encounter this product in Dyson's equation in the term ΣG and at the vertices of many interactions, for example potential scattering. Secondly, we have the parallel product

$$F(1,1')=A(1,1')B(1,1')\ . \tag{63}$$

This product is needed for describing the interaction of electrons with phonons or photons. There, let us say, A corresponds to an electron diagram (i.e., it has one electron line running in and one out) and B to a phonon (photon) Green's function. Another important application is an instantaneous two-particle interaction like the Coulomb interaction. Here we have to insert the Coulomb potential, which contains a δ function on the contour c^*, for B.

Let us first investigate the serial product. Considering all possibilities for the inner contour argument τ_2, the matrix representation of F is given by the matrix product

$$\begin{aligned}\hat{F}(1,1')=&\left[\int_{t_0}^{\infty}dt_2+\int_0^{-i\lambda}d\nu_2\right]\\ &\times\int d\mathbf{x}_2\hat{A}(1,2)\hat{V}_0(2)\hat{B}(2,1')\ ,\end{aligned} \tag{64}$$

where the vertex matrix

$$\hat{V}_0(2)\equiv\begin{bmatrix}V_{H_0}(2)P_c(2) & 0 & 0\\ 0 & -V_{H_0}(2)P_c(2) & 0\\ 0 & 0 & V_{B_0}(2)P_{c'}(2)\end{bmatrix} \tag{65}$$

has to be inserted between the matrices $\hat{A}$ and $\hat{B}$. Here we have simplified the integration along the three branches as $d\tau_2=(dt_2,-dt_2,d\nu_2)$, and the projectors P_c, $P_{c'}$ defined on the contour c^* as

$$\begin{aligned}P_c(1)&\equiv\begin{cases}1, & \tau_1 \text{ on } c\\ 0, & \tau_1 \text{ on } c'\end{cases}\\ P_{c'}(1)&\equiv\begin{cases}0, & \tau_1 \text{ on } c\\ 1, & \tau_1 \text{ on } c'\end{cases}\end{aligned} \tag{66}$$

are used to restrict the contour integrals properly.

The matrix representation of the parallel function is quite simple. Since the arguments $\tau_1,\tau_{1'}$ of the functions A and B are the same, the representation of their product is given by

$$\hat{F}^{ij}(1,1')=\hat{A}^{ij}(1,1')\hat{B}^{ij}(1,1')\ . \tag{67}$$

It should be noted here that this derivation of the representation of products of c^*-contour-ordered functions does not rely on any special properties of c^*-contour-ordered functions. Especially they do not need to be Green's functions. This reflects the fact that strictly speaking the matrix is a representation of two arguments on the contour, but not of the c^*-contour-ordered function itself.

It is easy to see that regular and irregular matrices transform in a different way when the representation is changed. It is therefore important to know whether a given diagram is regular or irregular, if its components are known to be regular or irregular. To decide this question we note that each diagram can be decomposed into nested serial and parallel products, which may be investigated one after another. It is easily proved that the serial product $\hat{\tau}_3 F\hat{\tau}_3$ is irregular only if both of its components A and B are irregular; otherwise it is regular. Similarly one shows that the parallel product $\hat{\tau}_3 F\hat{\tau}_3$ is regular only if both of its components A and B are regular; otherwise it is irregular. Hence, if the basic constituents (i.e., Green's functions and vertices) are regular or irregular, then all resulting diagrams are either regular or irregular. With that we have proved that the decomposition of the self-energy into a regular and an irregular part is exact.

By now we have derived a (3×3)-matrix representation for two-point functions defined on the contour c^*. With the representations of the c^*-contour-ordered Green's function G and the self-energy Σ it is possible to write the Dyson's equation (49) as a matrix equation

$$\begin{aligned}\hat{G}(1,1')=&\ \hat{G}_0(1,1')\\ &+\int(dt_2+d\nu_2)d\mathbf{x}_2\\ &\quad\times\int(dt_3+d\nu_3)d\mathbf{x}_3\\ &\quad\quad\times\hat{G}_0(1,2)\hat{\Sigma}(2,3)\hat{G}(3,1')\ .\end{aligned} \tag{68}$$

From this set of nine equations we will extract in the following section a subset of five independent equations, which may be interpreted physically.

IV. A MINIMAL SET OF EQUATIONS

To avoid the cumbersome notation of four-dimensional integrals let us first adopt a notation similar to that used by Rammer and Smith.[9] We define the (fourfold) convolution for c^*-contour-ordered functions as

$$(\mathcal{A}\otimes\mathcal{C})(1,1')\equiv\int_{c^*}d\tau_2 d\mathbf{x}_2\mathcal{A}(1,2)\mathcal{C}(2,1')\ , \tag{69}$$

and the combination of this convolution with the commutator as

$$[\mathcal{A}\otimes\mathcal{C}]^{\pm}(1,1')\equiv(\mathcal{A}\otimes\mathcal{C})(1,1')\pm(\mathcal{C}\otimes\mathcal{A})(1,1')\ . \tag{70}$$

This is readily extended to the case of the matrix representation. There the projectors $P_c, P_{c'}$ occurring at each vertex [compare Eqs. (64)–(66)] lead to

$$(\hat{\mathcal{A}}^{ij}\otimes\hat{\mathcal{C}}^{jk})(1,1')$$
$$=\begin{cases}\int dt_2 d\mathbf{x}_2\hat{\mathcal{A}}^{ij}(1,2)\hat{\mathcal{C}}^{jk}(2,1'), & j=1,2\\ \int d\nu_2 d\mathbf{x}_2\hat{\mathcal{A}}^{ij}(1,2)\hat{\mathcal{C}}^{jk}(2,1'), & j=3\ .\end{cases} \tag{71}$$

With the help of notion (69) Dyson's equation (68) can be written as

$$(\hat{G}_0^{-1}-\hat{\Sigma})\otimes\hat{G}=\hat{\delta} \tag{72}$$

and its adjungate as

$$\hat{G}\otimes(\hat{G}_0^{-1}-\hat{\Sigma})=\hat{\delta}\ . \tag{73}$$

The right-hand side $\hat{\delta}$ denotes the four-dimensional δ function defined in Eq. (59). The inverse free Green's function $\hat{G}_0^{-1}$ is defined to be

$$\hat{G}_0^{-1}(1,1')\equiv\left[i\frac{\partial}{\partial\tau_1}-K_0(1)\right]\hat{\delta}(1-1')$$
$$=\left[-i\frac{\partial}{\partial\tau_{1'}}-K_0(1')\right]\hat{\delta}(1-1')\ . \tag{74}$$

However, the inverse free Green's function $\hat{G}_0^{-1}$ and the irregular self-energy transform in the same way, since both contain δ functions on the contour. To simplify the following equations, it is therefore useful to combine them by redefining

$$\hat{G}_0^{-1}(1,1')\equiv\left[i\frac{\partial}{\partial\tau_1}-K_0(1)\right]\hat{\delta}(1-1')-\hat{\Sigma}^{\text{irreg}}(1,1')$$
$$=\left[-i\frac{\partial}{\partial\tau_{1'}}-K_0(1')\right]\hat{\delta}(1-1')-\hat{\Sigma}^{\text{irreg}}(1,1')\ . \tag{75}$$

Then we have the modified Dyson's equation

$$(\hat{G}_0^{-1}-\hat{\Sigma}^{\text{reg}})\otimes\hat{G}=\hat{\delta} \tag{76}$$

and its adjungate

$$\hat{G}\otimes(\hat{G}_0^{-1}-\hat{\Sigma}^{\text{reg}})=\hat{\delta}\ . \tag{77}$$

This matrix representation of the Dyson's equation yields a set of nine coupled equations for nine matrix elements. Unfortunately, it has two disadvantages. Firstly, some of the matrix elements are not directly related to physical quantities. And secondly, by inspecting the definitions we notice that there are only five independent matrix elements in the (3×3) matrix. It is therefore desirable to transform the matrix so that the number of nonvanishing matrix elements is minimized. A convenient way to do this is the following (nonunitary) transformation:

$$\underline{G}(1,1')=L\hat{\tau}_3\hat{G}(1,1')L^{\dagger}\ . \tag{78}$$

Here

$$L=\frac{1}{\sqrt{2}}\begin{bmatrix}1 & -1 & 0\\ 1 & 1 & 0\\ 0 & 0 & \sqrt{2}\end{bmatrix}\ . \tag{79}$$

The resulting matrix is

$$\underline{G}(1,1')=\begin{bmatrix}G^r(1,1') & G^k(1,1') & \sqrt{2}\hat{G}^{13}(1,1')\\ 0 & G^a(1,1') & 0\\ 0 & \sqrt{2}\hat{G}^{31}(1,1') & \hat{G}^{33}(1,1')\end{bmatrix}\ . \tag{80}$$

The Keldysh part of the matrix has been transformed into the *rak* representation,[10] which as matrix elements has the retarded and advanced Green's function and the Keldysh function

$$G^r(1,1')=\hat{G}^{11}(1,1')-\hat{G}^{12}(1,1')$$
$$=\Theta(t_1-t_{1'})[\hat{G}^{21}(1,1')-\hat{G}^{12}(1,1')]\ ,$$
$$G^a(1,1')=\hat{G}^{12}(1,1')-\hat{G}^{22}(1,1')$$
$$=-\Theta(t_{1'}-t_1)[\hat{G}^{21}(1,1')-\hat{G}^{12}(1,1')]\ , \tag{81}$$
$$G^k(1,1')=\hat{G}^{12}(1,1')+\hat{G}^{21}(1,1')\ .$$

The representation (80) still has more than five nonvanishing matrix elements, but anyway, it seems to be the best one attainable. Accordingly, the regular self-energy is transformed into

$$\underline{\Sigma}^{\text{reg}}(1,1')=\begin{bmatrix}\Sigma^r(1,1') & \Sigma^k(1,1') & \sqrt{2}\hat{\Sigma}^{13}(1,1')\\ 0 & \Sigma^a(1,1') & 0\\ 0 & \sqrt{2}\hat{\Sigma}^{31}(1,1') & \hat{\Sigma}^{33}(1,1')\end{bmatrix} \tag{82}$$

with

$$\Sigma^r(1,1')=\hat{\Sigma}^{11}(1,1')+\hat{\Sigma}^{12}(1,1')$$
$$=-\Theta(t_1-t_{1'})[\hat{\Sigma}^{21}(1,1')-\hat{\Sigma}^{12}(1,1')]$$
$$\Sigma^a(1,1')=-\hat{\Sigma}^{12}(1,1')-\hat{\Sigma}^{22}(1,1')$$
$$=\Theta(t_{1'}-t_1)[\hat{\Sigma}^{21}(1,1')-\hat{\Sigma}^{12}(1,1')] \tag{83}$$
$$\Sigma^k(1,1')=-\hat{\Sigma}^{12}(1,1')-\hat{\Sigma}^{21}(1,1')\ .$$

The transformation of the irregular self-energy is easy

$$\underline{\Sigma}^{\text{irreg}}(1,1')$$
$$=\begin{bmatrix}\hat{\Sigma}^{11}(1,1') & 0 & 0\\ 0 & -\hat{\Sigma}^{22}(1,1') & 0\\ 0 & 0 & \hat{\Sigma}^{33}(1,1')\end{bmatrix}\ . \tag{84}$$

As a set of five independent matrix elements we choose the c'-ordered Green's function $\hat{G}^{33}$, the correlations $\hat{G}^{13}$ and $\hat{G}^{31}$, the Keldysh function G^k, and the spectral density A, which is defined as

$$A(1,1')\equiv i[G^r(1,1')-G^a(1,1')] \ . \tag{85}$$

This function is independent of the correlation functions $\hat{G}^{12}(1,1')$ and $\hat{G}^{21}(1,1')$—at least in the lowest order in the interaction. We see, for example, that the commutation rules give for $t_{1'}=t_1$

$$A(1,1')|_{t_{1'}=t_1}=\delta(\mathbf{x}_1-\mathbf{x}_{1'}) \ . \tag{86}$$

The Keldysh function G^k contains information about the distribution function, i.e., about the occupation of the states described by the spectral density A. With Eqs. (81) and (85) we have

$$G^k(1,1')=2\hat{G}^{12}(1,1')-iA(1,1') \ , \tag{87}$$

where $n(1)=-i\hat{G}^{12}(1)$ is the particle density in $\mathbf{x}$ space. To show the qualitative behavior of the correlation functions $\hat{G}^{13}$ and $\hat{G}^{31}$ let us inspect, for example, $\hat{G}^{13}(1,1')$ [compare Eq. (55)]. It contains two operators. The first one has a real-time argument, whereas the second one has its argument on the hook c'. However, we can associate a real time even to the second operator if we utilize the fact that the interaction picture on the real time (with respect to H_0) and that on the contour c' (with respect to B_0) coincides for $t_{1'}=t_0$ and $\nu_{1'}=0$ [compare Eq. (42)]. Therefore we can qualitatively take the real time t_0 for operators on the contour c', and the correlation is roughly a function of t_1-t_0

$$\hat{G}^{13}(1,1')\simeq F(t_1-t_0) \ . \tag{88}$$

Hence these correlations measure the long-time effect of the many-particle contributions in the initial density matrix $\rho(t_0)$. They are therefore called "initial correlations." The c'-ordered Green's function $\hat{G}^{33}$ generates initial conditions on the (real-time) Green's functions and correlations at t_0. With Eqs. (42) and (52) we have

$$\begin{aligned}&\lim_{\nu_1\to 0}\lim_{\nu_{1'}\to 0}\hat{G}^{33}(1,1')=\hat{G}^{21}(1,1')|_{t_1=t_{1'}=t_0} \ ,\\ &\lim_{\nu_{1'}\to 0}\lim_{\nu_1\to 0}\hat{G}^{33}(1,1')=\hat{G}^{12}(1,1')|_{t_1=t_{1'}=t_0} \ .\end{aligned} \tag{89}$$

Before deriving differential equations for these five independent quantities, it is convenient to define some other related functions such as the symmetric parts of the Green's function

$$G^{r+a}(1,1')\equiv\tfrac{1}{2}[G^r(1,1')+G^a(1,1')] \tag{90}$$

and of the self-energy

$$\Sigma^{r+a}(1,1')\equiv\tfrac{1}{2}[\Sigma^r(1,1')+\Sigma^a(1,1')] \ . \tag{91}$$

These quantities are well known; they describe renormalization effects. In the gradient approximation they are equal to the familiar functions ReG and ReΣ, respectively. (In general, however, they are not real.) Finally we define the linewidth function Γ as

$$\Gamma(1,1')\equiv i[\Sigma^r(1,1')-\Sigma^a(1,1')] \ . \tag{92}$$

Now the 33-component of Dyson's equation in the representation (78) immediately yields

$$(\underline{G}_0^{-1}-\hat{\Sigma}^{33})\otimes\hat{G}^{33}=\delta \tag{93}$$

for the c'-ordered Green's function $\hat{G}^{33}$. [According to Eq. (71) the convolution $\otimes$ is restricted to c'.] It is important to notice that (93) is an equation for $\hat{G}^{33}$ only, since other components of our (3×3) matrix do not occur in an expansion of $\hat{\Sigma}^{33}$. Since parallel products do not mix the matrix elements, it is sufficient for showing this to consider the 33-component of a typical serial product of two functions $\hat{A}$ and $\hat{B}$

$$\hat{F}^{33}(1,1')=\int_{t_0}^{\infty}dt_2d\mathbf{x}_2V_{H_0}(2)[\hat{A}^{31}(1,2)\hat{B}^{13}(2,1')-\hat{A}^{32}(1,2)\hat{B}^{23}(2,1')]+\int_0^{-i\lambda}d\nu_2d\mathbf{x}_2\hat{A}^{33}(1,2)V_{B_0}(2)\hat{B}^{33}(2,1') \ . \tag{94}$$

With Eqs. (57) and (60) we have the identities

$$\hat{A}^{31}=-\hat{A}^{32}, \quad \hat{B}^{13}=-\hat{B}^{23} \tag{95}$$

irrespectively of $\hat{A}$ and $\hat{B}$ being regular or irregular matrices. With that the first two terms in (94) cancel each other and only the term

$$\hat{F}^{33}(1,1')=\int_0^{-i\lambda}d\nu_2\hat{G}^{33}(1,2)V_{B_0}(2)\hat{G}^{33}(2,1') \tag{96}$$

remains. Hence the equation for the 33-component, i.e., $\hat{G}^{33}$, is closed, regardless of the initial density matrix $\rho(t_0)$ used for averaging. The physical reason is causality: The initial preparation does not depend on the further time development of the system. Once Eq. (93) is solved, the real-time correlations and Green's functions at t_0, corresponding to the chosen density matrix $\rho(t_0)$, are determined via Eq. (89). The evaluation of $\hat{G}^{33}(1,1')$ may take advantage of the periodic boundary conditions (53) and of the fact that $\hat{G}^{33}(1,1')$ depends on $\nu_1-\nu_{1'}$ only [Eq. (54)].

The 32- and 13-components of Dyson's equation yield equations of motion for the initial correlations $\hat{G}^{13}$ and $\hat{G}^{31}$

$$\begin{aligned}&(\underline{G}_0^{-1}-\Sigma^r)\otimes\hat{G}^{13}-\hat{\Sigma}^{13}\otimes\hat{G}^{33}=0 \ ,\\ &(\underline{G}_0^{-1}-\hat{\Sigma}^{33})\otimes\hat{G}^{31}-\hat{\Sigma}^{31}\otimes G^a=0 \ .\end{aligned} \tag{97}$$

These equations couple the initial correlations to the Green's function $\hat{G}^{33}$ and to the real-time development of the system.

This real-time development is described by two further equations. We arrive at an equation for the spectral density A by performing some algebraic manipulations on the 11- and 22-components of Dyson's equation and its adjungate

$$[(\underline{G}_0^{-1}-\Sigma^{r+a})\otimes_{,} A]^- - [\Gamma\otimes_{,} G^{r+a}]^- = 0 \; . \qquad (98)$$

Here the integrals are with Eq. (71) restricted to the real-time domain and therefore the equation does not explicitly depend on the initial preparation at t_0. It has formally the same structure as the corresponding equations discussed by Kadanoff and Baym[8] or Rammer and Smith.[9] However, in general it is coupled to Eq. (97) and the following transport equation for G^k, which can be derived from the 12-components of Dyson's equation and its adjungate

$$\begin{aligned}[(\underline{G}_0^{-1}-\Sigma^{r+a})\otimes_{,} G^k]^- - [\Sigma^k\otimes_{,} G^{r+a}]^- &= \frac{i}{2}([\Sigma^k\otimes_{,} A]^+ - [\Gamma\otimes_{,} G^k]^+)\\ &\quad + 2(\hat{G}^{13}\otimes\hat{\Sigma}^{31}+\hat{\Sigma}^{13}\otimes\hat{G}^{31}) \; . \end{aligned} \qquad (99)$$

The left-hand side and the first two terms of the right-hand side involve, according to Eq. (71), integrals over real time only. They describe the evolution of the system in time due to physical interactions and have extensively been discussed in literature (for example Refs. 8 and 9). The last two terms are connected with the initial correlations; therefore $\otimes$ denotes an integral over c'. These terms are not known in the Keldysh theory. They are the reminiscence of the initial preparation of the system at t_0.

The set of equations (93) and (97)–(99) constitutes a complete description of a system with an arbitrary initial preparation at t_0 [described by $\mathcal{B}(t_0)$], and a following transient behavior governed by a time-dependent Hamiltonian $\mathcal{H}(t)$. The determination of the five independent quantities eventually yields the real-time correlations (6), from which every one-particle property of the system can be deduced.

To calculate the stationary state for $\lim_{t\to\infty}$ we often may utilize a considerably simplified system of equations. If for one reason or another we assume the initial correlation functions to be exponentially decaying with

$$F(t-t_0)\propto \exp[-\alpha(t-t_0)] \; , \qquad (100)$$

then they will damp out in the transport equation, and the stationary state can be calculated with the reduced transport equation

$$[(\underline{G}_0^{-1}-\Sigma^{r+a})\otimes_{,} G^k]^- - [\Sigma^k\otimes_{,} G^{r+a}]^- = \frac{i}{2}([\Sigma^k\otimes_{,} A]^+ - [\Gamma\otimes_{,} G^k]^+) \qquad (101)$$

and the equation for the spectral density, Eq. (98). With that we only have to determine a self-consistent solution for the Keldysh function G^k and the spectral density A, which satisfies the two equations (98) and (101).

The complete set of five equations is necessary, however, if we are interested in the transient behavior of the system a short time after the preparation, or if the initial correlations do not decay (due to symmetry and conservation laws). For example, the initial correlations will not decay in systems where a many-particle interaction induces various metastable ground (or steady) states. Here the initial correlations determine which of these metastable states will be the final state.

V. CONNECTIONS TO OTHER GREEN'S-FUNCTION THEORIES

It is instructive to inspect the matrix representation for the c^*-contour-ordered Green's function a bit further, because we will then find that it comprises the Green's functions defined by Feynman, Matsubara, and Keldysh. The Green's-function formalism most often used is the one introduced by Feynman.[11] It is employed to calculate ground-state properties of time-independent systems. The Green's function utilized there is the expectation value of the time-ordered product of an annihilation and a creation operator taken in the ground state of the system. Approximations are derived by expanding the time-development operator in an interaction picture with respect to a noninteracting Hamiltonian H_0. This treatment is based on two crucially important theorems. The first one is the Gell-Mann and Low theorem concerning the adiabatic time development of the states;[12] and secondly, Wick's theorem (in its original version) is used.[13]

The component $\hat{G}^{11}$ is also a real-time-ordered Green's function [compare Eq. (51)] and therefore very similar to that defined by Feynman. They only differ in the density matrix used for averaging. Due to the matrix structure of the Dyson's equation, the 11-component is generally coupled to the other components. A Dyson's equation closed for $\hat{G}^{11}$ may be set up if the initial density matrix is a projector on a pure one-particle state, $\rho_0 = |n\rangle_{0\,0}\langle n|$, and the theorem of Gell-Mann and Low applies. Firstly, we notice that in this case the components $\hat{G}^{13}$, $\hat{G}^{23}$, $\hat{G}^{31}$, and $\hat{G}^{32}$ do not contribute to $\hat{G}^{11}$, since for $\rho\equiv\rho_0$ no expansion of ρ is necessary. Therefore we have

$$\begin{aligned} i\hat{G}^{11}(1,1') &= {}_0\langle n|S^{-1}TS\Psi_{H_0}(1)\Psi^{\dagger}_{H_0}(1')|n\rangle_0 \\ &= \sum_m {}_0\langle n|S^{-1}|m\rangle_0 \\ &\qquad \times {}_0\langle m|TS\Psi_{H_0}(1)\Psi^{\dagger}_{H_0}(1')|n\rangle_0 \; , \end{aligned} \qquad (102)$$

where the S matrix is restricted to the upper branch of the contour, i.e., $S=S(+\infty,-\infty)$. Now the theorem of Gell-Mann and Low says that the states $|+\infty\rangle$ and $|-\infty\rangle$ are the same up to a phase factor, i.e., the summation is restricted to $|m\rangle_0 = |n\rangle_0$. This yields

$$i\hat{G}^{11}(1,1') = \frac{{}_0\langle n|TS\Psi_{H_0}(1)\Psi^{\dagger}_{H_0}(1')|n\rangle_0}{{}_0\langle n|S|n\rangle_0} \; , \qquad (103)$$

which allows for an expansion closed for $\hat{G}^{11}$. We recover the special case of the Feynman Green's function if the average is taken over the ground state, i.e., $|n\rangle_0 = |0\rangle_0$.

In 1964 Keldysh proposed a Green's-function technique for explicitly time-dependent systems in nonequilibrium.[6] (The Keldysh theory is reviewed in some excellent articles, for example Refs. 1, 14, and 15.) It relies on a Green's function defined as the contour-ordered product of an annihilation and a creation operator averaged over an arbitrary one-particle density matrix. The ordering is done along a contour which runs from an initial point t_0 to infinity and back to t_0 again (this is our contour c). The contour-ordered Green's function may be represented by a (2×2) matrix. As in the Feynman formalism, approximations are derived from an expansion of the time-development operator in terms of a noninteracting Hamiltonian H_0. Wick's theorem holds, since in the Keldysh theory an initial one-particle density matrix is assumed. Therefore the resulting many-particle Green's functions may again exactly be contracted to one-particle Green's functions.

It is easily proved that our (3×3)-matrix representation includes the (2×2) matrix of the Keldysh formalism in the left upper edge. If the statistical average is taken over a one-particle density matrix as given in Eq. (11), then B' vanishes according to Eq. (9), since no expansion of ρ is necessary. Hence the vertices V_{B_0} which connect the Keldysh matrix to the correlations $\hat{G}^{13}$, $\hat{G}^{23}$, $\hat{G}^{31}$, and $\hat{G}^{32}$ are zero, and the Dyson's equation for the (3×3) matrix decouples into a Dyson's equation for the usual (2×2) Keldysh matrix and a Dyson's equation for $\hat{G}^{33}$. With that we only have to solve the equation for the spectral density A [Eq. (98)] and the reduced transport equation (101).

The arguments for using one-particle density matrices at t_0 (usually for $t_0\to-\infty$) in the Feynman and Keldysh formalisms have their origin in scattering theory. If the many-particle interactions are assumed to be switched on adiabatically, then the time-development operator may be traced back to $t\to-\infty$, where the interaction eventually vanishes and a one-particle density matrix may be used. However, this approach is strictly speaking not applicable in solid-state physics. An adiabatic switching on of interactions such as the electron-electron interaction appears to be quite artificial. Nevertheless it is usually argued that this procedure is sufficient to calculate steady-state properties a long time after the initial preparation.

The proper way to deal with initial many-particle density matrices has already been shown by Matsubara.[5] His theory does not rely on any assumptions about time-development operators being switched on or off. Instead he resorts to a mathematical device by expanding the many-particle density matrix in terms of a one-particle density matrix. Matsubara's method may be used to calculate equilibrium properties of time-independent systems. His Green's function is defined as the τ-ordered product of an annihilation and a creation operator averaged over an equilibrium density matrix $\rho=(1/Z)\exp[-\beta(\mathcal{H}-\mu\mathcal{N})]$. Here the quantity τ has formally the same structure as a negative imaginary part of time. The determination of this Green's function is faciliated by three facts. Firstly, the Green's function depends on its relative τ arguments only. Secondly, it obeys boundary conditions periodic in β, which lead to a discrete Fourier transform. And thirdly, a generalized Wick's theorem has again been derived for the contraction of many-particle Green's functions in the interaction picture.[5,16]

Our last diagonal component $\hat{G}^{33}$ is a Green's function ordered along the hook $c'=[0,-i\lambda]$. It therefore much resembles the τ-ordered Green's function introduced by Matsubara, which is ordered along $c'=[0,-i\beta]$, where $\beta=1/(kT)$ is the inverse temperature. And indeed, they coincide for the special choice of a thermal initial density matrix

$$\rho(t_0)=\frac{1}{Z}\exp[-\beta(\mathcal{H}-\mu\mathcal{N})] \tag{104}$$

with

$$Z=\mathrm{Tr}\exp[-\beta(\mathcal{H}-\mu\mathcal{N})]\ , \tag{105}$$

i.e., $\mathcal{B}=\mathcal{H}-\mu\mathcal{N}$ and $\lambda=\beta$. Then we have

$$\hat{G}^{33}(1,1')=\mathcal{G}(\mathbf{x}_1,i\nu_1,\mathbf{x}_{1'},i\nu_{1'})\ , \tag{106}$$

where $\mathcal{G}$ is the Matsubara Green's function and $i\nu_1, i\nu_{1'}$ are real. We mention at this point that most of the computational methods developed for the Matsubara Green's function are based on the periodic boundary conditions and on its dependence on $i\nu_1-i\nu_{1'}$. However, since we have seen that both of these properties are valid for an arbitrary operator $\mathcal{B}$ [compare Eqs. (53) and (54)], it is to be expected that these methods may be utilized to calculate $\hat{G}^{33}(1,1')$ in the general case as well.

We have already noticed that the system of equations is closed for the 33-component, i.e., $\hat{G}^{33}$, alone, regardless of the initial density matrix $\rho(t_0)$ used for averaging. This property and the fact that a complex-time plane may be introduced are utilized in Matsubara theory. There only $\hat{G}^{33}$ is calculated, while the other correlations and Green's functions with real-time arguments are derived from $\hat{G}^{33}$ by an analytical continuation. However, the latter is only possible for a thermal density matrix, where the contour-development operator is generated by a time-independent Hamiltonian $\mathcal{H}$ and does not change along the whole contour c^* (i.e., where $\mathcal{H}$ is continuous). In general, the link between the two parts c and c' may not be differentiated continuously and the Green's functions on c and c' are not related by an analytical continuation. In this case there is no complex-time plane.

We conclude that the c^*-contour-ordered Green's function as defined in (41) or (50) contains the well-known Green's functions used in the Keldysh, Matsubara, and Feynman theories, if the proper corresponding density matrix for averaging is used. We may summarize these results graphically as

$$\hat{G}\simeq\left(\begin{array}{c|c}\begin{array}{c|c}F & \\ \hline & K\end{array} & \\ \hline & M\end{array}\right)\ . \tag{107}$$

Besides these contour-path formalisms some other Green's-function formalisms based on other approaches exist, which we will not, however, discuss in detail here. Kadanoff and Baym[8] were the first who set up a closed set of two equations for the correlation functions $G^<$ and $G^>$ ("equations of Kadanoff and Baym"). Fujita[2,3] generalized these equations by including matrices χ_l, $l\geq2$, to account for arbitrary initial correlations of the density matrix at t_0. These matrices χ_l had to be provided as input parameters. In our approach we used instead the parameter B' which led, roughly speaking, to an exponential representation of the χ_l [compare Eqs. (17) and (15)]. Hall[4] introduced to the work of Fujita the concept of the Keldysh Green's functions, which simplified the notation considerably. To our knowledge, he was the first who pointed out that initial correlations may be described by three additional quantities, but he did not set up the corresponding closed set of equations. The theory developed by Fujita and Hall is equivalent to our theory; however, their approach is totally different. The main point is that they used different expansion schemes for the usual Green's function and the density matrix. This results in new graphic elements such as cluster bonds, which are not known in common Feynman diagrams. We do not need these new elements, since we used one expansion scheme for both the usual Green's function and the density matrix. However, the price to be paid is a set of five instead of two equations to be solved.

VI. CONCLUSION

We have presented a contour-path formalism for nonequilibrium Green's functions which comprises the Feynman, Matsubara, and Keldysh formalisms as special cases. In contrast to these theories neither the initial preparation of the system, i.e., the density matrix, nor the subsequent time development are restricted. In particular, no assumption about an adiabatic switching on of many-particle interactions is necessary, since we have used an appropriate expansion of the initial density matrix. With that Wick's theorem is valid for our Green's function defined on an enlarged contour c^*, and common diagrammatic analysis can be used. The diagrams are topologically identical with those introduced in the Feynman theory, but evaluated differently by using the c^*-contour-ordered Green's function and suitably modified vertices. Similarly to the Keldysh theory we have derived a (3×3)-matrix representation for this Green's function which explicitly contains the Feynman, Matsubara, and Keldysh Green's functions as diagonal block matrices, if the proper density matrix for averaging is used. Moreover, for a general density matrix a closed set of five coupled equations have been derived from a generalized Dyson's equation. In particular this set comprises an equation for the spectral density and a transport equation, both well known in the Keldysh theory. However, the consideration of arbitrary initial many-particle correlations leads to additional terms in the transport equation which have to be determined with the help of the remaining three equations. The formalism presented here may be used to study corrections to the theories of Feynman, Matsubara, and Keldysh. Possible applications are the investigation of the transient behavior of a system shortly after its preparation or systems where the initial many-particle correlations do not decay.

ACKNOWLEDGMENTS

The author would like to express his gratitude to Professor H. Heyszenau for his fruitful and encouraging advice, and in particular for a critical reading of the manuscript. He thanks R. Brückner for valuable suggestions and many helpful discussions. This work was partly sponsored by the Studienstiftung des deutschen Volkes.

APPENDIX

We will show in this appendix that the expansion (44) may conveniently be described by diagrams which are essentially identical with Feynman diagrams. To this end let us consider an arbitrary term to nth order in the interactions. This order is defined as $n=n_1+n_2+\cdots$, where $n_1,n_2,\ldots$ are the orders of the one-particle, two-particle, etc., interactions. First we draw the outer indices $1,1'$ and the $\hat{n}=n_1+2n_2+\cdots$ vertices $2_1,\ldots,2_{\hat{n}}$ corresponding to the interactions. Then we draw a directed solid line from i to j for each of the $1+\hat{n}$ one-particle Green's functions $G_0(i,j)$ occurring in the product. We will thus end up with a diagram where at each vertex one solid line is going in and one out. Then we represent the interactions V connecting the vertices with dashed lines. Depending on the nature of the interaction, i.e., one-particle $(V=V_1)$, two-particle $[V=(1/2!)V_2]$, etc., these lines connect one, two, etc., vertices. To evaluate a given diagram we do the reverse. We associate to each directed solid line from i to j a c^*-contour-ordered Green's function $G_0(i,j)$. For each dashed line connecting m vertices $i_1\cdots i_m$ we insert an interaction $(1/m!)V_m(i_1,\ldots,i_m)$. To take the permutation factor $(-1)^{|p|+|p'|}$ into account we add a factor -1 for each closed fermion loop. Finally we have to integrate each vertex 2_i over space and over the contour. The nth order is then given by the sum over all possible diagrams with $n_1+2n_2+\cdots$ vertices (so that $n=n_1+n_2+\cdots$) divided by $n!$ and multiplied by Z_0/Z.

The number of diagrams to be calculated is drastically reduced by noticing that the vertices $2_1\cdots2_{\hat{n}}$ may be permuted within one sort of interaction without changing the result. The corresponding diagrams are topologically the same. It is simply a counting problem to show that there exist $n!(1!)^{n_1}(2!)^{n_2}\cdots$ such permutations. Hence, if we consider topologically distinct diagrams only, the factor $1/n!$ in the nth order is canceled and only the factor $(1!)^{n_1}(2!)^{n_2}\cdots$ remains. This factor is in turn canceled if we use the vertex functions $V_1,V_2,\ldots$ instead of the functions $(1/1!)V_1,(1/2!)V_2,\ldots$. Then the nth order is given by the sum over all topologically distinct diagrams with n dashed interaction lines and vertex functions $V_1,V_2,\ldots$ finally multiplied by Z_0/Z. A further reduction is achieved by considering the disconnected diagrams. These are diagrams which may be split into two parts without cutting any solid or dashed line. By utilizing arguments similar to those used in the Matsubara theory it is easily seen that the entire class of disconnected diagrams only contributes a factor Z/Z_0 to the result given by the class of connected diagrams. This factor fortunately cancels the prefactor Z_0/Z in Eq. (44). Hence the exact c^*-contour-ordered Green's function is finally given by the sum over all topologically distinct connected diagrams with $\hat{n}=0\cdots\infty$ vertices and vertex functions $V_1,V_2,\ldots$.

We conclude that the diagrams used for describing the expansion (44) are similar to those introduced by Feynman. They only differ in the Green's and vertex functions used. It is therefore not surprising that the notion of a self-energy may be introduced. A self-energy diagram of order $n = n_1 + n_2 + \cdots$ is defined as a connected diagram with $n_1 + 2n_2 + \cdots$ vertices, two of which are outer vertices and the other inner vertices subject to (four-dimensional) integrations. The vertices are connected by $-1 + n_1 + 2n_2 + \cdots$ directed solid lines and $n = n_1 + n_2 + \cdots$ interaction lines. A *proper* self-energy diagram may not be split into two parts by cutting only one single solid line.

So far we have constructed diagrams with free Green's functions G_0 only. We may reduce the number of self-energy diagrams by performing partial summations thus contracting the diagrams to irreducible diagrams. The resulting diagrams are based on dressed Green's functions G. There every self-energy insertion within an irreducibe diagram is removed in order not to count a diagram twice.

---

[*] Present address: Hitachi Cambridge Laboratory, Hitachi Europe Ltd., Cambridge CB3 0HE, United Kingdom.

[1] P. Danielewicz, Ann. Phys. **152**, 239 (1984). (The proof given by Danielewicz can readily be extended to the c^* contour-ordered Green's function, since it does not rely on any details about the contour.)

[2] S. Fujita, J. Math. Phys. **6**, 1877 (1965); *Non-Equilibrium Quantum Statistical Mechanics* (Saunders, Philadelphia, 1966); J. Phys. Soc. Jpn. **27**, 1096 (1969); Phys. Rev. A **4**, 1114 (1971).

[3] S. Fujita, Physica **64**, 1 (1973); **64**, 23 (1973).

[4] A. G. Hall, J. Phys. A **8**, 214 (1975); Physica A **80**, 369 (1975).

[5] T. Matsubara, Prog. Theor. Phys. **14**, 351 (1955).

[6] L. V. Keldysh, Zh. Eksp. Teor. Fiz. **47**, 1515 (1964) [Sov. Phys.—JETP **20**, 1018 (1965)].

[7] R. Mills, *Propagators for Many-Particle Systems* (Gordon and Breach, New York, 1969).

[8] L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (Benjamin, New York, 1962).

[9] J. Rammer and H. Smith, Rev. Mod. Phys. **58**, 323 (1986). Many references are given here.

[10] A. I. Larkin and Yu. N. Ovchinnikov, Zh. Eksp. Teor. Fiz. **68**, 1915 (1975) [Sov. Phys.—JETP **41**, 960 (1975)].

[11] R. P. Feynman, Phys. Rev. **76**, 749 (1949); **76**, 769 (1949).

[12] M. Gell-Mann and F. Low, Phys. Rev. **84**, 350 (1951).

[13] G. C. Wick, Phys. Rev. **80**, 268 (1950).

[14] D. F. DuBois, *Nonequilibrium Quantum Statistical Mechanics of Plasma and Radiation,* in Lectures in Theoretical Physics Vol. IX C, edited by W. E. Brittin and A. D. Barut (Gordon and Breach, New York, 1967), p. 469.

[15] D. C. Langreth, in *Linear and Nonlinear Electron Transport in Solids,* edited by J. T. Devreese and V. E. van Doren, Vol. 17 of *Nato Advanced Study Institutes, Series B: Physics* (Plenum, New York, 1976).

[16] M. Gaudin, Nucl. Phys. **15**, 89 (1960).