Kadanoff-Baym equations with initial correlations

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(Received 10 August 1998)

Equilibrium and nonequilibrium properties of nonideal many-particle systems are strongly influenced by correlation effects that are well described by generalized quantum kinetic equations, in particular, the Kadanoff-Baym equations (KBE). However, these equations are usually derived under the assumption of the weakening of initial correlations (Bogolyubov's condition) and, therefore, fail to correctly describe the short time behavior. We demonstrate that this assumption is not necessary for the derivation of the KBE. Using functional derivatives techniques, we present a straightforward generalization of the KBE that allows us to include arbitrary initial correlations and that is more general than previous derivations. As a result, an additional collision integral is obtained, which is being damped out after a few collisions. Our results are complemented with numerical investigations showing the effect of initial correlations. [S1063-651X(99)11202-9]

PACS number(s): 05.20.Dd, 52.25.Dg

I. INTRODUCTION AND BASIC EQUATIONS

The Kadanoff-Baym equations (KBE) for the two-time correlation functions $g^{\gtrless}(1,1')$, $1=(\mathbf{r}_1 t_1 s_1)$ have been very successful in the description of the nonequilibrium properties of quantum many-body systems, thereby allowing for a high degree of generality. Knowing the temporal evolution of these correlation functions, most properties of the system can be calculated, including the Wigner distribution, the spectral function, the mean kinetic and interaction energy, and so on. However, despite their fundamental role in many-particle theory, the original KBE [1] have a principal weakness—they do not contain initial correlations. Indeed, for t and t' approaching the initial time t_0, the KBE yield the Hartree-Fock equations, thus describing an uncorrelated system. Furthermore, it can be shown [2] that the KBE follow from the exact equations of motion for the correlation functions (the Martin-Schwinger hierarchy) under the assumption of Bogolyubov's condition of weakening of the initial correlations. Therefore, the KBE are unable to describe the initial stage of the evolution ($t_0 \leqslant t \leqslant \tau_{cor}$, where τ_{cor} is the correlation time) and the influence of initial correlations, which can be important for ultrafast relaxation processes.

This shortcoming of the KBE has been first pointed out by Fujita [3]. Fujita proposed generalized Kadanoff-Baym equations that, unfortunately, turned out to be inconsistent with the exact equations of motion for the correlation functions. Further investigations of these problems have been performed by Craig [4] and Hall [5] who used a generalized perturbation theory, which incorporates initial correlations. A convincing solution has been presented by Danielewicz [6]. He developed a *perturbation theory for a general initial state* and derived generalized KBE, which take into account arbitrary initial correlations [7].

In this paper, we present a derivation of closed equations of motion for the one-particle Green's functions (correlation functions), which is *not based on perturbation theory*. Instead, we use a straightforward and very intuitive method, which was proposed in Refs. [2,8], to generalize the KBE to the case of *arbitrary* initial correlations.

The starting point of this nonperturbative method is the Martin-Schwinger hierarchy, a system of coupled equations for the s-particle Green's function that is defined on the Keldysh contour $\mathcal{C}$ by

$$g_{1,\ldots,s}(1,\ldots,s;1',\ldots,s') = \left(\frac{1}{i}\right)^s \langle T_{\mathcal{C}}[\Psi(1)\cdots\Psi(s)\Psi^+(s')\cdots\Psi^+(1')]\rangle, \quad (1)$$

where Ψ is the field operator, $T_{\mathcal{C}}$ the time ordering operator on the contour, and $\langle\cdots\rangle$ denotes averaging over the density operator ρ. The first hierarchy equation is the equation of motion for the single-particle Green's function

$$\int_{\mathcal{C}} d\bar{1}\{g_1^{0^{-1}}(1\bar{1}) - U(1\bar{1})\} g_1(\bar{1}1',U) = \delta(1-1') \pm i\int d2\, V(1-2) g_{12}(121'2^+), \quad (2)$$

with U being an external potential and $g_1^{0^{-1}}$ the inverse Green's function

$$g_1^{0^{-1}}(11') = \left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right)\delta(1-1'). \quad (3)$$

Equation (2) is not a closed equation for $g_1(11')$, because the interaction leads to a coupling of the one-particle to the two-particle function and so on. The general form of the resulting hierarchy is

$$\int_{\mathcal{C}} d\bar{1}\{g_1^{0^{-1}}(1\bar{1}) - U(1\bar{1})\} g_s(\bar{1},\ldots,s;1',\ldots,s') = \sum_{\nu'=1}^{n} (\pm 1)^{\nu'-1}\delta(1-\nu') \times g_{s-1}(2,\ldots,s;1',\ldots,\nu'-1,\nu'+1,\ldots,s') \pm i\int d\alpha\, V(1-\alpha) g_{s+1}(1,\ldots,\alpha;1',\ldots,s,\alpha^+), \quad (4)$$

with $\alpha = s+1, V(1-2) = V(r_1-r_2)\delta(t_1-t_2)$, and $V(1-\alpha) = V(r_1-r_{s+1})\delta(t_1-t_{s+1})$.

To make further progress, the hierarchy has to be decoupled by means of suitable approximations, which leads to a closed system of equations for the first s Green's functions. This requires us to find formal solutions for the higher-order functions.

The system (4) constitutes first-order differential equations with respect to the time; therefore, initial (or boundary) conditions are required, which constrain the solution. We further remark that in the derivation of the hierarchy, no assumptions about the density operator ρ, which appears in Eq. (1), have been made. On the other hand, the explicit form of ρ has an influence on the boundary conditions. For example, in thermodynamic equilibrium with a grand canonical density operator, the solutions to Eqs. (4) are uniquely fixed by the Kubo-Martin-Schwinger condition. However, for real time nonequilibrium Green's functions this condition is not valid. In this case, the most general and natural choice is to supply initial conditions for the higher order Green's functions. In particular, we will be interested in a closed equation for the one-particle Green's function; then, the required initial condition is given by

$$g_{12}(121'2')|_{t_1=t_2=t_1'=t_2'=t_0}=g_{12}(t_0)=g_{12}^0. \tag{5}$$

The familiar condition of weakening of initial correlations, which is commonly used in kinetic theory, follows as a special case of Eq. (5) from the limit

$$\lim_{t_0\to-\infty} g_{12}(121'2')|_{t_1=t_2=t_1'=t_2'=t_0} =[g_1(11')g_1(22')\pm g_1(12')g_1(21')]|_{t_1=t_2=t_1'=t_2'=t_0}. \tag{6}$$

As was shown in Ref. [2], a decoupling of the hierarchy with condition (6) directly yields the original equations of Kadanoff and Baym. Therefore, the question arises how the KBE will change if in the derivation, condition (6) is replaced by Eq. (5).

II. SELF-ENERGY AND INITIAL CORRELATIONS

A formally closed equation for the one-particle Green's function can be derived by introducing the self-energy, which we define on the Keldysh contour, by

$$\int_{\mathcal{C}} d\bar{1}\Sigma(1\bar{1})g_1(\bar{1}1')=\pm i\int d2V(1-2)g_{12}(121'2^+). \tag{7}$$

Taking into account that g_{12} can be derived from g_1 by means of functional derivation, we can rewrite Eq. (7) as

$$\int_{\mathcal{C}} d\bar{1}\Sigma(1\bar{1})g_1(\bar{1}1') =\pm i\int d2V(1-2) \times\left\{\pm\frac{\delta g_1(11',U)}{\delta U(2^+2)}+g_1(11')g_1(22^+)\right\}. \tag{8}$$

Since the self-energy follows from the two-particle Green's function, definition (7) becomes unique only if the initial condition (5) is properly taken into account. With this definition of the self-energy, we have obtained a formally closed equation for the one-particle Green's function on the Keldysh contour, which may be cast into the form

$$\int_{\mathcal{C}} d\bar{1}\{g_1^{0^{-1}}(1\bar{1})-U(1\bar{1})-\Sigma(1\bar{1})\}g_1(\bar{1}1',U)=\delta(1-1'). \tag{9}$$

This equation is a compact notation of the Kadanoff-Baym equations and is sometimes called the Dyson-Schwinger equation. The same procedure for the adjoint of Eq. (2) leads to the adjoint Dyson equation with the self-energy $\hat{\Sigma}$. As we will see below, $\Sigma=\hat{\Sigma}$ for all times $t,t'>t_0$.

So far our considerations have been formal, and a number of questions remain open, among them: (a) Does the self-energy defined by Eq. (7) exist? (b) How do initial correlations affect the self-energy and, thus, the KBE? (c) How can one derive suitable approximations for the self-energy? To answer these questions, we return to the definition (8) of the self-energy. Further analysis of this equation requires us to evaluate the functional derivative

$$\frac{\delta g_1(11',U)}{\delta U(2'2)}=\pm\{g_{12}(121'2')-g_1(11')g_1(22')\} =\pm L(121'2'), \tag{10}$$

for which a simple procedure has been given [9]. Here, L is the density fluctuation function. The result is not an arbitrary four-point function, but it is restricted to $L(1,r_2t_2,1',r_2't_2)$ because of the temporally local character of the potential $U(2'2)=U(r_2'r_2)\delta(t_2-t_2')$. However, this restriction does not influence our further considerations, and so all four-point functions, which appear, can be regarded as formally nonlocal.

For $t,t'>t_0$, the Dyson equation can be written in the form

$$\int_{\mathcal{C}} d\bar{1}g_1^{-1}(1\bar{1})g_1(\bar{1}1')=\delta(1-1'), \tag{11}$$

where we introduced the inverse Green's function

$$g_1^{-1}(11')=g_1^{0^{-1}}(11')-U(11')-\Sigma(11'). \tag{12}$$

Functional differentiation of Eq. (11) for $t,t'>t_0$ yields easily

$$\int_{\mathcal{C}} d\bar{1}\frac{\delta g_1^{-1}(1\bar{1})}{\delta U(2'2)}g_1(\bar{1}1')=-\int_{\mathcal{C}} d\bar{1}g_1^{-1}(1\bar{1})\frac{\delta g_1(\bar{1}1')}{\delta U(2'2)}. \tag{13}$$

Using Eq. (12), the general solution of this equation is found immediately;

$$\frac{\delta g_1(11')}{\delta U(2'2)} = g_1(12')g_1(21') + \int_{\mathcal{C}} d\bar{1}d\bar{\bar{1}}g_1(1\bar{1}) \times \frac{\delta\Sigma(\bar{1}\bar{\bar{1}})}{\delta U(2'2)} g_1(\bar{\bar{1}}1') \pm C(121'2'), \quad (14)$$

where C is an arbitrary function, which obeys the homogeneous equation, i.e.,

$$\int_{\mathcal{C}} d\bar{1} g_1^{-1}(1\bar{1})C(\bar{1}21'2') = 0. \quad (15)$$

There are three similar conditions, one following from the crossing symmetry ($1 \leftrightarrow 2$) and two from the adjoint Dyson equation.

Let us now analyze the physical and mathematical consequences of the function $C(121'2')$. To this end, we consider Eq. (14) in the limit $t, t' \to t_0$. In this case, the integral over the Keldysh contour vanishes, and it directly follows

$$L(r_1, r_2, r_1', r_2', t_0) = C(r_1, r_2, r_1', r_2', t_0) \pm g_1(r_1, r_2', t_0)g_1(r_2, r_1', t_0). \quad (16)$$

Hence, the function $C(t_0)$ is to be identified with initial binary correlations. Furthermore, using the commutation relations for the field operators at equal times, it is readily verified that all Keldysh components of L differ only by one-particle functions. This means, $C(t_0)$ is a universal initial correlation, that is the same for the correlation functions and for the causal and anticausal Green's functions as well.

After having given a physical interpretation to the function $C(t_0)$, we now explore its temporal evolution. For that purpose, we consider the four conditions for C, Eq. (15) and the three analogous relations, which are valid on the Keldysh contour. Taking into consideration that (a), the inverse function g^{-1} acts only on one variable of C and (b), the initial value is universal for all Keldysh components, one readily verifies the following two properties of C: (i) C is a function, which does not depend on the positioning of the times on the Keldysh contour. That means it is completely determined by its values on the physical time axis. (ii) C obeys four equations, which follow from Eq. (15), by using the identity $\Sigma^c - \Sigma^< = \Sigma^R$,

$$\int d\bar{1} g_1^{R^{-1}}(1\bar{1})C(\bar{1}21'2') = 0, \quad \text{with} \quad g_1^{R^{-1}}(1\bar{1}) = g_1^{0^{-1}}(1\bar{1}) - U(1\bar{1}) - \Sigma^R(1\bar{1}), \quad (17)$$

and analogously for the other three conditions.

The four equations of the type (17) have to be solved together with the initial condition

$$C(121'2')|_{t_1 = t_2 = t_1' = t_2' = t_0} = C(t_0). \quad (18)$$

This is done conveniently by introducing the function g_1^R, which is the retarded function of the homogeneous differential Eq. (17), and satisfies

$$\int d\bar{1} g_1^{R^{-1}}(1\bar{1})g_1^R(\bar{1}1') = \delta(1-1'). \quad (19)$$

As a result, the solution of the initial value problem (17) and (18) can be written as

$$C(121'2') = \int d\bar{r}_1 d\bar{r}_2 d\bar{\bar{r}}_1 d\bar{\bar{r}}_2 g_1^R(1,\bar{r}_1 t_0)g_1^R(2,\bar{r}_2 t_0) \times C(\bar{r}_1 t_0, \bar{r}_2 t_0, \bar{\bar{r}}_1 t_0, \bar{\bar{r}}_2 t_0)g_1^A(\bar{\bar{r}}_1 t_0, 1') \times g_1^A(\bar{\bar{r}}_2 t_0, 2'), \quad (20)$$

where $C(\bar{r}_1 t_0, \bar{r}_2 t_0, \bar{\bar{r}}_1 t_0, \bar{\bar{r}}_2 t_0)$ denotes the coordinate representation of the correlation part of the two-particle density operator. With this result, the density fluctuation function L is formally defined too.

In order to rewrite all relations in a compact way on the Keldysh contour, we take into account that for a function $C(121'2')$, which is uniquely defined on the physical time axis, it holds

$$\int_{\mathcal{C}} d\bar{1} g_1(1\bar{1})C(\bar{1}21'2') = \int d\bar{1} g_1^R(1\bar{1})C(\bar{1}21'2'), \quad (21)$$

and, therefore, Eq. (20) can be rewritten in the form

$$C(121'2') = \int_{\mathcal{C}} d\bar{1}d\bar{2}d\bar{\bar{1}}d\bar{\bar{2}} g_1(1\bar{1})g_1(2\bar{2}) \times c(\bar{1}\bar{2}\bar{\bar{1}}\bar{\bar{2}})g_1(\bar{\bar{2}}2')g_1(\bar{\bar{1}}1'), \quad (22)$$

with

$$c(\bar{1}\bar{2}\bar{\bar{1}}\bar{\bar{2}}) = c(\bar{r}_1 t_0, \bar{r}_2 t_0, \bar{\bar{r}}_1 t_0, \bar{\bar{r}}_2 t_0)\delta(\bar{t}_1 - t_0) \times \delta(\bar{t}_2 - t_0)\delta(\bar{\bar{t}}_1 - t_0)\delta(\bar{\bar{t}}_2 - t_0). \quad (23)$$

Let us now come back to the self-energy. Introducing Eq. (14) with solution (22) into Eq. (8), the latter can be solved by acting on it with g^{-1}. The result is a functional equation for the self-energy:

$$\Sigma(11') = \pm i \int d2V(1-2)\Bigg\{ \pm \int_{\mathcal{C}} d\bar{1} g_1(1\bar{1}) \frac{\delta\Sigma(\bar{1}1')}{\delta U(2^+2)} + \delta(1-1')g_1(22^+) \pm \delta(2-1')g_1(12^+) + \int_{\mathcal{C}} d\bar{1}d\bar{2}d\bar{\bar{2}} g_1(1\bar{1})g_1(2\bar{2})c(\bar{1}2\bar{1}'\bar{\bar{2}})g_1(\bar{\bar{2}}2^+) \Bigg\}. \quad (24)$$

An analogous equation follows readily for $\hat{\Sigma}$. With Eq. (24), the self-energy is given as a functional of the interaction, the initial correlations, and the one-particle Green's function, where the initial correlations are contained in the last term. From the definition of c, Eq. (22), it is obvious that this contribution is local in time with a δ-type singularity at $t = t'$. Additional terms of this structure arise from the func-

tional derivative. A further important property of the self-energy follows from comparing Σ, Eq. (24), with the corresponding expression for $\hat{\Sigma}$. One verifies that $\Sigma=\hat{\Sigma}$ for all times $t,t'>t_0$, which means, in particular, that for these times, a well-defined inverse Green's function does exist.

Equation (24) is well suited to come to approximations for the self-energy. By iteration, a perturbation series for Σ in terms of g,V, and C can be derived, which begins with

$$\Sigma^1(11')=\pm i\delta(1-1')\int d2V(1-2)g_1(22^+)$$
$$\pm i\int d2V(1-2)\int_C d\bar{1}d\bar{2}d\bar{\bar{2}}g_1(1\bar{1})g_1(2\bar{2})$$
$$\times c(\bar{1}\bar{2}1'\bar{\bar{2}})g_1(\bar{\bar{2}}2^+)+(\text{exchange}). \quad (25)$$

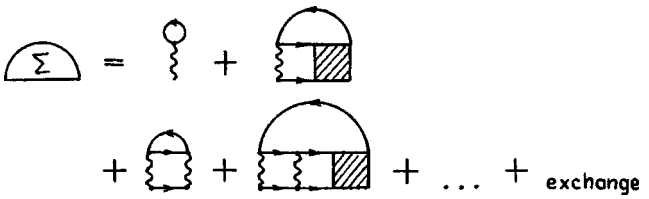
It is now instructive, to introduce Feynman diagrams, which allows for the following representation of formula (25):

(26)

In contrast to conventional diagram techniques, we have introduced the initial correlations as a new basic element, drawn as a shaded rectangle. Second-order contributions are evaluated straightforwardly, too, with the result

$$\Sigma^2(11')=\Sigma^1(11')\pm i^2\int_C d2d\bar{2}V(1-2)$$
$$\times g_1(11')g_1(2\bar{2})V(\bar{2}-1')g_1(\bar{2}2^+)$$
$$\pm i^2\int_C d2d\bar{1}d\bar{2}d\bar{\bar{1}}d\bar{\bar{2}}d\bar{\bar{\bar{2}}}V(1-2)$$
$$\times g_1(1\bar{1})g_1(2\bar{2})V(\bar{1}-\bar{2})g_1(\bar{\bar{1}}\bar{\bar{\bar{1}}})g_1(\bar{\bar{2}}\bar{\bar{\bar{2}}})$$
$$\times c(\bar{\bar{\bar{1}}}\bar{\bar{1}}1'\bar{\bar{\bar{2}}}\bar{\bar{2}})g_1(\bar{\bar{\bar{2}}}2^+)+\cdots+(\text{exchange}), \quad (27)$$

or, in terms of Feynman diagrams,



(28)

The analysis of the iteration scheme allows us to conclude that all contributions to the self-energy (all diagrams) fall into two classes: (i) the terms Σ^{HF} und Σ^c, which begin and end with a potential, and (ii) Σ^{in}—those which begin with a potential but end with an initial correlation. This means the self-energy has the structure

$$\Sigma(11')=\Sigma^{HF}(11')+\Sigma^c(11')+\Sigma^{in}(11'), \quad (29)$$

$$\Sigma^{in}(11')=\Sigma^{in}(1,r_1't_0)\delta(t_1'-t_0). \quad (30)$$

The initial correlation part of the self-energy turns out to be a temporally local contribution (similar to the Hartree-Fock term) that is nonzero only if t_1' (or, in the adjoint case, t_1) is equal to the initial time t_0.

Interestingly, the same result was obtained by Danielewicz based on his perturbation theory for general initial states [6], which was mentioned in the Introduction. The agreement of the two approaches becomes particularly obvious from the diagrammatic representation of Σ.

If one considers the first two iterations for the self-energy, Eqs. (25) and (27), more in detail, it becomes evident that, in the initial correlation contribution in front of the function c, appear just the ladder terms, which lead to the buildup of the two-particle Green's function. Thus, obviously, the iteration ''upgrades'' the product of retarded one-particle propagators in the function C to a full two-particle propagator, in the respective order, i.e., Σ^{in} is of the form

$$\Sigma^{in}(11')=\pm i\int d2V(1-2)\int d\bar{r}_1d\bar{r}_2d\bar{\bar{r}}_1d\bar{\bar{r}}_2$$
$$\times g_{12}^R(12,\bar{r}_1t_0,\bar{r}_2t_0)c(\bar{r}_1t_0,\bar{r}_2t_0,1',\bar{\bar{r}}_2t_0)$$
$$\times g_1^A(\bar{\bar{r}}_2t_0,2^+)\delta(t_1'-t_0). \quad (31)$$

Notice especially that this renormalization occurs not symmetrically, i.e., in the adjoint of Eq. (31), $\Sigma_{in}\equiv[\Sigma^{in}]^\dagger$ (Σ_{in} denotes the initial correlation contribution of $\hat{\Sigma}$) appears the adjoint propagator g_{12}^A.

III. GENERALIZED KADANOFF-BAYM EQUATIONS

Let us now come back to the Kadanoff-Baym equations. In order to discuss the influence of initial correlations, we insert expression (29) into Eq. (2) and find

$$\int_C d\bar{1}[g_1^{0^{-1}}(1\bar{1})-U(1\bar{1})-\Sigma^{HF}(1\bar{1})]g_1(\bar{1}1')$$
$$=\delta(1-1')+\int_C d\bar{1}[\Sigma^c(1\bar{1})+\Sigma^{in}(1\bar{1})]g_1(\bar{1}1'). \quad (32)$$

From this equation, we obtain the KBE for the correlation functions if we restrict the time arguments to opposite branches of the Keldysh contour:

$$\left(i\frac{\partial}{\partial t_1}+\frac{\nabla_1^2}{2m}\right)g_1^{\gtrless}(11')-\int d\bar{1}U(1\bar{1})g_1^{\gtrless}(\bar{1}1')$$
$$-\int d\bar{r}_1\Sigma^{HF}(1\bar{1})g_1^{\gtrless}(\bar{1}1')$$
$$=\int_{t_0}^{\infty}d\bar{1}\Sigma^R(1\bar{1})g_1^{\gtrless}(\bar{1}1')+\int_{t_0}^{\infty}d\bar{1}[\Sigma^{\gtrless}(1\bar{1})$$
$$+\Sigma^{in}(1\bar{1})]g_1^A(\bar{1}1'), \quad (33)$$

whereas the adjoint equation reads

$$\left(-i\frac{\partial}{\partial t_1'}+\frac{\nabla_{1'}^2}{2m}\right)g_1^{\gtrless}(11')-\int d\bar{1}\,g_1^{\gtrless}(1\bar{1})U(\bar{1}1')$$
$$-\int d\bar{r}_1 g_1^{\gtrless}(1\bar{1})\Sigma^{HF}(\bar{1}1')$$
$$=\int_{t_0}^{\infty}d\bar{1}\,g_1^{R}(1\bar{1})[\Sigma^{\gtrless}(\bar{1}1')+\Sigma_{in}(\bar{1}1')]$$
$$+\int_{t_0}^{\infty}d\bar{1}\,g_1^{\gtrless}(1\bar{1})\Sigma^{A}(\bar{1}1'). \tag{34}$$

In contrast to the original KBE, there are two important new properties, which have to be underlined here: Equations (33) and (34) are valid for an *arbitrary initial time point* t_0, and they explicitly contain the influence of *arbitrary initial correlations* in the additional self-energy term Σ^{in}.

The analytical properties of the retarded and advanced Green's functions give rise to a damping γ_{12} leading to a decay of the initial correlation term after a time of the order $t\sim 1/\gamma_{12}\sim\tau_{cor}$. Thus, there is no need at all to postulate Bogolyubov's weakening condition; for $t>\tau_{cor}$, the generalized Kadanoff-Baym equations switch from the initial regime into the kinetic, or Bogolyubov regime, ''automatically.''

As we have seen in the previous section, the term Σ^{in} contains all singular in time contributions to the self-energy (except the Hartree-Fock term, of course). The importance of this temporal structure becomes obvious if we consider the Kadanoff-Baym equations in the limit $t,t'\to t_0$. Then only the terms with δ singularities remain, and we get for the right-hand side,

$$\int dr_2 V(r_1-r_2)\{g_1(r_1r_1',t_0)g_1(r_2r_2',t_0)$$
$$\pm g_1(r_1r_2',t_0)g_1(r_2r_1',t_0)+c(r_1r_2r_1'r_2',t_0)\}, \tag{35}$$

which is just the right-hand side of the first hierarchy equation (2), for $t=t'=t_0$. This identity is an essential consistency criterion for the theory. This condition would be violated if weakening of initial correlations would be assumed, since then Eqs. (33) and (34) would go over into the usual Kadanoff-Baym equations, which in the limit $t,t'\to t_0$, yield the Hartree-Fock equations.

A further consistency criterion is, of course, the requirement that the equal time limit of the additional collision integral of Eq. (33) coincides with the well-known results of density operator theory, e.g., [10,11]. In order to explore this problem more in detail, we consider the approximation $g_{12}^{R/A}\sim g_1^{R/A}\cdot g_2^{R/A}$, i.e., the initial correlation part of the self-energy is taken in second-order Born approximation. Then, $I^{IC}(t)$ reads, in momentum representation,

$$I^{IC}(p_1,t)=\mp 2\hbar^5\int\frac{dp_2}{(2\pi\hbar)^3}\frac{d\bar{p_1}}{(2\pi\hbar)^3}\frac{d\bar{p_2}}{(2\pi\hbar)^3}$$
$$\times V(\bar{p_1}-p_1)(2\pi\hbar)^3\delta(p_1+p_2-\bar{p_1}-\bar{p_2})$$
$$\times\mathrm{Im}\{g_1^R(\bar{p_1},tt_0)g_1^R(\bar{p_2},tt_0)$$
$$\times c(\bar{p_1},\bar{p_2},p_1,p_2;t_0)g_1^A(p_2,t_0t)g_1^A(p_1,t_0t)\}, \tag{36}$$

which exactly agrees with the corresponding density operator result.

It is readily confirmed that the collision integral (36) conserves density and total energy and that it vanishes for $t\gg\tau_{cor}$; see, also, the numerical results below.

IV. NUMERICAL ILLUSTRATIONS AND DISCUSSION

For illustration of our theoretical results, we have performed numerical solutions of the Kadanoff-Baym equations including the initial correlation integral (36). We considered the relaxation of a weakly coupled electron gas with self-energies in second Born approximation. Starting from an initial nonequilibrium distribution, we compared the relaxation for two cases: (1) without initial correlations, $C(t_0)\equiv 0$, and (2) with nonzero initial correlations, which were chosen in the form of the Debye pair correlation function,

$$C(q,p_1,p_2,t_0)=-\frac{V_D(q)}{kT}f(p_1)f(p_2)$$
$$\times[1-f(p_1+q)][1-f(p_2-q)], \tag{37}$$

where $f\equiv f(t_0)$. As expected, the presence of initial correlations turns out to be important on short times. This becomes particularly clear from analyzing the time evolution of the mean potential and kinetic energy, Fig. 1. While for the uncorrelated initial state, potential energy starts with zero and builds up continuously, the picture changes if there exist initial correlations. With the choice of the form (37), the correlations are stronger than in equilibrium that corresponds to a larger magnitude of potential energy at $t=t_0$, which, consequently, is reduced in the course of the relaxation. Due to conservation of total energy, kinetic energy shows exactly the opposite trend. One clearly sees the decay of the initial correlation term as the curves for the two cases merge after times of the order of the correlation time. This confirms that, indeed, Bogolyubov's weakening principle is reproduced by

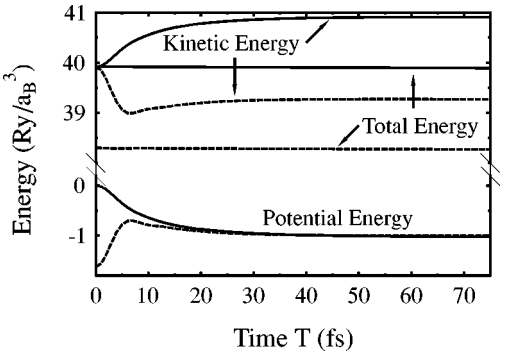


FIG. 1. Time evolution of kinetic, potential, and total energy for zero (solid lines) and nonzero (dashed lines) initial correlations. The initial distribution is an uncorrelated equilibrium (Fermi) distribution with $T=290$ K and $n=10^{18}$ cm^{-3}.

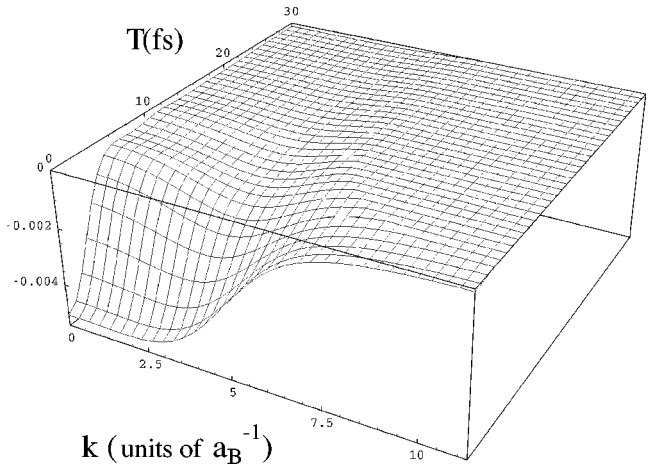


FIG. 2. Imaginary part of the initial correlation contribution to the τ derivative of the correlation function $g^<(tt')$ for $t=t'(\tau=0)$.

the presented generalized Kadanoff-Baym equations in a dynamic and self-consistent way.

The behavior of the initial correlation term can be analyzed directly by investigating its contribution to the correlation energy,

$$\langle V\rangle(t)=\frac{1}{4}\mathcal{V}\hbar\int\frac{d^3p}{(2\pi\hbar)^3}\left(i\hbar\frac{\partial}{\partial t}-i\hbar\frac{\partial}{\partial t'}-\frac{p^2}{m}\right)\times(\pm i)g^<(p,t,t')|_{t'=t}, \tag{38}$$

with $\mathcal{V}$ denoting the system volume. Since this quantity is essentially determined by the derivative of the correlation function $g^<(tt')$ perpendicular to the time diagonal for $t=t'$ (i.e., derivative with respect to $\tau\equiv t-t', \partial/\partial\tau=\partial/\partial t-\partial/\partial t'$), this derivative can be used to isolate the effect of initial correlations on $\langle V\rangle$. In fact, $\partial g/\partial\tau\sim 2i\,\mathrm{Im}(I+I^{IC})$, cf. Eqs. (33) and (34). We, therefore, show in Fig. 2 the evolution (along the time diagonal) of $\mathrm{Im}\,I^{IC}$ as a function of momentum. One clearly sees the decay of the initial correlations within the correlation time.

Our numerical results illustrate the effect of initial correlations on the short-time relaxation behavior for a simple model case. But our theoretical approach is completely general and allows for numerical investigations of far more complex initial correlations. Besides the fundamental interest in the problem of initial correlations in the Kadanoff-Baym equations, our results are also of practical importance. With the possibility to start quantum kinetic calculations from a general initial state, the scope of nonequilibrium processes in many-body systems, which are accessible for numerical investigation, is essentially extended. Although the determination of $C(t_0)$ can be complicated by itself, our approach allows us to separate this problem (the ''generation'' of the correlated state) from the relaxation dynamics.

ACKNOWLEDGMENTS

The authors acknowledge discussions with N. H. Kwong (Rostock) and V. I. Morozov (Moscow). This work was supported by the Deutsche Forschungsgemeinschaft (Grant No. SFB 198 and Schwerpunkt ''Quantenkohärenz in Halbleitern'').

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