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Short-Time Kinetics and Initial Correlations in Quantum Kinetic Theory

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Abstract. There are many reasons to consider quantum kinetic equations describing the evolution of a many-particle system on ultrashort time scales, e.g. correct energy conservation in nonideal plasmas, buildup of correlations (bound states), and kinetics of ultrafast processes in short-pulse laser plasmas. These problems have been always an central and important field of research of Yu. L. Klimontovich.

We present a quantum kinetic theory including initial correlations and being valid on arbitrary time scales. Various examples of short-time relaxation processes, such as relaxation of the distribution function and the energy, are shown. Furthermore, gradient expansions of the general equations and the role of bound states are discussed.

1. Introduction

This paper is devoted to Yu. L. Klimontovich who has given remarkable and important contributions to the development of theoretical physics, especially to the nonequilibrium statistical mechanics of nonideal gases and plasmas.

Nonequilibrium properties of many-particle systems are successfully described by kinetic equations of the Boltzmann type. In the quantum case, the Boltzmann equation has the shape

$$\left\{ \frac{\partial}{\partial t} + \frac{\partial E_a}{\partial \mathbf{p}} \frac{\partial}{\partial \mathbf{R}} + \frac{\partial E_a}{\partial \mathbf{R}} \frac{\partial}{\partial \mathbf{p}} \right\} f_a(\mathbf{pR}t) = I_a(\mathbf{pR}T), \tag{1}$$

where f_a is the Wigner distribution. The most interesting term in this equation is the collision integral $I_a(\mathbf{pR}T)$ given here in binary collision approximation

$$\begin{aligned} I(\mathbf{p}_1\mathbf{R}T) &= \frac{2}{\hbar} \int \frac{d\mathbf{p}_2 d\bar{\mathbf{p}}_1 d\bar{\mathbf{p}}_2}{(2\pi\hbar)^9} 2\pi\delta\left(E_{12} - \bar{E}_{12}\right) \left|\langle \mathbf{p}_1\mathbf{p}_2 | T^+ \left(E_{12} + i\varepsilon\right) | \bar{\mathbf{p}}_2\bar{\mathbf{p}}_1 \rangle\right|^2 \\ &\times \left(\bar{f}_1\bar{f}_2 \left(1 \pm f_1\right)\left(1 \pm f_2\right) - f_1 f_2 \left(1 \pm \bar{f}_1\right)\left(1 \pm \bar{f}_2\right)\right). \end{aligned} \tag{2}$$

We find the typical terms of a Boltzmann-like collision integral: the kinetic energy conserving delta function, the transition probability in two-particle collisions given by the on-shell T–matrix and the usual combination of Wigner functions describing the occupation at the beginning and the end of the collision.

In spite of the fundamental character of Boltzmann-like kinetic equations, which describe the irreversible relaxation of an arbitrary initial Wigner distribution to the equilibrium distribution and, moreover, are the basic equations of transport theory, there exist many principle shortcomings. This was pointed out already by Prigogine and Resibois [1], Kadanoff and Baym [2], Silin [3] and especially by Klimontovich [4]. The Boltzmann equation

(i) cannot describe the short-time behavior ($t < t_{corr}$) correctly,
(ii) conserves the kinetic energy $\langle T \rangle$ only instead of the total energy $\langle T \rangle + \langle V \rangle$ which is unphysical, especially for strongly correlated many-particle systems,
(iii) does not describe, because of the on-shell T–matrix, the influence of bound states on the kinetics,
(iv) gives as equilibrium solution the distribution for ideal particles.

To all these problems Klimontovich gave interesting remarks and solutions. Most of them were presented in his well-known book [4]

Kinetic Theory of Nonideal Gases and Plasmas.

In this book, Klimontovich pointed out that these shortcomings follow from a certain assumption necessary for the derivation of the Boltzmann equation from the basic equations of statistical mechanics. Let us consider this idea more in detail. The relaxation of a strongly correlated many-particle system from the initial state to the equilibrium state runs over several stages. In the vicinity of the initial time the evolution is strongly influenced by the initial condition, especially by the initial correlations.

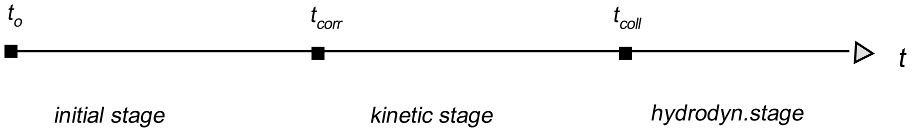


Figure 1. Stages of relaxation of a many-particle system

We observe in this initial stage the buildup of correlations and the kinetics is a non-Markovian one, i.e., we have memory effects. For times bigger then the correlation time, the time evolution of the system is determined only by the one-particle density operator. All higher density operators are now functionals of the latter one. Initial correlation and memory effects are damped out, the kinetics is Markovian. Finally, after the collision time, we have local equilibrium and, therefore, a reduction of the phase space to the configuration space description.

Let us consider first a simple description of the relaxation process. We start from the Bogolyubov hierarchy for the reduced density operators in binary collision approximation. In this approximation follows the closed system of equations

$$\frac{dF_1}{dt} + [H_1^{HF},\, F_1] \;=\; \mathrm{Tr}\,[V_{12}, g_{12}], \tag{3}$$

$$\frac{dg_{12}}{dt} + [H_{12}^{HF} + V_{12},\, g_{12}] \;=\; [V_{12},\, F_1 F_2]. \tag{4}$$

It is easy to find a formal solution of the second equation

$$\begin{aligned} & g_{12}(t) = U(t,t_0) g_{12}(t_0) U(t_0,t) \\ & + \frac{1}{i\hbar} \int_0^{t-t_o} d\tau U\left(t, t-\tau\right) \; [V_{12},\, F\left(t-\tau\right) F\left(t-\tau\right)]\, U\left(t-\tau, t\right). \end{aligned} \tag{5}$$

Here, the first term describes the influence of the initial correlations to the time evolution of the system. The $U(t, t_0)$ are two-particle propagators. The second term describes the non-Markovian buildup of correlations, i.e., the value of the correlation operator at the time t is determined by all previous times. If we insert now (5) into the first equation (3) we get a closed non-Markovian equation for the one-particle density operator which describes the short-time behavior and the influence of initial correlations.

The Boltzmann equation follows from this equation under very restrictive assumptions:

i) We apply the Bogolyubov condition of weakening of initial correlations (no correct short-time behavior), i.e.

$$\lim_{t_0 \to -\infty} g_{12}(t_0) = 0. \tag{6}$$

ii) We neglect the retardation (destruction of the correct energy conservation, influences strongly the short-time behavior).

With condition (6), the initial stage is completely neglected. But there are many reasons to extend the description into the initial region. We mention here only, for example, correct energy conservation in nonideal plasmas, buildup of correlations, and kinetics of ultrafast processes, e.g. in short pulse laser plasmas.

A first idea to take into account the influence of the initial stage was the gradient expansion with respect to the retardation [1, 2, 5, 6]. With this expansion, Klimontovich and Ebeling and also Baerwinkel obtained kinetic equations with conservation laws for nonideal systems. Further, with a modification of the Bogolyubov condition to a partial weakening of initial correlations, it was possible to include bound states [7].

Of course the pure binary collision approximation is too simple especially to describe the damping in the propagators U and, therefore, the weakening of initial correlations and other many-particle effects like Pauli blocking, self-energy, screening of the Coulomb potential in plasmas, lowering of the ionization energy etc. A generalization of the equations (3,4) are given in [8] and [9] but we will consider these problems from the more general point of view of the powerful real-time Green's functions.

The original scheme of real-time Green's functions contains no contribution of initial correlations. In order to include them, several methods have been used, e.g. analytical continuation to real times which allows to include equilibrium initial correlations [2, 10, 11, 12], and perturbation theory with initial correlations [13, 14, 10]. A convincing solution has been presented by Danielewicz [10]. He developed a perturbation theory for a general initial state and derived generalized Kadanoff–Baym equations which take into account arbitrary initial correlations. A straightforward and very intuitive method which is not based on perturbation theory [21, 15, 16, 17], uses the equations of motion for the Green's functions which we will present in the next section.

2. Martin–Schwinger hierarchy. Initial correlation

The formalism of real-time Green's functions describes the many-particle system by a system of single, two, and more-particle Green's functions. We consider the definition of the single-particle Green's function as an average over the time-ordered product of field operators $\psi(1)$ and $\psi^\dagger(1')$,

$$g(1,1') = \frac{\frac{1}{i\hbar}\mathrm{Tr}\left\{\varrho \mathrm{T}_C \left\{S(t_0,t_0)\psi(1)\psi^\dagger(1')\right\}\right\}}{\mathrm{Tr}\left\{\mathrm{T}_C S(t_0,t_0)\right\}} \tag{7}$$

with

$$S(t_0,t_0) = \mathrm{T}_C \exp\left\{-i\int_C d2d\bar{2}U(2,\bar{2})\psi^\dagger(2)\psi(\bar{2})\right\}.$$

T_C denotes ordering along the Keldysh contour [18, 19]. The field operators are given in the interaction picture with respect to a formal external potential $U(1,1')$. Their equation of motion is

$$\left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2\nabla_1^2}{2m}\right)\psi(1)=\pm\int d2\,V(1-2)\psi^\dagger(2)\psi(2)\psi(1)|_{t_1=t_2}. \tag{8}$$

The density operator is in general a nonequilibrium one. In this case the adiabatic theorem is not valid and, therefore, we have a causal and anticausal time ordering. In order to handle this problem, for nonequilibrium systems, the time ordering on the physical time axis is to replace by the ordering along the upper and lower branch of the Keldysh contour, see Fig. 2.

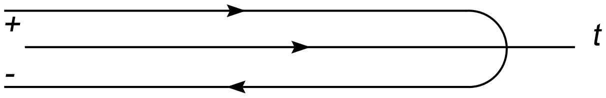


Figure 2. Keldysh time contour

Now we introduce the following notation: times t located on the upper (+) branch we denote by t_+, times located on the lower branch (–) by t_-. The function (7) is a very compact representation of the causal and anticausal single particle Green's functions $g^{c(a)}(1,1')$ and the two correlation functions $g^{>(<)}(1,1')$. In dependence on the position of the two times t and t' on the Keldysh contour we get these functions by

$$\begin{aligned} g(1_+,1'_+) &= g^c(1,1'), \qquad g(1_-,1'_+)=g^>(1,1'),\\ g(1_-,1'_-) &= g^a(1,1'), \qquad g(1_+,1'_-)=g^<(1,1'). \end{aligned} \tag{9}$$

Of special interest is the two-time correlation function $g^<(1,1')$. The time diagonal part of this function is just the Wigner function.

In order to derive the equations of motion for the Green's functions (7) on the Keldysh contour, we have to introduce the equation of motion for the field operators (8) into the definition of the single-particle Green's function (7). Then follows immediately

$$\begin{aligned} &\int d\bar{1}\left\{g_0^{-1}(1,\bar{1})-U(1,\bar{1})\right\}g(\bar{1},1';U)=\\ &= \delta(1-1')\pm i\hbar\int d2\,V(1-2)g_{12}(12,1'2^+;U)\,,\\ g_0^{-1}(1,1') &= \left(i\hbar\frac{\partial}{\partial t_1}+\frac{\hbar^2\nabla_1^2}{2m}\right)\delta(1-1')\,. \end{aligned} \tag{10}$$

This equation is not closed. Due to the interaction between the particles we have a coupling with the two-particle Green's function and so on. Equation (10) is therefore a member of an infinite chain of equations for many-particle Green's functions, well known as Martin–Schwinger hierarchy [20].

To find a closed equation for the one-particle Green's function we proceed in well-known manner. First, we define the self-energy by

$$\begin{aligned} &\int_{\mathcal{C}} d\bar{1}\,\Sigma(1,\bar{1})g(\bar{1},1')=\pm i\hbar\int d2\,V(1-2)g_{12}(12,1'2^+)\\ &= \pm i\hbar\int d2\,V(1-2)\left\{\pm\frac{\delta g(1,1';U)}{\delta U(2^+,2)}+g(1,1')g(2,2^+)\right\}. \end{aligned} \tag{11}$$

Here we took into account that g_{12} can be derived from g by means of functional derivation. Next, we introduce this definition into the first equation of the Martin–Schwinger hierarchy. Then follows immediately

$$\int\limits_C d\bar{1}\left\{g_0^{-1}(1,\bar{1}) - U(1,\bar{1}) - \Sigma(1,\bar{1})\right\} g(\bar{1},1') = \delta(1-1'). \tag{12}$$

This equation is a Dyson equation for nonequilibrium systems and was for the first time derived by Kadanoff and Baym [2] and by Keldysh [18].

Of course, all problems are now transferred into the self-energy. We, therefore, have to consider the properties of this function and to find a possibility to determine appropriate approximations for Σ.

Let us first consider the dependence of Σ on the initial value of the two-particle Green's function. From (11) it is obvious that the self-energy has, in the limit $t \to t_0$, to fulfill the important relation

$$\begin{aligned}\lim_{t_1=t_1'=t_0} \int\limits_C d\bar{1}\Sigma(1,\bar{1})g(\bar{1},1') = \pm i \int d\mathbf{r}_2\, V(\mathbf{r}_1-\mathbf{r}_2)\, g(\mathbf{r}_1\mathbf{r}_2,\mathbf{r}_1'\mathbf{r}_2;t_0) \;= \\ \pm i\hbar \int d\mathbf{r}_2\, V(\mathbf{r}_1-\mathbf{r}_2)\, \left\{g(1,1')g(2,2^+)_{t_0} \pm g(1,2^+)g(2,1')_{t_0}\right. \\ \left. +c(\mathbf{r}_1\mathbf{r}_2,\mathbf{r}_1'\mathbf{r}_2;t_0)\,\right\}\end{aligned} \tag{13}$$

what means that Σ is dependent on an arbitrary initial value $g(\mathbf{r}_1\mathbf{r}_2,\mathbf{r}_1'\mathbf{r}_2;t_0)$ of the two-particle correlation function. Consequently, it is necessary to introduce initial conditions in order to determine the self-energy uniquely.

Now we have to take into consideration that the integral over the Keldysh contour for a regular integrand vanishes in the limit $t, t' \to t_0$. Therefore, the equation (13) can be fulfilled only if the self-energy has a contribution proportional to a δ–function with respect to the times. Such a term is the Hartree–Fock contribution Σ^{HF}. But this term only produces the uncorrelated contribution to the initial binary density matrix. This means that the self-energy must contain a second part with a δ–like singularity. The general structure of the self-energy is thus given by

$$\begin{aligned}\Sigma(1,1') &= \Sigma^{\mathrm{HF}}(1,1') + \Sigma^{c}(1,1') + \Sigma^{in}(1,1'), \\ \Sigma^{in}(1,1') &= \Sigma^{in}(1,\mathbf{r}_1't_0)\delta(t_1'-t_0).\end{aligned} \tag{14}$$

We should note here that the self-energy $\hat{\Sigma}$ in the adjoint Dyson equation differs from Σ just in the initial contribution.

Let us come back to the Kadanoff–Baym/Keldysh equation (12). In order to discuss the influence of the initial correlations on the time evolution of the single-particle Green's function we insert (14) into Eq. (12) and fix the time arguments to opposite branches on the contour. Then we get the Kadanoff–Baym equations (KBE) for the correlation functions

$$\begin{aligned}\left(i\hbar\frac{\partial}{\partial t_1} + \frac{\hbar^2\nabla_1^2}{2m}\right) g^{\gtrless}(1,1') - \int d\bar{1}\, U(1,\bar{1})g^{\gtrless}(\bar{1},1') = \\ \int d\bar{r}_1\, \Sigma^{\mathrm{HF}}(1,\bar{1})g^{\gtrless}(\bar{1},1') - \int\limits_{t_0}^{t_1} d\bar{1}\,[\Sigma^{>}(1,\bar{1}) - \Sigma^{<}(1,\bar{1})]g^{\gtrless}(\bar{1},1') \\ + \int\limits_{t_0}^{t_{1'}} d\bar{1}\left[\Sigma^{\gtrless}(1,\bar{1}) + \Sigma^{in}(1,\bar{1})\right][g^{<}(\bar{1},1') - g^{>}(\bar{1},1')].\end{aligned} \tag{15}$$

In contrast to the original KBE [2], there are two new properties: (i) the equations are valid for arbitrary initial times t_0, (ii) they contain an additional self-energy contribution Σ^{in} which describes the influence of initial correlations. These equations are very general and contain, in the time-diagonal form and for special approximations for the self-energy, all the well-known kinetic equations for the Wigner distribution.

In order to determine the self-energy uniquely, boundary or initial conditions are necessary. Under the condition $t_{\mathrm{corr}} < t_{\mathrm{coll}}$ the Bogolyubov condition of weakening of initial correlations

$$\lim_{t_0 \to -\infty} g(12, 1'2')|_{t_0} = \left[g(1,1')g(2,2') \pm g(1,2')g(2,1') \right]_{t_0}$$

may be applied. With this condition follows $\Sigma^{in} = 0$, and we get the original KBE. This was shown in [21].

The most general and natural idea to fix the solution of the hierarchy for real times, however, is an initial condition,

$$g(12, 1'2')|_{t_0} = g(1,1')g(2,2')|_{t_0} \pm g(1,2')g(2,1')|_{t_0} + c(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2'; t_0)\,. \tag{16}$$

Here, $c(\mathbf{r}_1\mathbf{r}_2, \mathbf{r}_1'\mathbf{r}_2'; t_0)$ is the initial correlation.

3. Self-energy and initial correlations

Let us come back now to the central problem, the determination of the self-energy including initial correlations. In order to find the self-energy function, we start from (11). Therefore, we need the functional derivative $\delta g/\delta U$. Fortunately, a simple procedure for the calculation of this quantity is available [2]. We start from the equation (12) which, for $t_1, t_1' > t_0$, can be written in the form

$$\int_C g^{-1}(1,\bar{1})g(\bar{1},1')d\bar{1} = \delta(1-1')\,. \tag{17}$$

Here, the inverse Green's function g^{-1} is given by

$$g^{-1}(1,\bar{1}) = g_0^{-1}(1,\bar{1}) - U(1,\bar{1}) - \Sigma(1,\bar{1})\,. \tag{18}$$

Functional differentiation of (17) with respect to the external potential easily yields

$$\int_{\mathcal{C}} d\bar{1}\, \frac{\delta g^{-1}(1,\bar{1})}{\delta U(2',2)} g(\bar{1},1') = -\int_{\mathcal{C}} d\bar{1}\, g^{-1}(1,\bar{1}) \frac{\delta g(\bar{1},1')}{\delta U(2',2)}. \tag{19}$$

Using (18), the general solution of this equation and its adjoint can be found:

$$\begin{aligned} \frac{\delta g(1,1')}{\delta U(2',2)} &= \pm L(12,1'2') \\ &= g(1,2')g(2,1') + \int_{\mathcal{C}} d\bar{1} d\bar{\bar{1}}\, g(1,\bar{1}) \frac{\delta \left[\Sigma(\bar{1},\bar{\bar{1}}) + \Sigma_{in}(\bar{1},\bar{\bar{1}}) \right]}{\delta U(2',2)} g(\bar{\bar{1}},1') \\ &\quad \pm C(12,1'2'), \end{aligned} \tag{20}$$

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

$$\int_{\mathcal{C}} d\bar{1}\, g^{-1}(1,\bar{1}) C(\bar{1}2,1'2') = 0, \tag{21}$$

where Σ_{in} is the initial correlation contribution to $\hat{\Sigma}$. There are three similar conditions to (21), one following from the crossing symmetry $(1 \leftrightarrow 2)$ and two from the adjoint equation (12).

The function $C(12, 1'2')$ gives the possibility to take into account initial correlations. To show this we consider Eq. (20) in the limit $t_1, t_1' \to t_0$. Because the integral over the contour vanishes, it follows directly

$$L(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2', t_0) = c(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_1', \mathbf{r}_2', t_0) \pm g(\mathbf{r}_1, \mathbf{r}_2', t_0) g(\mathbf{r}_2, \mathbf{r}_1', t_0). \tag{22}$$

Hence, the function $c(t_0)$ has to be identified with initial binary correlations.

In order to explore the temporal evolution of the function $C(12, 1'2')$, we solve Eq. (21) (and the three analogous relations) together with the initial condition

$$C(12, 1'2')|_{t_1=t_2=t_1'=t_2'=t_0} = C(t_0). \tag{23}$$

The result is

$$C(12, 1'2') = \int\limits_{\mathcal{C}} d\bar{1} d\bar{2} d\bar{\bar{1}} d\bar{\bar{2}}\, g(1, \bar{1}) g(2, \bar{2})\, c(\bar{1}\bar{2}, \overline{\overline{12}})\, g(\bar{\bar{2}}, 2') g(\bar{\bar{1}}, 1'), \tag{24}$$

with

$$\begin{aligned} c(\bar{1}\bar{2}, \overline{\overline{12}}) \;&=\; c(\bar{\mathbf{r}}_1 t_0, \bar{\mathbf{r}}_2 t_0, \bar{\bar{\mathbf{r}}}_1 t_0, \bar{\bar{\mathbf{r}}}_2 t_0) \\ &\quad \times \delta(\bar{t}_1 - t_0) \delta(\bar{t}_2 - t_0) \delta(\bar{\bar{t}}_1 - t_0) \delta(\bar{\bar{t}}_2 - t_0). \end{aligned} \tag{25}$$

Let us now come back to the self-energy. Introducing Eqs. (20) and (24) into (11), we find the following functional equation for Σ:

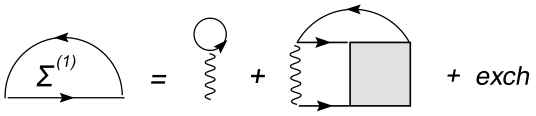
$$\begin{aligned} \Sigma(1, 1') \;=\; \pm i\hbar \int d2\, V(1-2) \Bigg\{ &\pm \int\limits_{\mathcal{C}} d\bar{1}\, g(1, \bar{1}) \frac{\delta[\Sigma(\bar{1}, 1') + \Sigma_{in}(\bar{1}, 1')]}{\delta U(2^+, 2)} \\ &+ \delta(1-1') g(2, 2^+) \pm \delta(2-1') g(1, 2^+) \\ &+ \int\limits_{\mathcal{C}} d\bar{1} d\bar{2} d\bar{\bar{2}}\, g(1, \bar{1}) g(2, \bar{2})\, c(\bar{1}\bar{2}, 1'\bar{\bar{2}})\, g(\bar{\bar{2}}, 2^+) \Bigg\}. \end{aligned} \tag{26}$$

For $\hat{\Sigma}$, an analogous equation follows readily. With Eq. (26), the self-energy is given as a functional of the interaction, the initial correlations, and the one-particle Green's function. From the definition of c, Eq. (25), it is obvious that the last contribution on the r.h.s. is local in time with a δ–type singularity at $t = t'$. Additional terms of this structure arise from the functional derivative. A further important property of the self-energy follows from comparing Σ, Eq. (26), with the corresponding expression for $\hat{\Sigma}$. One verifies that $\Sigma = \hat{\Sigma}$ for all times $t_1, t_1' > t_0$, which means, in particular, that for these times, a well defined inverse Green's function does exist.

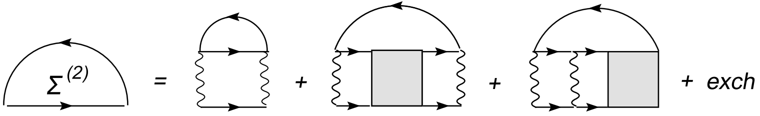
Eq. (26) is well suited to come to approximations for the self-energy. By iteration, a perturbation series for Σ in terms of g, V, and C can be derived which begins with

$$\begin{aligned} &\Sigma^1(1, 1') = \pm i\hbar \delta(1-1') \int d2\, V(1-2) g(2, 2^+) \\ &\pm i\hbar \int d2 V(1-2) \int\limits_{\mathcal{C}} d\bar{1} d\bar{2} d\bar{\bar{2}}\, g(1, \bar{1}) g(2, \bar{2})\, c(\bar{1}\bar{2}, 1'\bar{\bar{2}})\, g(\bar{\bar{2}}, 2^+) \\ &+\text{exchange}, \end{aligned}$$

or, in terms of Feynman diagrams,



Second order contributions are evaluated straightforwardly, too, with the result



In contrast to the conventional diagram technique, we have now the initial correlation as a new basic element, drawn by a shaded rectangle. 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 conclusion verifies the structure of the self-energy, Eqs. (14), as we discussed in the previous section. The same result was obtained by Danielewicz based on his perturbation theory for general initial states [10].

If one considers the first two iterations for the self-energy 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[1]

$$\begin{aligned}\Sigma^{in}(1,1') = \pm i\hbar \int d2\, V(1-2) \int d\bar{\mathbf{r}}_1 d\bar{\mathbf{r}}_2 d\bar{\bar{\mathbf{r}}}_1 d\bar{\bar{\mathbf{r}}}_2 \\ \times g^R_{12}(12, \bar{\mathbf{r}}_1 t_0, \bar{\mathbf{r}}_2 t_0) c(\bar{\mathbf{r}}_1 t_0, \bar{\mathbf{r}}_2 t_0, 1', \bar{\bar{\mathbf{r}}}_2 t_0) g^A(\bar{\bar{\mathbf{r}}}_2 t_0, 2^+) \delta(t_1' - t_0). \qquad (27)\end{aligned}$$

The analytical properties of $g^R_{12}(12, \bar{\mathbf{r}}_1 t_0, \bar{\mathbf{r}}_2 t_0)$ give rise to a damping γ_{12} leading to a decay of the initial correlation for times $t > 1/\gamma_{12} \sim t_{corr}$. Thus, after the initial stage of relaxation, the Bogolyubov condition of weakening of initial correlations is reproduced automatically.

The method to include initial binary correlations presented here is, undoubtedly, mathematically rigorous. The question arises which initial conditions are physically meaningful, i.e., which restrictions exist concerning the form of the function $c(t_0)$. The answer to that question has, in principle, to be given by the actual experimental situation. It can be shown, however, that a sufficient condition on the initial state is that it can be produced by a preceding evolution from another, in particular an uncorrelated, state, see [22]. The latter statement is again tangent to another question—why do not include the description of such a preceding evolution instead of constructing an initial correlation? The decision, of course, depends on the physical situation. However, there exist a variety of cases where the formation of the "initial" correlation is much more complicated than the result itself, consider, for example, the generation of a dense partially ionized plasma from a solid state target by an intense laser pulse. In such cases, the formalism developed above can be of high interest and usability.

4. Kinetic equation in first order gradient expansion. Bound states

Let us now discuss the transition from the Kadanoff–Baym equations to the usual kinetic equations for the Wigner function. The equation for the Wigner function follows from (15) and its adjoint equation in the time diagonal case $t_1 = t_1' = t$,

$$\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m_a} \nabla_{\mathbf{R}} - \nabla_{\mathbf{R}} U_a^{eff}(\mathbf{R}, t) \nabla_{\mathbf{p}} \right) f_a(\mathbf{p}, \mathbf{R}, t) =$$

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[1] Explicit expressions for Σ and Σ^{in} in T–matrix approximation have been given in [16].

$$
\int_{t_0}^{t} d\bar{t} \left\{ \left[\Sigma^<(t,\bar{t}) + \Sigma^{in}(t,\bar{t})\right] g^A(\bar{t},t) + \Sigma^R(t,\bar{t}) g^<(\bar{t},t) \right.
$$

$$
\left. - g^<(t,\bar{t}) \Sigma^A(\bar{t},t) - g^R(t,\bar{t}) \left[\Sigma^<(\bar{t},t) + \Sigma_{in}(\bar{t},t)\right] \right\} . \tag{28}
$$

This time-diagonal Kadanoff–Baym equation is the most general quantum mechanical kinetic equation. Like in the case of the two-time Kadanoff–Baym equations, we retained still (i) the influence of initial correlations, (ii) the effect of retardation, and (iii) the validity of conservation laws. The r.h.s. of Eq. (28) represents a rather far-reaching generalization of usual collision integrals. Unfortunately, the kinetic equation for the Wigner function is not closed because the single-particle Green's function arises on the right-hand side. In order to get a closed kinetic equation in explicit form, one has to solve still two problems: (i) The self energy Σ has to be determined as a functional of $g^{\gtrless}$ by perturbation theory. Here, the standard two-particle collision approximation (T–matrix approximation) will be used. (ii) The two-time correlation functions have to be reconstructed from the single-time single-particle density matrix. This is the so-called reconstruction problem, which was addressed first by Lipavský, Špička, and Velický [23].

In this section we will not consider the full non-Markovian kinetic equations. This was done e.g. in [8, 16]. Some effects of the initial stage can be taken into account already by expansions with respect to the retardation. Further we eliminate the correlation functions using the extended quasi-particle reconstruction concept according to [24].

Then, after some formal manipulations, the Boltzmann equation in first order retardation follows,

$$
\left(\frac{\partial}{\partial t} + \frac{\mathbf{p}}{m_a} \nabla_{\mathbf{R}} - \nabla_{\mathbf{R}} U_a^{eff}(\mathbf{R},t) \nabla_{\mathbf{p}} \right) f_a(\mathbf{p},\mathbf{R},t) =
$$

$$
= \lim_{\varepsilon \to 0} \left(1 + \frac{1}{2} \frac{d}{dt} \frac{d}{d\varepsilon} \right) I^0(\mathbf{p}\varepsilon) = I^0(\mathbf{p}) + I^1(\mathbf{p}) \, . \tag{29}
$$

Here, $I^0(\mathbf{p}\varepsilon)|_{\varepsilon\to 0} = I^0(\mathbf{p})$ is the Boltzmann collision integral with

$$
I^0(\mathbf{p}_1\varepsilon) = -\int d\mathbf{p}_2 d\bar{\mathbf{p}}_1 d\bar{\mathbf{p}}_2 \int d\omega \frac{1}{\pi} \frac{\varepsilon}{(\omega - E_{12})^2 + \varepsilon^2} \frac{1}{\pi} \frac{\varepsilon}{(\omega - \bar{E}_{12})^2 + \varepsilon^2} \times
$$

$$
\left| \langle \mathbf{p}_1 \mathbf{p}_2 | T^R(\omega + i\varepsilon) | \bar{\mathbf{p}}_2 \bar{\mathbf{p}}_1 \rangle \right|^2 \left[\bar{f}_1 \bar{f}_2 \left(1 \pm f_1\right)\left(1 \pm f_2\right) - f_1 f_2 \left(1 \pm \bar{f}_1\right)\left(1 \pm \bar{f}_2\right) \right] . \tag{30}
$$

The first order retardation contributions are collected in I^1 [24, 8]

$$
I^1 = \frac{\partial}{\partial t} \int \frac{d\mathbf{p}_2}{(2\pi)^3} \left\{ \frac{\partial}{\partial \omega} \mathrm{Re} \langle \mathbf{p}_1 \mathbf{p}_2 | T^R(\omega) | \mathbf{p}_2 \mathbf{p}_1 \rangle |_{\omega = E(\mathbf{p}_1) + E(\mathbf{p}_2)} f_1 f_2 \right.
$$

$$
\left. - \int \frac{d\omega}{2\pi} \langle \mathbf{p}_1 \mathbf{p}_2 | T^<(\omega + \epsilon(\mathbf{p}_2)) | \mathbf{p}_2 \mathbf{p}_1 \rangle \frac{P'}{\omega - E(\mathbf{p}_1)} (1 - f_1 - f_2) \right\} . \tag{31}
$$

It is important to remark that the second term in (31) is determined by the off-shell T–matrix. Therefore, it can be expected that this term contains bound state contributions. In order to separate the bound state parts, the off-shell term $T^<$ is written as a bilinear expansion with respect to the bound and scattering eigenstates of the two particle Hamiltonian

$$
I^1 = I^1_{scatt} + \frac{\partial}{\partial t} \int \frac{d\mathbf{p}_2}{(2\pi)^3} \sum_{jP} \langle \mathbf{p}_1 \mathbf{p}_2 | jP \rangle \langle Pj | \mathbf{p}_2 \mathbf{p}_1 \rangle N_j(P). \tag{32}
$$

Bound states can be considered now as a new species of composed particles. Then it is obvious to introduce the distribution function of the bound states $f^B(\mathbf{p}_1)$ and the free particles by the relations [7, 24]

$$\begin{aligned} f^B(\mathbf{p}_1) &= \int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3} \sum_{jP} \langle \mathbf{p}_1\mathbf{p}_2|\Psi^{jP}\rangle \left\langle \tilde{\Psi}^{jP}|\mathbf{p}_2\mathbf{p}_1\right\rangle N_j(P)\,, && (33) \\ f(\mathbf{p}_1) &= f^B(\mathbf{p}_1) + f^F(\mathbf{p}_1). && (34) \end{aligned}$$

Using these definitions, we get for the kinetic equation for the free particle distribution function $f^F(\mathbf{p}_1)$

$$\left(\frac{\partial}{\partial t}\frac{\mathbf{p}}{m_a}\nabla_{\mathbf{R}} - \nabla_{\mathbf{R}} U_a^{eff}(\mathbf{R},t)\nabla_{\mathbf{p}}\right) f_a^F(\mathbf{p},\mathbf{R},t) = I^B + I^1_{scatt}. \tag{35}$$

This equation is the basic equation of the kinetic theory with reactions, e.g. ionization and recombination, in plasmas. But we have to take into account that the kinetic equation is influenced by bound states only if there are changes of the bound state occupation $N_j(P)$ with respect to the time. That is the case only in collisions of at least three particles or for external fields. The approximation of the self-energy is therefore to extend to a cluster expansion up to three or more particles, see e.g. [7, 25, 26, 27].

In summary, we can conclude that the inclusion of first order gradient corrections gives an essential generalization of the usual Boltzmann equation. Especially, this equation conserves the total energy in binary collision approximation as was shown in [24, 8]. Furthermore, in (29) off-shell contributions appear which enable to investigate long-living correlations such as bound states.

5. Numerical illustration and discussion

Let us come back to the Kadanoff–Baym equations (15). Analytical solutions of these complex equations are available only for free particles. But also numerical solutions are possible up to now only for relatively simple approximations for the self-energy [28]. A short review of the numerical scheme for the solution of the Kadanoff–Baym equations and some results are given in papers of Köhler et al. [29, 30], and a text book [31]. We consider now the numerical solution of the Kadanoff–Baym equations in second Born approximation for the self-energy. Here, V_D is the statically screened Coulomb potential. The initial correlation contribution is given by

$$\begin{aligned} &\Sigma^{in}(\mathbf{p}_1;t_1,t_1') = -i\hbar^5 \int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\frac{d\mathbf{q}}{(2\pi\hbar)^3} V_D(\mathbf{q}) \\ &\times g^R(\mathbf{p}_1+\mathbf{q};t_1,t_0) g^R(\mathbf{p}_2-\mathbf{q};t_1,t_0) \\ &\times c(\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q},\mathbf{p}_1,\mathbf{p}_2;t_0) g^A(\mathbf{p}_2;t_0,t_1)\delta(t_1'-t_0). \end{aligned} \tag{36}$$

The initial correlations were chosen in the form of the Debye pair correlation:

$$\begin{aligned} &c(\mathbf{p}_1,\mathbf{p}_2;\mathbf{p}_1+\mathbf{q},\mathbf{p}_2-\mathbf{q};t_0) = \\ = \;& -\frac{1}{(i\hbar)^2}\frac{V_D(\mathbf{q})}{k_{\mathrm{B}}T} f(\mathbf{p}_1)f(\mathbf{p}_2)[1-f(\mathbf{p}_1+\mathbf{q})][1-f(\mathbf{p}_2-\mathbf{q})]|_{t_0}. \end{aligned} \tag{37}$$

Let us consider here, as a model system, the electrons in a hydrogen plasma with the density $n = 10^{21}$ cm^{-3} and the initial temperature $T_0 = 10000$ K. Figure 3 shows the result of the numerical computation for the full time dependence of $\mathrm{Im}\, g^<(\mathbf{p},t,t')$ for a fixed momentum. The time evolution of the Wigner function for a fixed momentum is given on the time diagonal $t = t'$. The spectral properties are shown perpendicular to the diagonal. We observe here

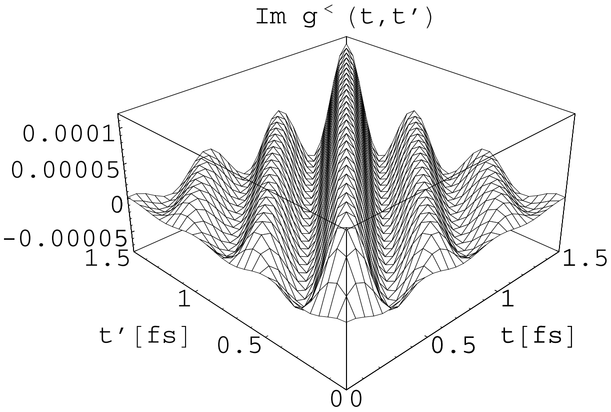

Figure 3. Temporal evolution of the imaginary part of $g^{<}(t,t')$, momentum $k = 0.8/a_B$, for electrons in hydrogen. The initial distribution is a Fermi distribution with $T = 10000$ K and $n = 10^{21}$ cm^{-3}.

oscillations which are determined by the single-particle energy and a damping of the amplitude which characterizes the damping of the single-particle states.

Macrophysical quantities are directly computed from the correlation function. For example, the kinetic energy is given by

$$\langle T\rangle(t) = \mathcal{V}\int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\frac{p^2}{2m}(-i\hbar)g^{<}(\mathbf{p},t,t) \tag{38}$$

and the potential energy follows from

$$\begin{aligned}\langle V\rangle(t) \;&=\; \frac{1}{4}\mathcal{V}\int \frac{d\mathbf{p}}{(2\pi\hbar)^3}\left\{\left(i\hbar\frac{\partial}{\partial t} - i\hbar\frac{\partial}{\partial t'}\right) - \frac{p^2}{m}\right\}\\ &\quad (-i\hbar)\, g^{<}(\mathbf{p},t,t')_{t=t'}.\end{aligned} \tag{39}$$

Here, $\mathcal{V}$ is the system volume.

Figure 4 shows the time evolution of kinetic, potential, and total energy for electrons in a hydrogen plasma in comparison of the initially correlated and uncorrelated case [17]. The following analogies and differences can be observed:

- In spite of the same initial density and temperature, the initial state is principally different. In the case free of correlations, the correlation energy is zero at $t_0 = 0$. If there exist initial correlations, it has already a finite value, leading e.g. to a different total energy.
- The behavior for short times ($t < t_{corr}$) is completely different, too. In both cases, this stage is determined by the correlation buildup. In the case of nonzero initial correlations, however, this buildup is superposed by their decay. Therefore, the value of the correlation energy is decreased.
- The evolution in the kinetic stage, i.e. after the correlation time t_{corr}, is independent on the initial correlation. Thus, Bogolyubov's weakening condition [cf. Eq. (6)] comes out automatically in that stage without postulating it, i.e., the system has “forgotten” about the initial state.
- Due to total energy conservation, different final kinetic energies (and therefore, final temperatures) are reached. Thus, the equilibrium state is influenced by the initial correlation due to its contribution to the total energy.

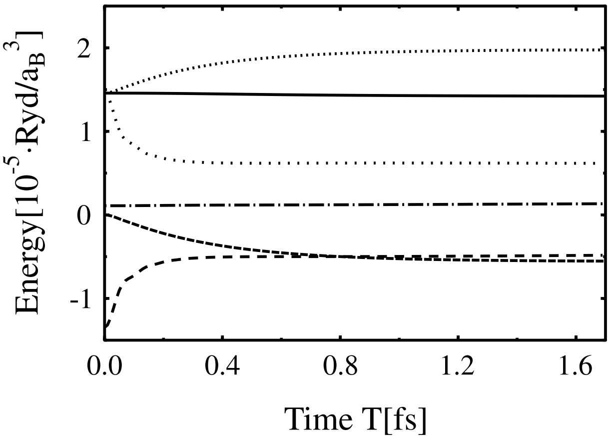

Figure 4. Temporal evolution of the kinetic energy without (narrow-dotted line) and with initial correlations (wide-dotted line), potential energy w/o (narrow-dashed line) and with initial correlations (wide-dashed line) and total energy without (solid line) and with initial correlations (dash-dotted line) for electrons in a hydrogen plasma. Parameters see Fig. 3.

- The equilibrium correlations agree approximately. They are nearly independent on the initial state.

We can conclude that the energy evolution on short time scales strongly depends on the initial state of the system, especially on the initial binary correlations. In the example shown above, the initial state is overcorrelated and, thus, causes a reduction of the kinetic energy. It can be easily verified by a simple energy balance that an *overcorrelated* initial state will always cause a decrease of kinetic energy while an *undercorrelated* initial state leads to its increase. Apart from contributions due to correlations built up in the system, the kinetic energy is closely connected with the temperature. Thus, we can conclude that, by preparing an overcorrelated initial state, it should be possible to cool down a system [32, 33, 34]. This cooling effect can be of experimental importance e.g. for ultracold ions in traps in order to reach still lower temperatures.

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