

# Quantum kinetic equations, memory effects, conservation laws

D. Kremp<sup>a,\*</sup>, Th. Bornath<sup>a</sup>, M. Bonitz<sup>a</sup>, M. Schlages<sup>b</sup>

<sup>a</sup> *Fachbereich Physik, Rostock University, D-18051 Rostock, Germany*

<sup>b</sup> *Institut für Physik, Ernst-Moritz-Arndt-University Greifswald, D-17489 Greifswald, Germany*

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## Abstract

In the framework of real-time Green's functions, a general non-Markovian Boltzmann equation including initial correlations, full time retardation (memory) and self energy is considered. This equation conserves the total (kinetic plus potential) energy. Two approximations of this very general equation are investigated: (i) the first order expansion with respect to the retardation and (ii) the first Born approximation for the scattering  $T$ -matrix (non-Markovian Landau equation). The influence of memory and damping effects on the relaxation of the one-particle distribution and of the kinetic energy is demonstrated by a numerical analysis.

**Keywords:** Quantum kinetic equations; Memory effects; Conservation laws

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## 1. Introduction

Though the Boltzmann equation is one of the fundamental equations in statistical physics, as it describes the irreversible relaxation to stationary states and is the basis of transport theory, this equation has many essential shortcomings. Two of these are:

- (i) The Boltzmann equation is valid only on time-scales larger than the correlation time  $\tau^{\text{corr}}$ .
- (ii) The Boltzmann equation conserves the kinetic energy or the quasiparticle energy only, instead of the total (kinetic plus potential) energy.

Especially, the second point is a serious problem in strongly correlated many-particle systems. In such systems, thermodynamic functions, as for example the internal energy, are essentially determined by correlation effects. Any kinetic theory of strongly correlated systems has to describe the relaxation to the nonideal thermodynamic properties. Now it is well known since papers of Bärwinkel [1] and Klimontovich [2] that this

defect of Boltzmann-type equations is essentially connected with the approximations with respect to time. Boltzmann-like kinetic equations are approximations local in time (Markovian equations) of the most general nonlocal form of kinetic equations given by Prigogine, Resibois, Zwanzig, Kadanoff and Baym and others [3–5]. In order to overcome the shortcomings, generalizations of Boltzmann-like Markovian kinetic equations are necessary. This will be done here in the framework of real-time Green's functions. Specifically, the connection between memory and the conservation laws shall be considered. Further, the influence of the memory and the memory depth on the relaxation of the momentum distribution and of the energy will be investigated solving numerically the non-Markovian Landau equation.

## 2. Non-Markovian Boltzmann equation

Within the frame work of real-time Green's functions, the equilibrium and nonequilibrium

\* Corresponding author.

properties of a many-particle system are determined by the two-time correlation functions  $\pm ig^<(1, 1') = \langle \Psi^+(1') \Psi(1) \rangle$  and  $ig^>(1, 1') = \langle \Psi(1) \Psi^+(1') \rangle$  with the abbreviation  $1 = r_1, s_1^3, t_1$ . These functions contain the statistical and spectral information on the system. From the Martin–Schwinger-hierarchy of equations of motion for the correlation functions, one can, specifying an initial condition for the two-particle correlation function, give a generalization of the time-diagonal Kadanoff–Baym equations. The equation for the Wigner function  $f(t) = \pm ig^<(t, t)$  has the form

$$\left\{ \frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \nabla_R \right\} f(\mathbf{p}, t) = F^+(t) + \int_{t_0}^t d\tilde{t} [\Sigma^<(t\tilde{t})g^A(\tilde{t}t) + \Sigma^R(t\tilde{t})g^<(\tilde{t}t) - g^<(t\tilde{t})\Sigma^A(\tilde{t}t) - g^R(t\tilde{t})\Sigma^<(\tilde{t}t)]. \quad (1)$$

Here  $\Sigma$  is the self energy determined by the potential and the two-particle correlation functions. The contribution  $F^+(t)$  is determined by

$$F^+(t) = \int d^3r_2 \{ V(r_1 - r_2) - V(r'_1 - r_2) \} \times \int d^3\tilde{r}_1 d^3\tilde{r}_2 d^3\tilde{r}_1 d^3\tilde{r}_2 g_{12}^R(r_1 r_2 t, \tilde{r}_1 \tilde{r}_2 t_0) \times g_{12}^<(\tilde{r}_1 \tilde{r}_2 t_0, \tilde{r}_1 \tilde{r}_2 t_0) g_{12}^A(\tilde{r}_1 \tilde{r}_2 t_0, r'_1 r_2 t). \quad (2)$$

The collision integral describes the different collision processes in the system and includes memory effects because it is nonlocal in time.

In order to derive explicit expressions for the collision integral, one has to solve two problems: The self energy has to be determined in an appropriate approximation and the so-called reconstruction problem has to be solved, i.e. the two-time correlation functions have to be determined as a functional of the time-diagonal part. The first problem can be solved within standard approximations [6,7] as for instance the binary collision approximation. The self energy in this approximation reads with help of the  $T$ -matrix

$$\Sigma^{\lessgtr}(\mathbf{r}_1 t, \mathbf{r}'_1 t') = \int d^3r_1 d^3\tilde{r}_2 \langle \mathbf{r}_1 \mathbf{r}_2 | T^{\lessgtr}(t, t') | \mathbf{r}'_1 \tilde{r}_2 \rangle \times (\pm i) g^{\lessgtr}(\tilde{r}_2 t', \mathbf{r}_2 t). \quad (3)$$

The  $T^{\lessgtr}$ -matrices are given by the generalized optical theorem

$$T^{\lessgtr}(t, t') = \int_{-\infty}^{\infty} d\tilde{t} d\tilde{t}' T^R(t, \tilde{t}) \mathcal{G}_{12}^{\lessgtr}(\tilde{t}, \tilde{t}') T^A(\tilde{t}, t'). \quad (4)$$

Thus they can be expressed in terms of the correlation functions  $\mathcal{G}^{\lessgtr} = ig_1^{\lessgtr} g_2^{\lessgtr}$  and the retarded and advanced  $T$ -matrices  $T^{R/A}$  which describe the in-medium scattering. The latter have to be determined from a generalized Lippmann–Schwinger equation

$$T^{R/A}(t, t') = V\delta(t - t') + i \int d\tilde{t} V \mathcal{G}^{R/A}(t, \tilde{t}) T^{R/A}(\tilde{t}, t'). \quad (5)$$

Another standard approximation for the self energy is the random phase approximation (RPA).

Let us consider now the reconstruction problem. Because we are interested in memory effects, the simple Kadanoff–Baym ansatz is not applicable. In a quasiparticle approximation, the so-called generalized Kadanoff–Baym ansatz (GKBA) can be used [8], i.e.

$$\pm g^{\lessgtr}(t_1, t_2) = f^{\lessgtr}(t_1) g_1^A(t_1 t_2) - g_1^R(t_1 t_2) f^{\lessgtr}(t_2) \quad (6)$$

with  $f^< = f$  and  $f^> = 1 \pm f$ .

A solution of the reconstruction problem going beyond the quasiparticle approximation but restricted to a first order expansion with respect to retardation is given by [9]

$$\begin{aligned} \pm ig^<(\omega, T) &= 2\pi\delta(\omega - E) f(T) - \frac{P'}{\omega - E} \frac{\partial}{\partial T} f(T) \\ &- \frac{P'}{(\omega - E)} (\pm i) \Sigma^<(\omega, T) + 2\pi\delta(\omega - E) \\ &\times \int \frac{d\tilde{\omega}}{2\pi} \frac{P'}{(\tilde{\omega} - E)} (\pm i) \Sigma^<(\tilde{\omega}, T). \end{aligned} \quad (7)$$

Using the GKBA and the binary collision approximation, we get the non-Markovian generalization of the Boltzmann equation

$$\left( \frac{\partial}{\partial t} + \frac{\mathbf{p}}{m} \nabla_R \right) f(pRt) = F^+(t) + Tr \int_{t_0}^t d\tilde{t} d\tilde{t}' \times \left\{ T^R(t\tilde{t}) \tilde{U}^A(\tilde{t}\tilde{t}') T^A(\tilde{t}\tilde{t}') U^A(\tilde{t}\tilde{t}') \right.$$

$$\begin{aligned}
& \times \left[ F^<(\tilde{t})\tilde{F}^>(\hat{t}) - \tilde{F}^>(\tilde{t})\tilde{F}^<(\hat{t}) \right] \\
& + T^R(\hat{t}\tilde{t})U^R(\tilde{t}\hat{t})T^A(\hat{t}\tilde{t})U^A(\hat{t}\tilde{t}) \\
& \times \left[ F^<(\tilde{t})\tilde{F}^>(\hat{t}) - F^>(\tilde{t})\tilde{F}^<(\hat{t}) \right] \\
& + U^R(\hat{t}\tilde{t})T^R(\tilde{t}\hat{t})U^R(\tilde{t}\hat{t})T^A(\hat{t}\tilde{t}) \\
& \times \left[ F^<(\tilde{t})\tilde{F}^>(\hat{t}) - F^>(\tilde{t})\tilde{F}^<(\hat{t}) \right] \\
& + U^R(\hat{t}\tilde{t})T^R(\tilde{t}\hat{t})U^A(\tilde{t}\hat{t})T^A(\hat{t}\tilde{t}) \\
& \times \left[ F^<(\tilde{t})\tilde{F}^>(\hat{t}) - F^>(\tilde{t})\tilde{F}^<(\hat{t}) \right] \Big\}, \quad (8)
\end{aligned}$$

with the abbreviations  $F^< = f_1^< f_2^<$  and  $F^> = f_1^> f_2^> = (1 \pm f_1)(1 \pm f_2)$ . The propagators are given by

$$U^{R/A}(\hat{t}\tilde{t}) = \Theta(\pm(\hat{t} - \tilde{t}))e^{i(E_1 + E_2 - i\gamma_1 - i\gamma_2)(\hat{t} - \tilde{t})}. \quad (9)$$

with the quasiparticle energies  $E_j$  and the damping  $i\gamma_j = \text{Im } \Sigma$ .

The most important properties of this kinetic equation are:

- The full energy, i.e. the sum of averaged kinetic and potential energy, in binary collision approximation is conserved by this equation. This follows from the fact that the binary collision approximation is a conserving one [5] and that there was no further approximation with respect to time.
- The equation includes memory effects with a memory depth given by  $1/\gamma_{12} = 1/(\gamma_1 + \gamma_2)$ .
- With the contribution  $F^+(t)$ , the influence of initial correlations is described. Because of the inclusion of damping in the propagators (9), the initial correlations are weakened in times  $t \sim 1/\gamma_{12}$ , i.e. the Bogoljubov condition is realized here by the interaction.

For applications this equation is very complicated due to the three time integrations in addition to the integrations with respect to momenta. We will therefore discuss two useful approximations in the following.

### 3. First order gradient expansion, conservation laws

An essential simplification of the non-Markovian Boltzmann equation can be reached if all the terms are expanded up to the first order with respect to

the retardation. The result can be written in the form

$$\frac{df}{dt} = I^B(p_1) + I^R(p_1), \quad (10)$$

where the local term, the Boltzmann collision integral, is given by

$$\begin{aligned}
I^B = & \int \frac{d^3 p_2 d^3 \tilde{p}_1 d^3 \tilde{p}_2}{(2\pi)^9} |\langle p_1 p_2 | T(E_{12} + i\varepsilon) | \tilde{p}_2 \tilde{p}_1 \rangle|^2 \\
& \times 2\pi\delta(E_{12} - \tilde{E}_{12}) (\tilde{f}_1 \tilde{f}_2 (1 \pm f_1)(1 \pm f_2) \\
& - f_1 f_2 (1 \pm \tilde{f}_1)(1 \pm \tilde{f}_2)). \quad (11)
\end{aligned}$$

First order retardation corrections, based on a Green's function approach, were given first by Bärwinkel [1]. But this result was not complete because Bärwinkel used the Kadanoff–Baym ansatz.

Considering for simplicity only the case of a non-degenerate many-particle system, the scattering  $T$ -matrices are dependent only on time differences, and we get

$$\begin{aligned}
I^R(p_1) = & \int \frac{d^3 p_2 d^3 \tilde{p}_1 d^3 \tilde{p}_2}{(2\pi)^9} \\
& \times \left\{ [|\langle p_1 p_2 | T(\tilde{E}_{12}) | \tilde{p}_1 \tilde{p}_2 \rangle|^2 \right. \\
& \quad \left. + |\langle p_1 p_2 | T(E_{12}) | \tilde{p}_1 \tilde{p}_2 \rangle|^2] \right. \\
& \times \frac{P'}{E_{12} - \tilde{E}_{12}} - 2\pi\delta(E_{12} - \tilde{E}_{12}) \\
& \left. \times \text{Im}(T^R T^{A'}) \right\} \left( \frac{dF^<}{dT} - \frac{d\tilde{F}^<}{dT} \right). \quad (12)
\end{aligned}$$

There is an interesting relation between  $I^B$  and  $I^R$  in the nondegenerate case. For this reason we define

$$\begin{aligned}
I^B(\varepsilon) = & \int \frac{d^3 p_2 d^3 \tilde{p}_1 d^3 \tilde{p}_2}{(2\pi)^9} \int \frac{d\omega}{2\pi} \frac{2\varepsilon}{(E - \omega)^2 + \varepsilon^2} \\
& \times \frac{2\varepsilon}{(\tilde{E} - \omega)^2 + \varepsilon^2} |\langle p_1 p_2 | T(\omega + i\varepsilon) | \tilde{p}_2 \tilde{p}_1 \rangle|^2 \\
& \times (\tilde{F}_{12}^< - F_{12}^<). \quad (13)
\end{aligned}$$

The kinetic equation in first order retardation then has the compact shape

$$\frac{d}{dT} f(p_1 T) = \left( 1 + \frac{1}{2} \frac{d}{dT} \frac{d}{d\varepsilon} \right) I^B(p_1, \varepsilon, T) \Big|_{\varepsilon \rightarrow 0}. \quad (14)$$

This relation holds also in the random phase approximation for the self energy, but in this case  $I^B(\varepsilon)$  has to be replaced by  $I^{LB}(\varepsilon)$

$$I^{LB}(\varepsilon) = \int \frac{dp_2 d\bar{p}_1 d\bar{p}_2}{(2\pi)^9} \int \frac{d\omega}{2\pi} \left\{ \frac{2\varepsilon}{(\omega - E_1 + \bar{E}_1)^2 + \varepsilon^2} \times \frac{2\varepsilon}{(\omega + E_2 - \bar{E}_2)^2 + \varepsilon^2} \left| \frac{V(p_1 - \bar{p}_1)}{\varepsilon^R(p_1 - \bar{p}_1, \omega)} \right|^2 \times \left[ \bar{F}_{12}^< F_{12}^> - \bar{F}_{12}^> F_{12}^< \right] \right\}. \quad (15)$$

It is easy to show that the kinetic equation (10) leads to conservation of the total density given by  $n = \int (dp/(2\pi)^3) f(p)$ .

Multiplying the kinetic equation with  $p^2/2m$  and integrating, we find

$$\frac{\partial}{\partial T} \langle T \rangle = - \frac{\partial}{\partial T} \langle V \rangle, \quad \text{i.e.} \quad \frac{\partial}{\partial T} \langle H \rangle = \frac{\partial}{\partial T} \langle T + V \rangle = 0, \quad (16)$$

with the mean potential energy in binary collision approximation

$$\langle V \rangle = \langle V \rangle^{\text{HF}} + \frac{1}{2} \text{Tr}_{12} \left[ |T^R(\bar{E})|^2 \frac{P}{E - \bar{E}} \left\{ F_{12}^< - \bar{F}_{12}^< \right\} \right]. \quad (17)$$

Thus the total energy in a binary collision approximation is a conserved quantity.

#### 4. Non-Markovian Landau equation

The first order expansion of the non-Markovian Boltzmann equation is not suited for the description of

short-time kinetics, i.e. details of the relaxation processes near the initial state cannot be described. In order to get a simplified kinetic equation, but without any approximation with respect to the times, we use the first Born approximation for the  $T$ -matrices

$$\langle p_1 p_2 | T^R(t_1, t_2) | \bar{p}_1 \bar{p}_2 \rangle = V(p_1 - \bar{p}_1) \delta(t_1 - t_2) \delta(p_1 + p_2 - \bar{p}_1 - \bar{p}_2). \quad (18)$$

The collision integral is now much simpler because of the  $\delta$ -function  $\delta(t_1 - t_2)$ . We get the non-Markovian Landau equation

$$\frac{d}{dt} f(p_1 t) = I^+(p_1 t) + I(p_1 t). \quad (19)$$

$I(p_1 t)$  is the non-Markovian Landau collision integral given by

$$I = 2n \int_0^{t-t_0} d\tau \int \frac{d\bar{p}_1 d\bar{p}_2 dp_2}{(2\pi)^9} |V(p_1 - \bar{p}_1)|^2 (2\pi)^3 \times \delta(p_1 + p_2 - \bar{p}_1 - \bar{p}_2) e^{-(\gamma_{12} + \bar{\gamma}_{12})\tau} \times \cos((\bar{E}_{12} - E_{12})\tau) \left[ \bar{F}_{12}^< F_{12}^> - \bar{F}_{12}^> F_{12}^< \right]_{t-\tau}. \quad (20)$$

The influence of initial correlations is described by  $I^+$

$$I^+ = 2n \int \frac{d\bar{p}_1 d\bar{p}_2 dp_2}{(2\pi)^9} V(p_1 - \bar{p}_1) (2\pi)^3 \times \delta(p_1 + p_2 - \bar{p}_1 - \bar{p}_2) e^{-(\gamma_{12} + \bar{\gamma}_{12})(t-t_0)} \times \text{Im} \{ \exp(i(\bar{E}_{12} - E_{12})(t-t_0)) g_{12}(t_0) \}. \quad (21)$$

Let us summarize the main properties of Eq. (19): the generalized Landau equation contains Pauli blocking and self energy effects, and it is valid for all times. The term  $I^+$  describes the influence of (arbitrary) initial correlations. The time integral in (20) corresponds to correlation build up. Eq. (19) contains energy broadening of the form  $\cos((\bar{E}_{12} - E_{12})t)$  and includes retardation (memory effects) in the distribution functions. Self energy effects give rise to the damping exponents ( $\gamma_{12} \sim \text{Im} \Sigma_1 + \text{Im} \Sigma_2$ ). This assures time irreversibility and the correct long-time behaviour (damping of initial correlations and finite memory depth).

In many cases, the memory depth is sufficiently small, so that damping and memory can be neglected.

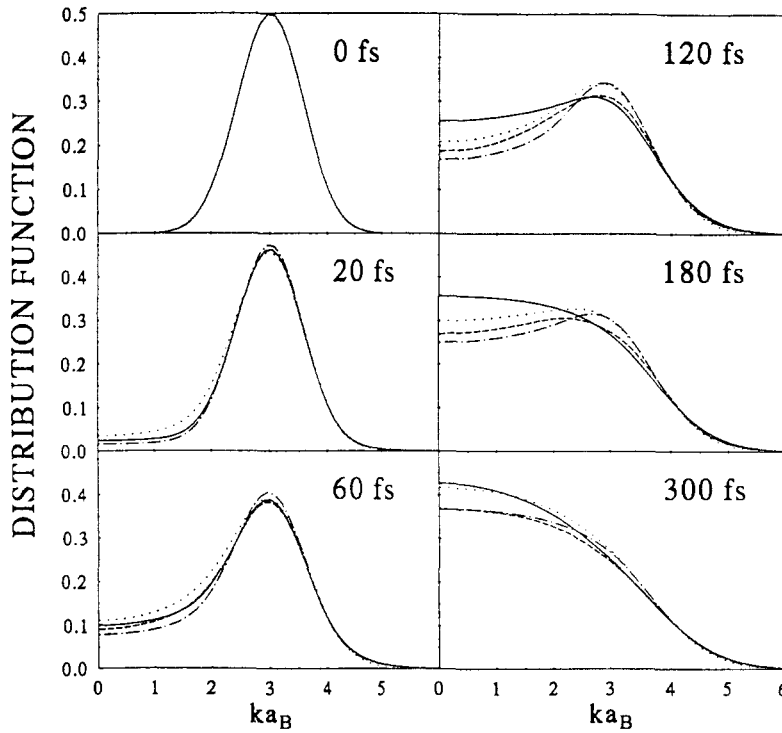


Fig. 1. Relaxation for a screened potential with  $\kappa a_B = 1.16$ . The different parts of the figure represent the different time steps. Relaxation is calculated in four different approximations for the collision integral: Markovian Landau equation (dotted line), collisional broadening approximation [Eq. (22)] (full line), the non-Markovian equation (20) with  $\gamma_{12} = 0$  (dashed line) and the Kadanoff–Baym equation in the first Born approximation [12] (dash-dotted line).

Then the  $\tau$ -integration can be performed in (20) with the result

$$I = 2n \int \frac{d\bar{p}_1 d\bar{p}_2 dp_2}{(2\pi)^9} |V(p_1 - \bar{p}_1)|^2 (2\pi)^3 \times \delta(p_1 + p_2 - \bar{p}_1 - \bar{p}_2) \times \frac{\sin(\bar{E}_{12} - E_{12})(t - t_0)}{\bar{E}_{12} - E_{12}} \times \left[ \bar{F}_{12}^< F_{12}^> - \bar{F}_{12}^> F_{12}^< \right]_t. \quad (22)$$

Eq. (19) conserves density, momentum and the total energy in second Born approximation. The general expression for the potential energy, including Pauli blocking, self energy and initial correlations, is

$$\langle V \rangle(t) = -\frac{nN}{2} \int \frac{dp_1 dp_2 d\bar{p}_1 d\bar{p}_2}{(2\pi)^{12}} V(p_1 - \bar{p}_1) \times (2\pi)^3 \delta(p_1 + p_2 - \bar{p}_1 - \bar{p}_2)$$

$$\times \left\{ \int_0^{t-t_0} d\tau e^{-(\gamma_{12} + \bar{\gamma}_{12})\tau} \sin((\bar{E}_{12} - E_{12})\tau) \times V(p_1 - \bar{p}_1) \left[ \bar{F}_{12}^< F_{12}^> - \bar{F}_{12}^> F_{12}^< \right]_{t-\tau} - e^{-(\gamma_{12} + \bar{\gamma}_{12})(t-t_0)} \times \text{Im}[\exp(i(\bar{E}_{12} - E_{12})(t-t_0)) g_{12}(t_0)] \right\}. \quad (23)$$

The non-Markovian Landau equation is “simple” enough for a numerical evaluation. Fig. 1 shows results of the numerical solution of the non-Markovian Landau equation for a one-component 3D isotropic system starting from a nonequilibrium initial distribution (Gaussian) with zero initial correlations. For the calculation, we used a screened potential  $V(r) = 2/r e^{-\kappa r}$ . The relaxation is compared for different approximations, including the Markovian collision integral and also the solution of the two-time Kadanoff–Baym equations for the correlation functions in the Born approximation [5,10–12]. Fig. 2 shows the relaxation of the corresponding kinetic en-

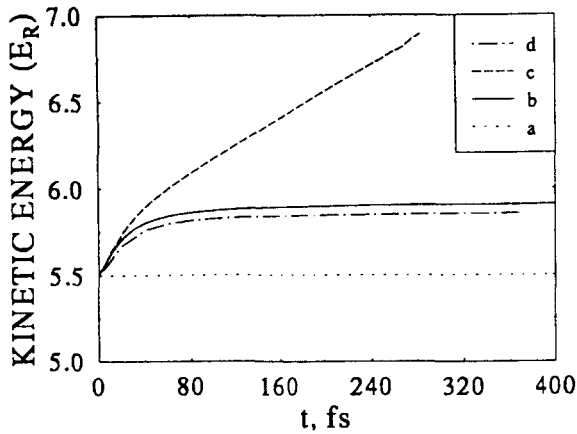


Fig. 2. Relaxation of the kinetic energy. The same approximations, and line styles denoting them, as in Fig. 1 are used.

ergy. As a result of energy broadening and correlation build up, the kinetic energy in the system increases. It is interesting that there is a good agreement between the zeroth order retardation approximation [cf. (22)] and the Kadanoff–Baym equation. On the other hand, the full kinetic equation (19) without self

energy, which is time reversible, strongly overestimates memory effects.

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