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Correlation time approximation in non-Markovian kinetics

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Abstract

A new approximation to kinetic equations is derived which has a broad range of applicability. It allows one to take into account dominant memory and correlation effects while solving only Markovian instead of complicated non-Markovian kinetic equations. It furthermore yields a drastic simplification of kinetic equations for spatially inhomogeneous systems. The approximation is illustrated numerically on examples based on the quantum Boltzmann equation with, respectively, a static and a dynamically screened interaction potential (Lenard–Balescu equation).

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Short-time phenomena are currently of high interest in the context of laser–plasma interaction, ultrafast optical response of semiconductors [1] and in nuclear matter as well [2,3]. Laser pulses have become so short that they do not only influence the carrier relaxation (one-particle properties), but also modify the interaction and the correlations between the particles (two-particle properties). Therefore, to understand the experimentally measured response of a many-particle system to ultra-short optical excitation (for a review, see, e.g., Ref. [4]), requires insight in the formation of binary correlations [5,6], the build-up of plasma screening [7,8] and the formation of bound states [9].

These phenomena are best described in the framework of the Kadanoff–Baym equations for the two-time correlation functions [10]. However, these equations are of rather complex structure and are currently accessible only on supercomputers, and yet only within the Born approximation [3,5]. One may therefore try to deal with the simpler equations for the one-time Wigner distribution function f (see, e.g., Refs. [2,11]) or, alternatively, coupled equations for the distribution and the binary correlation function g_{12} [6]. However, still these equations are very complicated due to their non-Markovian structure and they have been solved only within the Born approximation [12,5]. More realistic models like the binary collision (T-matrix) approximation [9] or the random phase approximation (RPA) [11] increase the numerical effort by orders of magnitude, since, due to the intrinsic dynamics of the scattering matrix and the screened potential, respectively, they contain two additional time integrals in the collision terms.

On the other hand, though recent experiments have been successfully explained using non-Markovian kinetic equations [1], many other experiments show only a weak signature of memory effects and agree well with "classical" Markovian models. This suggests that, in many situations of short-time relaxation, a full non-Markovian treatment is not necessary. Instead, one might try to look for simpler models which are based

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on Markovian kinetics and account for memory effects approximately. One possible approach is to perform retardation expansions of the full kinetic equations [12,5,6]. The analysis within the Born approximation showed that keeping only the lowest two expansion terms or even only the lowest one, yields in many cases sufficiently accurate results [5]. However, the resulting collision integrals are still essentially more complicated than their "classical" counterparts since they contain energy broadening instead of a kinetic energy (quasi-particle) conserving delta function, what again becomes a problem if one goes beyond the Born approximation.

For this reason, in this paper a different approach is proposed which is applicable to non-Markovian equations in general. The basic idea is to take advantage of the fact that generalized kinetic equations describe processes on several time scales (correlation time τ_{cor} and relaxation time t_{rel}), which are often very different from each other. It turns out that if the correlation dynamics is much faster than that of the one-particle properties (as is the case in most situations), a drastic simplification of the kinetic description is possible. At the same time, in an spatially inhomogeneous system, a separation of time scales translates into separated length scales, what again allows for a significant simplification of the description.

The concept of time scales is among the most fruitful for theoretical modelling of physical phenomena [13]. The separation of fast processes (e.g. in oscillation theory) or the identification of "master" processes (self-organization, nonequilibrium phase transitions) allows one not only to simplify the model, but often yields far deeper insight into the underlying physics. Though the situation in kinetic theory is more complicated by the fact that the number of variables is large (e.g. continuous dependence of the Wigner distribution on coordinates and momentum), this concept is well established in the relaxation time approximation (RTA), where the collision term I in the kinetic equation is approximated by a single (total) collision rate $\nu = t_{rel}^{-1}$,

$$\frac{\mathrm{d}f(\boldsymbol{p},t)}{\mathrm{d}t} = I(\boldsymbol{p},t) \approx -\frac{f(\boldsymbol{p},t) - f^{EQ}(n,T;\boldsymbol{p})}{t_{rel}(n,T)}. \tag{1}$$

Here f^{EQ} is the (local) equilibrium distribution function which depends on density (n) and temperature (T). Taking advantage of the existence of different time scales, this approximation was very successful for incorporating the effect of collisions (fast process) into macroscopic balance equations, describing diffusion, electrical and heat conductivity etc. (slow processes) qualitatively correct. Among the well-known representatives of this approach we mention the Drude theory of dielectric and optical properties of solids and the relaxation time approximation to the semiconductor Bloch equations [15]. The relaxation time t_{rel} in Eq. (1) is calculated as the inverse of the sum of all collision rates, accounting for different types of scattering processes and different particle species as well. The collision rates are taken from experiment or are derived from kinetic theory. Alternatively, comparison with the solution of the full kinetic equation allows one to determine t_{rel} as a fit to the momentum dependent scattering rates and reproduces the exact relaxation properties to a high degree of accuracy [14]. Of course, there are other situations where a relaxation time approximation is not applicable, i.e. when details of the momentum dependence of the scattering rates are important, especially if the system is far from equilibrium.

To extend this concept to non-Markovian kinetics we use a density operator representation of generalized kinetic equations, because this allows for a clear distinction of the relevant time scales. The starting point are the first two equations of the BBGKY-hierarchy for the one-particle density operator F_1 and the binary correlation operator $g_{12} = F_{12} - F_1 F_2$,

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F_1 - [H_1 + U_1^{HF}, F_1] = n\,\mathrm{Tr}_2[V_{12}, g_{12}], \tag{2}$$

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}g_{12} - [H_{12}^0 + V_{12}, g_{12}] - [V_{12}, F_1F_2] = n\,\mathrm{Tr}_3([V_{13}, F_1 g_{23}] + [V_{23}, F_2 g_{13}] + [V_{13} + V_{23}, g_{123}]), \tag{3}$$

with the Hartree–Fock contributions, $U_1^{HF} = n\,\mathrm{Tr}_2 V_{12}F_2$ and the effective free two-particle Hamiltonian $H_{12}^0 = H_1 + H_2 + U_1^{HF} + U_2^{HF}$, n is the density and V_{12} the binary interaction potential. Eqs. (2) and (3) are exact.

They couple to the higher order hierarchy equations via g_{123}. Details of the spin statistics will not be important below, so we use the classical form (2), (3) of the hierarchy equations.

Eqs. (2), (3) contain all possible generalized (non-Markovian) kinetic equations, including the Landau equation (second Born approximation), the Boltzmann (T-matrix) equation, the Lenard–Balescu equation (polarization approximation) and the screened ladder approximation. The choice of the model is governed by the approximation for the three-particle correlation operator g_{123}, i.e. the hierarchy is decoupled on the level of ternary correlations with $g_{123} = g_{123}(\{F_1\}, \{g_{12}\})$, and by the neglect of various terms in Eq. (3). Furthermore, self-energy effects may be included also [5].

Let us consider in the following the spatially homogeneous situation, extension to inhomogeneous systems will be discussed below. Then we introduce the momentum representation, with f and g being the matrix elements of the operators F_1 and g_{12}, respectively. Eqs. (2), (3) can now be rewritten in the form

$$\frac{\mathrm{d}}{\mathrm{d}t} f(\boldsymbol{p}_1, t) = I(\boldsymbol{p}_1, t) = \frac{2\mathcal{V}^2}{\hbar} \int \frac{\mathrm{d}\boldsymbol{p}_2}{(2\pi\hbar)^3} \frac{\mathrm{d}\bar{\boldsymbol{p}}_1}{(2\pi\hbar)^3} \frac{\mathrm{d}\bar{\boldsymbol{p}}_2}{(2\pi\hbar)^3} V\left(\frac{\boldsymbol{p}_1 - \bar{\boldsymbol{p}}_1}{\hbar}\right) \operatorname{Im} g(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t), \tag{4}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} g(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t) = J(\{f(t)\}, \{g(t)\}), \qquad \boldsymbol{p}_1 + \boldsymbol{p}_2 = \bar{\boldsymbol{p}}_1 - \bar{\boldsymbol{p}}_2, \tag{5}$$

where $\mathcal{V}$ is the volume. The formal solution of Eq. (5) can, due to linearity in g, be written as

$$g(t) = J_0(\{g_0\}, t) + J_s(\{f(t)\}, t), \tag{6}$$

where J_0 is related to the initial correlations $g_0 = g(t_0)$ and J_s is a source term which arises from terms in Eq. (3) that do not contain g_{12}. The time dependence of all quantities is indicated explicitly. In particular, the source contribution J_s contains a two-fold time dependence: an explicit dependence and a dependence via the one-particle distribution function. This two-fold dependence has been studied in detail in Ref. [6] and will only briefly be summarized here: Typically, the relaxation can be divided into (at least) three distinct stages. At the initial stage, the two-particle and possibly higher correlations relax until they have reached an equilibrium form after the correlation time $t = \tau_{\mathrm{cor}}$, while $f(t)$ changes only insignificantly. In the time interval $\tau_{\mathrm{cor}} < t < t_{\mathrm{rel}}$, the one-particle distribution function relaxes towards its equilibrium form. Still the correlation function changes, but only weakly, via the implicit time dependence $g(t) = g\{f(t)\}$, $t > \tau_{\mathrm{cor}}$. The third major stage is that of hydrodynamic relaxation, $t_{\mathrm{rel}} < t < t_{\mathrm{mac}}$, where the relaxation towards the stationary state proceeds on a macroscopic scale, given by the evolution of density, temperature, pressure, etc. The main statement is now that, in most situations [13,6],

$$\tau_{\mathrm{cor}} \ll t_{\mathrm{rel}} \ll t_{\mathrm{mac}}. \tag{7}$$

Whereas the last inequality is the basis for the relaxation time approximation, Eq. (1), in analogy, the first inequality allows for deriving the correlation time approximation (CTA). Before we proceed we have to eliminate physical situations for which the correlation time might be comparable to or even exceed the relaxation time. This is the case for long-range correlations, which are related to bound states, hydrodynamic modes (turbulent vortices) or plasma turbulence, and also correlations in the vicinity of phase transitions, which we will not consider in this paper.

The reason for the complexity of non-Markovian kinetic equations is the complicated dynamics of g_{12} on times $t < \tau_{\mathrm{cor}}$. When time approaches the correlation time, the deviation of g_{12} from its equilibrium form gradually vanishes. Then we may expect a linear approximation to be sufficiently accurate, so we define the CTA as

$$\frac{\mathrm{d}g(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t)}{\mathrm{d}t} \approx -\frac{g(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t) - g^{\mathrm{EQ}}(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, \{F(t)\})}{\tau_{\mathrm{cor}}}, \tag{8}$$

where g^{EQ} is an equilibrium (Markovian) binary correlation function, which still depends on time via the nonequilibrium distributions. The correlation time is momentum and time independent, though we may permit a slow time dependence (as a function of density or via the distribution functions, as is the case e.g. for pulsed excitation of carriers in semiconductors). g^{EQ} and τ_{cor} will be specified below. The solution of Eq. (8) together with the initial condition $g(t_0) = g_0$ is readily found (we drop the momentum arguments)

$$g_{CTA}(t) = g^{EQ}\{F(t)\} + [g_0 - g^{EQ}\{F(t)\}]e^{-t/\tau_{cor}}. \tag{9}$$

g_{CTA} evolves from g_0 at the initial moment, approaching g^{EQ} for long times, while the influence of the initial correlations decays exponentially. In case of zero initial correlations ($g_0 = 0$), the solution is particularly simple

$$g_{CTA}(t) = g^{EQ}\{F(t)\}(1 - e^{-t/\tau_{cor}}). \tag{10}$$

Let us now consider the collision integral of the kinetic equation which follows from the CTA. Taking into account Eq. (4) and the solution (9) we obtain

$$I_{CTA} = e^{-t/\tau_{cor}} \frac{2\mathcal{V}^2}{\hbar} \int \frac{d\boldsymbol{p}_2}{(2\pi\hbar)^3} \frac{d\bar{\boldsymbol{p}}_1}{(2\pi\hbar)^3} \frac{d\bar{\boldsymbol{p}}_2}{(2\pi\hbar)^3} V\left(\frac{\boldsymbol{p}_1 - \bar{\boldsymbol{p}}_1}{\hbar}\right) \operatorname{Im} g_0(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2)$$
$$+ (1 - e^{-t/\tau_{cor}}) \frac{2\mathcal{V}^2}{\hbar} \int \frac{d\boldsymbol{p}_2}{(2\pi\hbar)^3} \frac{d\bar{\boldsymbol{p}}_1}{(2\pi\hbar)^3} \frac{d\bar{\boldsymbol{p}}_2}{(2\pi\hbar)^3} V\left(\frac{\boldsymbol{p}_1 - \bar{\boldsymbol{p}}_1}{\hbar}\right) \operatorname{Im} g^{EQ}(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t). \tag{11}$$

Of course, the choice of a single scalar correlation time means a drastic simplification of the true dynamics and will not allow one to describe all situations of non-Markovian relaxation, in particular, on the very first stage of evolution, where $t \ll \tau_{cor}$. However, for times of the order of magnitude of the correlation time, which is sufficient in many cases, we may expect approximations that are based on Eq. (8) to qualitatively and quantitatively correctly reproduce the main features of the exact non-Markovian dynamics. This will be confirmed by the numerical examples below.

Let us now summarize properties of non-Markovian kinetic equations and discuss how they are reproduced by approximations of the type of Eq. (8).

(1) Decay of initial correlations as well as correlation build-up on times of the order of τ_{cor}: This is correctly reproduced by the CTA if τ_{cor} in Eq. (8) is sufficiently close to the true correlation time of the system. Similarly as with the RTA, this time may be taken from experiment or from full non-Markovian calculations. A simple way to calculate τ_{cor} within the Born approximation was given in Ref. [6]. For systems with short-range (r_{int}) interaction, $\tau_{cor} \approx r_{int}/v_0$, where v_0 is a characteristic velocity determined by the initial distribution function. For long-range interaction (e.g. Coulomb interaction), $\tau_{cor} \approx 2\pi/\omega_{pl}$, where ω_{pl} is the plasma frequency [7].

(2) In the limit of long times ($t > \tau_{cor}$) the "classical" Markovian kinetics is recovered, including the kinetic (quasi-particle) energy conserving delta function: This is guaranteed if g^{EQ} in Eq. (8) is taken to be the correct "classical" correlation function,

$$\operatorname{Im} g_0^{EQ}(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t) = V\left(\frac{\boldsymbol{p}_1 - \bar{\boldsymbol{p}}_1}{\hbar}\right) \Phi(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t), \qquad \text{Born},$$
$$= \frac{V((\boldsymbol{p}_1 - \bar{\boldsymbol{p}}_1)/\hbar)}{|\varepsilon(E_1 - \bar{E}_1, \boldsymbol{p}_1 - \bar{\boldsymbol{p}}_1)|^2} \Phi(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t), \qquad \text{RPA},$$
$$= \frac{|T(E_{12} + i\epsilon)|^2}{V((\boldsymbol{p}_1 - \bar{\boldsymbol{p}}_1)/\hbar)} \Phi(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t), \qquad \text{BCA}. \tag{12}$$

where $\Phi(\boldsymbol{p}_1, \boldsymbol{p}_2, \bar{\boldsymbol{p}}_1, \bar{\boldsymbol{p}}_2, t) = (2\pi\hbar)^3 \delta(\boldsymbol{p}_1 + \boldsymbol{p}_2 - \bar{\boldsymbol{p}}_1 - \bar{\boldsymbol{p}}_2) 2\pi\delta(E_{12} - \bar{E}_{12})(\bar{f}_1\bar{f}_2 - f_1 f_2)$, E_1 is the one-particle (quasiparticle) energy, $E_{12} = E_1 + E_2$, $f_1 = f(\boldsymbol{p}_1)$ and $\bar{f} = f(\bar{\boldsymbol{p}})$. Furthermore, "Born", "RPA" and "BCA" denote the second Born approximation, the random phase approximation and the binary collision approximation

(ladder approximation), respectively. ε is the dielectric function and T the T-matrix (scattering matrix). Inserting g_0^{EQ} from Eq. (12) into the collision integral (11), yields the "classical" Markovian collision integral in the respective approximation modified by a switch-on factor accounting for the correlation build-up. This approximation will be studied numerically below for the Born approximation and for the RPA.

(3) Non-Markovian kinetic equations conserve density: this is also fulfilled by the CTA.

(4) Non-Markovian kinetic equations, in a proper formulation, conserve total energy [5]: With the choice of Eq. (12), due to the energy delta function, obviously only kinetic (quasi-particle) energy is conserved. However, it is well-known that total energy conservation may be achieved also with Markovian collision integrals [16,17,6]. For this it is sufficient to include into g^{EQ} an additional contribution which can be derived from a retardation expansion of the distribution functions in the non-Markovian expression for the correlation function, Eq. (6). Keeping the first two terms, $f(t-\tau) \approx f(t) - \tau f'(t)$, the result in the long-time limit $t \longrightarrow \infty$, is [1]

$$\mathrm{Im}\, g_1^{EQ}(t) = \left(1 + \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right) \mathrm{Im}\, g_\varepsilon^{EQ}(t)|_{\varepsilon\to 0}, \tag{13}$$

where the limit $\varepsilon \to 0$ is to be taken after the differentiation. g_ε^{EQ} is identical to g_0, except that the energy delta function is replaced by a broadened function $\delta_\varepsilon = 2\varepsilon/[(E_{12} - \bar{E}_{12})^2 + \varepsilon^2]$. The first term on the r.h.s. of Eq. (13) yields just $\mathrm{Im}\, g_0^{EQ}$, from Eq. (12), whereas the second term gives the first order retardation correction. With $g^{EQ} = g_1^{EQ}$ in Eq. (8) total energy is conserved in the long time limit.

(5) Non-Markovian kinetic equations contain memory (retardation) effects: Using $g^{EQ} = g_1^{EQ}$ accounts for memory effects in first order (linear in the retardation time τ), which is sufficient in most cases, because the actual memory depth is limited by the damping effect.

(6) Non-Markovian kinetic equations exhibit collisional energy broadening, which is due to the replacement of the energy delta function by oscillating exponents of the form $\exp[\mathrm{i}(E_{12} - \bar{E}_{12})t/\hbar]$, and causes kinetic energy (quasi-particle energy) to increase in carrier–carrier scattering on short times $t < \tau_{cor}$ [5]: In choosing "classical" Markovian expressions for g^{EQ}, such as g_0^{EQ} or g_1^{EQ}, of course, this effect is lost. On the other hand, in systems with strong coupling, i.e. where the mean interaction energy is comparable to the mean kinetic energy, this can be an important and even the dominant effect. As a result, the system will relax towards a stationary state with significantly increased temperature, compared to the "classical" prediction. Therefore, in some cases, it may be highly desirable to incorporate this effect into the CTA. This can be done in the following phenomenological way: Suppose the kinetic energy at the initial moment is

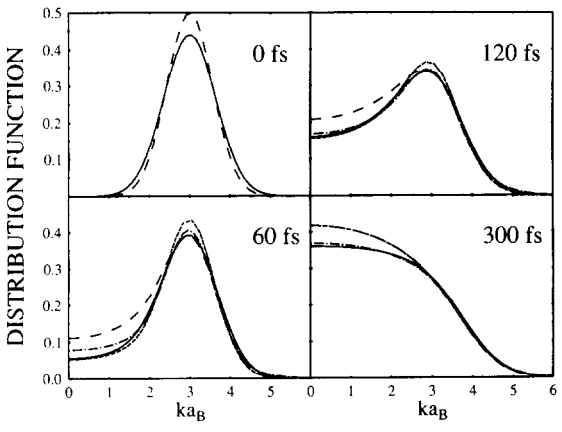
$$E_{KIN}^0 = \mathcal{V} \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi\hbar)^3} \frac{p^2}{2m} f(\boldsymbol{p}, t_0)$$

and increases by ΔE_{KIN} to

$$E_{KIN}^c = \mathcal{V} \int \frac{\mathrm{d}\boldsymbol{p}}{(2\pi\hbar)^3} \frac{p^2}{2m} f(\boldsymbol{p}, \tau_{cor})$$

(due to the, basically, "classical" kinetics, for $t > \tau_{cor}$, it will not change significantly further). If $f(\tau_{cor})$ would be an equilibrium distribution $f^{EQ}(n,T)$, we would simply use E_{KIN}^c for the temperature, e.g. $3k_BT/2 = E_{KIN}^c$. But in general this is not the case and $f(\tau_{cor})$ is unknown. We know, however, the zeroth and second momenta of $f(\tau_{cor})$, density (which is conserved) and kinetic energy (E_{KIN}^c), respectively. Furthermore we know that $f(\tau_{cor})$ is only slightly different from $f(t_0)$. Then we may write

[1] This result is always true for the second Born approximation. In the case of the binary collision approximation and the RPA, such a simple relation has, so far, been found only for the nondegenerate case [18].



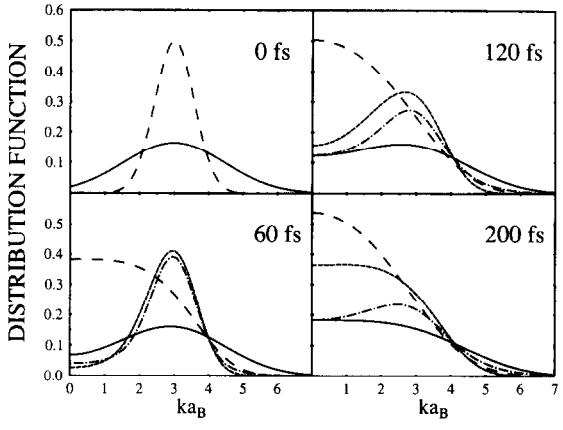


Fig. 1. Relaxation of the distribution function in the second Born approximation for a weak static potential ($\kappa a_B = 1.16$). The relaxation corresponding to four different scattering approximations is shown: "classical" kinetic equation (long dashes), Kadanoff–Baym equations (dash-dotted line), CTA without and with energy increase (short dashes and full line, respectively).

Fig. 2. The same as Fig. 1 but for the strong interaction potential ($\kappa a_B = 0.2$).

$$f(\tau_{cor}) \approx f(t_0) + \left.\frac{\delta f(t_0)}{\delta E_{KIN}}\right|_n \Delta E_{KIN}, \tag{14}$$

where the derivative is to be calculated at fixed density. Finally, we may reverse the question: How do we need to modify the initial distribution in order to obtain from the CTA-dynamics after $t = \tau_{cor}$ a distribution of the original density but with a modified kinetic energy equal to E^c_{KIN}? The answer is to just replace $f(t_0) \rightarrow \tilde{f}(t_0) = f(\tau_{cor})$ from Eq. (14). Taking, for example, a pulse-shaped initial nonequilibrium distribution, this procedure means to "renormalize" it by increasing the width and reducing the height of the peak. This is also physically transparent: Due to energy broadening, the particles "see" an energetically broadened distribution. Like the correlation time, the value of ΔE_{KIN} has to be obtained from non-Markovian calculations [6].

Thus, basic phenomena of non-Markovian calculations can be included into the correlation time approximation. The numerical calculations below will show that even good quantitative agreement can be achieved.

It is further possible to upgrade the CTA, by self-consistently calculating the correlation time from the "classical" total scattering rates $\Gamma = \Gamma^{IN} + \Gamma^{OUT}$ according to [6]

$$\frac{\hbar}{\tau_{cor}} = \alpha \Gamma(p_0, t_0), \tag{15}$$

where α and p_0 are free parameters. Our numerical analysis shows that, at least for weak interaction potentials, it is always possible to choose α and p_0 such that the correlation time is well reproduced.

We illustrate the use of the CTA on three numerical examples. First, we consider the simplest model of two-particle scattering, the second Born approximation. For this case, extensive numerical investigations of non-Markovian carrier relaxation have been performed. In particular, correlation build-up and kinetic energy relaxation have been studied in detail within different models, including the two-time Kadanoff–Baym equations [5,6]. Results from the latter should be regarded as the most accurate model and will, therefore, be used to test the results from the CTA.

Figs. 1 and 2 show calculations with the same parameters as in Ref. [5], which were chosen to model the intraband relaxation of electrons in bulk-GaAs. The interaction potential is of Yukawa type (Debye potential) with the Fourier transform $V(q) = 4\pi e_0^2/\mathcal{V}\epsilon_b/(q^2 + \kappa^2)$, where e_0 is the free electron charge and $\epsilon_b = 13.998$ the background dielectric constant. Fig. 1 shows calculations with a weak interaction potential, $\kappa = 1.16 a_B^{-1}$ ($a_B = 132$ Å is the exciton Bohr radius), which corresponds to the static long wavelength limit of the

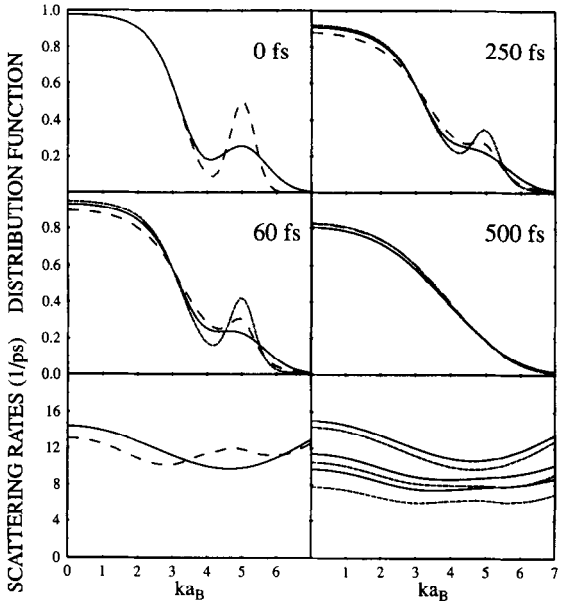


Fig. 3. Relaxation of the distribution function and total scattering rates in RPA. The relaxation corresponding to three different scattering approximations is shown: "classical" kinetic equation (long dashes), CTA without and with energy increase (short dashes and full line, respectively). The bottom left figure shows the total scattering rates for the "classical" calculation at the initial time (long dashes) and after 500 fs (full line). The bottom right figure shows the total scattering rates for the CTA without and with energy increase (short dashes and full line, respectively). Times are, from bottom to top, 60, 250 and 500 fs. At $t = 0$, the scattering rates are equal to zero.

RPA polarization. The distribution function is shown for different times for four approximations: the classical scattering integral, the Kadanoff–Baym equations and two different variants of the CTA based on $\mathrm{Im}\, g_0^{\mathrm{EQ}}$, Eq. (12). The correlation time was calculated self-consistently according to Eq. (15), where p_0 was chosen to be the peak position of the initial distribution, and $\alpha = 1$, the result was $\tau_{\mathrm{cor}} = 56$ fs. The difference between both CTA calculations is that in the second variant, a kinetic energy increase of about 8% (based on the results of Ref. [5]) was included. The results of Fig. 1 show that for short times, $t < \tau_{\mathrm{cor}}$, the CTA-relaxation is slower than the other models. After that time, the relaxation is faster than that based on the Kadanoff–Baym equations. With a proper choice of τ_{cor} the cross-over from the "slow" to the fast relaxation can be optimized. For long times, the CTA without kinetic energy increase approaches the "classical" relaxation, whereas the result with kinetic energy increase (broadened initial distribution in Fig. 1) is almost identical to the Kadanoff–Baym result.

In a second calculation, we changed only the potential, choosing $\kappa = 0.2 a_{\mathrm{B}}^{-1}$, thus making the interaction very strong. In that case, a self-consistent calculation of τ_{cor} is difficult. We chose the value $\tau_{\mathrm{cor}} = 300$ fs, when the kinetic energy increase in the Kadanoff–Baym calculations saturated [5,6]. In this case, correlation time and relaxation time are close to each other: After 300 fs the distribution function is almost thermalized. Thus, we cannot expect that the CTA is a good approximation. Nevertheless, Fig. 2 shows that the CTA again shows good results when time approaches the correlation time. However, after that time the relaxation is already almost finished. In this case, kinetic energy increases by about 80%, so the broadened version of the CTA is significantly closer to the Kadanoff–Baym result than the other.

As a third calculation, we apply the CTA to the quantum Boltzmann equation with dynamically screened potential (Lenard–Balescu equation, RPA). This is of high interest for thermalization of optically excited semiconductors. In particular, solutions of the "classical" Balescu equation have yielded very high scattering and dephasing rates, which were explained by plasmon undamping due to nonequilibrium carrier distributions

[14]. One may expect that these high dephasing rates are, at least in part, due to an overestimate of collective plasma effects, since the classical Balescu collision term replaces the true build-up of polarization effects by an instantaneous process (see, e.g., Refs. [7,8]). Unfortunately, the non-Markovian generalization of the Balescu equation [11] and of the Kadanoff–Baym equations in RPA is still numerically not feasible. Therefore, calculations using the CTA can yield some first insight into the effect of correlation build-up on the RPA relaxation. Fig. 3 shows the relaxation of the electron distribution in an equilibrium plasma where, e.g. by optical excitation, additional nonequilibrium carriers have been generated. In this case, one observes plasmon undamping and increased scattering rates. Along with the "classical" relaxation, CTA-calculations with and without energy increase are shown, where the correlation time was calculated by formula (15) using the "classical" RPA scattering rates. The result was $\tau_{\rm cor} = 98$ fs. As one can see from Fig. 3, indeed, a gradual increase of the scattering rates is found which reduces the previously observed very high dephasing rates and gives, at least, an estimate for the full non-Markovian result.

After discussing numerical results for homogeneous systems, let us, finally, consider implications of the CTA for spatially inhomogeneous systems. If $\tau_{\rm cor} \ll t_{\rm rel}$, then everything said above about the hierarchy of scales may be extended to scales in space also. Then, at $t > \tau_{\rm cor}$ the dependence of the correlations on fine-scale structures is lost and only large-scale space dependence via the distribution function remains, $g(\boldsymbol{R}, t) = g\{f(\boldsymbol{R}, t)\} \approx g_{\rm CTA}\{f(\boldsymbol{R}, t)\}$. This means that we may use exactly the same functional expressions for $g_{\rm CTA}$ as in the homogeneous case (momentum delta function), where now space dependence appears, but only parametrically via the distribution functions (zeroth order gradient expansion). In the same way, also the collision integral $I_{\rm CTA}$ become space dependent. This means, if spatial inhomogeneities of the size $v_0/\tau_{\rm cor}$ and smaller are not important, one may solve a kinetic equation for the space dependent Wigner function using the essentially simpler collision integrals for homogeneous systems. Moreover, correlation build-up in space may be included by making g_0 and $\tau_{\rm cor}$ space dependent.

We have thus shown that most phenomena typical for non-Markovian relaxation may be successfully incorporated into the correlation time approximation. Extension to quantum systems and to several particle species is straightforward. While the current discussion is aimed at illustrating the general concept of the CTA, for particular situations modifications will be necessary. Good agreement can be expected for a weak static interaction (Born approximation). Beyond that, the dynamics of bound state formation (ladder approximation) [9] or screening build-up [7,8] may be reproduced by the current version of the CTA if the spectral properties (of the bound states or of the screened potential) are close to that at $t = \tau_{\rm cor}$. Otherwise, the scalar correlation time has to be replaced by a more complex quantity. If the correlation build-up involves more than one time scale, one has to generalize the ansatz (8) to involve several time constants. A typical example is the process of femto-second optical excitation of carriers, described by the non-Markovian generalization of the Bloch equations [15]. In the same way as the "classical" (Markovian) coupled relaxation of carrier distribution and optical polarization has been successfully approximated by a RTA with two times T_1 and T_2 (see, e.g., Ref. [15]) the concept of the CTA can easily be generalized, including a weakly time-dependent correlation time [19].

In summary, we have proposed a new approximation scheme to generalized kinetic equations. It allows one to incorporate dominant non-Markovian effects, such as correlation build-up, decay of initial correlations and energy broadening, into much simpler and well understood "classical" Markovian kinetic equations. Not only may a drastic simplification of the numerical treatment become possible, at the same time, the resulting collision integrals, Eq. (11), give a physically very transparent picture of correlation dynamics on short times.

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