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Quantum Kinetic Equations: Correlation Dynamics and Selfenergy

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Abstract

The derivation of non-Markovian quantum kinetic equations is reconsidered in the framework of density operators. Conventional derivations use for the decoupling of the BBGKY-hierarchy the assumption of vanishing three-particle correlations $g_{123} = 0$. This yields non-Markovian kinetic equations with infinite memory depth. We discuss a different closure relation to the hierarchy, which overcomes this difficulty without assumptions on weakening of initial correlations and in fact corresponds to the inclusion of selfenergy effects (beyond Hartree-Fock).

1 Introduction

For the last decades, quantum kinetic properties of many-particle systems have successfully been described on the basis of Markovian kinetic equations, such as the Landau, Lenard-Balescu or Boltzmann equation. However, these equations have several principal shortcomings:

1. They are valid on time-scales larger than the correlation time τ_{cor} only,
2. they neglect initial correlations and
3. they conserve only kinetic energy (quasi-particle energy) instead of the total (kinetic+potential) energy of the system.

The last point becomes a serious problem, if strongly correlated systems are considered. Then, the behavior, both on a microscopic and macroscopic scale, is essentially influenced by many-body effects. In particular, hydrodynamic, thermodynamic and transport properties will contain additional correlation contributions. If driven out of equilibrium, the system will relax towards a strongly coupled stationary state. To describe the relaxation of nonideal systems correctly requires generalized kinetic equations that conserve total energy. On the other hand, the first point seems to be of quite specific relevance, confined to ultra-fast relaxation phenomena. However, this is not the case. As is well known, both points are linked together inseparably. Total energy conservation can be achieved only in the framework of non-Markovian kinetic equations. Even in situations, where short-time phenomena are not of interest or experimentally not (yet) accessible, details of the initial relaxation phase may be essential for the correct description of the asymptotic state. Therefore, progress in non-Markovian kinetic equations is a central problem of many-body theory in general.

Generalized kinetic theories including memory effects have been derived already in the 60ies by Zwanzig [1], Prigogine and Resibois [2], Balescu [3], Silin [4], Klimontovich [5], Kadanoff and Baym [6] and others. Substantial contributions are also due to Bärwinkel [7] and Zubarev [9]. Explicit non-Markovian collision integrals were derived by Silin [4] and by

Klimontovich and Ebeling [8, 5] for the classical Landau equation (statically screened Born approximation).

For the application to nonideal quantum systems, the non-Markovian Landau equation [5] has to be generalized in several directions:

I. to include effects of the spin statistics for fermions or bosons,

II. to incorporate many-particle effects, such as selfenergy, and

III. to permit the inclusion of arbitrary initial correlations existing in the system at the starting point of the relaxation.

This can be accomplished in the framework of Green's functions, where the first two points follow straightforwardly [14, 16, 17]. However, these derivations encounter two principal problems. The first ist the question of arbitrary initial correlations, which despite interesting concepts [14, 15] is not yet solved satisfactorily. The reason is that the Green's functions approach, in one way or another, incorporates asymptotic conditions for $t \to -\infty$. The second problem is that for the derivation of kinetic equations for the Wigner function, certain reconstruction ansatzes for the two–time correlation functions in terms of the one–time Wigner functions, such as the generalized Kadanoff-Baym ansatz [18], have to be used.

These problems do not occur within the alternative approach of the quantum generalization of the Bogolyubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy for the reduced density operators [11, 12]. We therefore will use this approach here. The density operator method easily allows us to incorporate initial correlations into the kinetic equations. On the other hand, inclusion of selfenergy effects into this concept was, so far, an open question. We solve this important problem here by identifying the appropriate approximation for the three-particle correlation operator[1]. The final kinetic equations are fully equivalent to the time-diagonal Green's functions results and provide a useful confirmation for the mentioned above reconstruction ansatz in second Born approximation, which follows directly as a result of our theory.

2 Density Operator Approach to Generalized Kinetic Equations with Selfenergy

The starting point for the density operator approach to quantum-kinetic theory is the Liouville–von Neumann equation for the N-particle density operator

$$i\hbar\frac{\partial}{\partial t}\rho_{1\ldots N} - [H_{1\ldots N}, \rho_{1\ldots N}] = 0, \quad H_{1\ldots N} = \sum_{i=1}^{N}\frac{p_i^2}{2m_i} + \sum_{1\leq i<j\leq N} V_{ij}. \tag{1}$$

From eq. (1) follows the BBGKY-hierarchy for the reduced density operators F_1, F_{12}, ..., $F_{1\ldots s}$, which are normalized according to $\mathcal{V}^{-s}\mathrm{Tr}_{1\ldots s}F_{1\ldots s} = 1$, by calculating the partial trace, [11, 12],

$$i\hbar\frac{\partial}{\partial t}F_{1\ldots s} - [H_{1\ldots s}, F_{1\ldots s}] = n\mathrm{Tr}_{s+1}\sum_{i=1}^{s}[V_{i,s+1}, F_{1\ldots s+1}]. \tag{2}$$

Here, $H_{1\ldots s}$ is the s-particle Hamiltonian, V_{ij} the binary interaction potential between particles i and j, $\mathcal{V}$ is the volume and n the density. The *complete* hierarchy (2) has all the properties of the von Neumann equation (1), including time reversibility and total energy conservation. It is advantageous to rewrite eq. (2) in terms of correlation operators, and also to include spin statistics effects explicitly [12],

$$F_{12} = F_1F_2\Lambda^{\pm}_{12} + g_{12} \tag{3}$$

$$F_{123} = F_1F_2F_3\Lambda^{\pm}_{123} + F_3g_{12}\Lambda^{\pm}_{3(12)} + F_2g_{13}\Lambda^{\pm}_{2(13)} + F_1g_{23}\Lambda^{\pm}_{1(23)} + g_{123}, \tag{4}$$

[1] This concept has been derived together with D. Kremp [20] and did also benefit from similar ideas for the carrier-phonon problem [19].

with the (anti-)symmetrization operators $\Lambda^{\pm}_{12} = 1 \pm P_{12}$, $\Lambda^{\pm}_{123} = (1 \pm P_{12} \pm P_{13})\Lambda^{\pm}_{12}$, $\Lambda^{\pm}_{1(23)} = \Lambda^{\pm}_{123}/\Lambda^{\pm}_{12}$ etc. The first two hierarchy equations are now:

$$i\hbar \quad \frac{\partial}{\partial t}F_1 - [H_1 + U_1^{HF}, F_1] = n\mathrm{Tr}_2[V_{12}, g_{12}], \tag{5}$$

$$\begin{aligned} i\hbar \quad & \frac{\partial}{\partial t}g_{12} - [\bar{H}^0_{12}, g_{12}] + \left\{\hat{V}_{12}g_{12} - g_{12}\hat{V}^{\dagger}_{12}\right\} = \left\{V_{12}F_1F_2 - F_1F_2\hat{V}^{\dagger}_{12}\right\}\Lambda^{\pm}_{12} \\ + \quad & n\mathrm{Tr}_3\left\{[V_{13}, F_1 g_{23}]\Lambda^{\pm}_{12} + [V_{23}, F_2 g_{13}]\Lambda^{\pm}_{12} + [V_{13} + V_{23}, g_{123}]\right\}, \end{aligned} \tag{6}$$

with the Hartree-Fock contributions, $U_1^{HF} = n\mathrm{Tr}_2 V_{12} F_2 \Lambda^{\pm}_{12}$ and the effective free two-particle Hamiltonian $\bar{H}^0_{12} = \bar{H}^0_1 + \bar{H}^0_2, \bar{H}^0_1 = H_1 + U_1^{HF}$. $\hat{V}_{12}$ is the operator of the shielded potential which includes phase space occupation effects $\hat{V}_{12} = (1 \pm nF_1 \pm nF_2)\,V_{12}$.

2.1 Non-Markovian Quantum Landau Equation

A quite general conserving closing approximation to the hierarchy is to neglect three-particle correlations, $g_{123} = 0$. Then eqs. (5) and (6) are sufficient to derive a large variety of generalized non-Markovian kinetic equations, including the Boltzmann equation (binary collision approximation, [24]), the Lenard-Balescu equation [25] or the Landau equation. To demonstrate the concept, we derive the quantum Landau equation which plays a central role in plasma and solid state theory, since it is, at the same time, the static limit of the Lenard-Balescu equation and the weak coupling limit of the ladder approximation. Neglecting ladder and polarization terms and three-particle correlations (third term on the l.h.s. and all terms on the r.h.s. of eq. (6)), we obtain the hierarchy closure which corresponds to the static second Born approximation,

$$i\hbar\frac{\partial}{\partial t}g_{12} - [\bar{H}^0_{12}, g_{12}] = \left\{V_{12}F_1F_2 - F_1F_2\hat{V}^{\dagger}_{12}\right\}\Lambda^{\pm}_{12}. \tag{7}$$

eqs. (5) and (7), together with the initial conditions $F_1(t_0) = F^0$ and $g_{12}(t_0) = g^0$, form a closed system of local in time equations for F_1 and g_{12}. They describe the dynamics of the particle pair $1-2$ including the effect of initial correlations and correlation build-up. We can solve eq. (7) for $g_{12}(t)$

$$g_{12}(t) = U_{12}^{0+}(tt_0)\, g^0\, U_{12}^{0-}(t_0 t) + \frac{1}{i\hbar}\int_{t_0}^{\infty} d\bar{t}\, U_{12}^{0+}(t\bar{t})\left\{\hat{V}_{12}F_1F_2 - F_1F_2\hat{V}^{\dagger}_{12}\right\}|_{\bar{t}}\Lambda^{\pm}_{12}\, U_{12}^{0-}(\bar{t}t), \tag{8}$$

where $U_{12}^{0\pm}$ are retarded/advanced propagators which have the properties $U_{12}^{0\pm} = U_1^{0\pm}\,U_2^{0\pm}$, $U^{0\pm}(tt') = [U^{0\mp}(t't)]^{\dagger}$. U_1^{0+} is defined by

$$\left\{i\hbar\frac{\partial}{\partial t} - \bar{H}^0_1\right\}U_1^{0+}(tt') = i\hbar\,\delta(t-t'). \tag{9}$$

If $\bar{H}^0_1$ is just the free-particle Hamiltonian, $\bar{H}^0_1 \to E^0_1 = p_1^2/2m_1$, the solution of eq. (9) is particularly simple, with the matrix elements

$$U_1^{0+}(t-t') = \Theta(t-t')\,e^{-\frac{i}{\hbar}E^0_1(t-t')}. \tag{10}$$

Inserting the result for g_{12}, eq. (8), with the propagators (10) into the r.h.s. of the first hierarchy equation (5), we obtain the non-Markovian Landau equation for a spatially homogeneous system, $\frac{d}{dt}f_1(t) = I(\mathbf{p}_1, t) + I^{IC}(\mathbf{p}_1, t)$, with the collision integral

$$\begin{aligned} I(\mathbf{p}_1,t) &= \frac{2}{\hbar^2}\int\limits_0^{t-t_0} d\tau \int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3}(2\pi\hbar)^3\delta(\mathbf{p}_{12}-\bar{\mathbf{p}}_{12}) \\ &\times\ V(\bar{\mathbf{p}}_1-\mathbf{p}_1)\Big(V(\mathbf{p}_1-\bar{\mathbf{p}}_1)\pm V(\mathbf{p}_1-\bar{\mathbf{p}}_2)\Big)\cos\left\{\frac{E_{12}^0-\bar{E}_{12}^0}{\hbar}\tau\right\} \\ &\times\ \Big\{\bar{f}_1\bar{f}_2[1\pm f_1][1\pm f_2]\ -\ f_1f_2[1\pm\bar{f}_1][1\pm\bar{f}_2]\Big\}\Big|_{t-\tau}, \end{aligned} \tag{11}$$

and an additional collision integral due to the initial correlations

$$\begin{aligned} I^{IC}(\mathbf{p}_1,t) &= \frac{2}{\hbar}\int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3}V(\bar{\mathbf{p}}_1-\mathbf{p}_1)\,(2\pi\hbar)^3\delta(\mathbf{p}_{12}-\bar{\mathbf{p}}_{12}) \\ &\times\ Im\Big\{e^{-\frac{i}{\hbar}(E_{12}^0-\bar{E}_{12}^0)(t-t_0)}g_0(\mathbf{p}_1,\mathbf{p}_2,\bar{\mathbf{p}}_1,\bar{\mathbf{p}}_2)\Big\}, \end{aligned} \tag{12}$$

where we denoted $E_{12}^0 = E_1^0 + E_2^0$. This kinetic equation is an important extension of the conventional Landau equation to times shorter than the correlation time and generalizes the non-Markovian result of Silin [4] and Klimontovich and Ebeling [8] to systems with initial correlations and spin statistics. We will discuss its properties in Sec. 3. Here we point out only the problems with the collision integrals (11) and (12): These integrals describe a time–reversible dynamics of the Wigner distribution. The collision integrals are nonlocal in time with an unlimited memory depth, and the initial correlations in the system are not being weakened. This is, of course, an unphysical long–time behavior. The reason is that the coupled equations (8) and (5) describe the isolated dynamics of the particle pair $1-2$ what corresponds to two–particle states of infinite lifetime. We will show in the following, how finite lifetime (damping) effects can be incorporated into the BBGKY–hierarchy.

2.2 Selfenergy in Density Operator Approach

Instead of neglecting three-particle correlations, we now take into account those terms from g_{123}, that describe the coupling between a particle pair and the surrounding medium to lowest order. These terms will contribute to a renormalization of the Hamiltonian $\bar{H}_{12}^0 \longrightarrow H_{12}^{eff}$. Inspection of the equation of motion for g_{123} (third hierarchy equation), leads to the following approximation

$$i\hbar\frac{\partial}{\partial t}g_{123} - \left\{H_{123}^{eff}g_{123} - g_{123}H_{123}^{eff\,\dagger}\right\} = [V_{13}+V_{23}, F_3\,g_{12}]. \tag{13}$$

where the effective Hamiltonian is, in general non-hermitean with $H_{123}^{eff} = \bar{H}_1 + \bar{H}_2 + \bar{H}_3$, and $\bar{H}_1$ is yet to be defined selfconsistently. Solving for g_{123}, we obtain

$$g_{123}(t) = U_{123}^{+}(tt_0)\,g_{123}^0\,U_{123}^{-}(t_0t) + \frac{1}{i\hbar}\int\limits_{t_0}^{t} d\bar{t}\,U_{123}^{+}(t\bar{t})\,[V_{13}+V_{23}, F_3g_{12}]|_{\bar{t}}\,U_{123}^{-}(\bar{t}t), \tag{14}$$

where $U_{123}^{\pm} = U_1^{\pm}\,U_2^{\pm}\,U_3^{\pm}$ and U_1^{+} is defined by

$$\left\{i\hbar\frac{\partial}{\partial t} - \bar{H}_1\right\}U_1^{+}(tt') = i\hbar\,\delta(t-t'). \tag{15}$$

To shorten the notation, we will not write the term with g_{123}^0, but restore it in the final expression (21). We will not proceed in the operator notation here [20], but, for sake of transparence, use the momentum representation assuming spatial homogeneity. Furthermore, we consider only the local approximation of eq. (15). Then, introducing the matrix elements of the renormalized Hamiltonian $\bar{H}_1|p_1\rangle = \epsilon_1|p_1\rangle$ which are complex, $\epsilon_1(t) = E_1^0+\Delta_1(t)+i\gamma_1(t)$, **the renormalized one–particle propagator has the form**

$$U_1^+(tt_0) = U_1^+(t-t_0) = e^{-\frac{i}{\hbar}\int_{t_0}^{t} d\tau \epsilon_1(\tau)} . \tag{16}$$

The momentum representation of the solution (14) is given by (we denote $p_1 \to 1$ and use $1+2+3 = 1'+2'+3'$)

$$\begin{aligned} g_{123}(1,2,3,1',2',3',t) &= \frac{1}{i\hbar}\int_0^{t-t_0} d\tau e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_{123}(\bar{\tau})-\epsilon^{*\prime}_{123}(\bar{\tau})\right)} V(3-3') \\ &\times \left\{f_3'\Big(g(1+3-3',2,1',2')+g(1,2+3-3',1',2')\Big)\right. \\ &- \left. f_3\Big(g(1,2,1'+3'-3,2')+g(1,2,1',2'+3'-3)\Big)\right\}\Big|_{t-\tau}, \end{aligned} \tag{17}$$

with $\epsilon_{123} = \epsilon_1+\epsilon_2+\epsilon_3$. Now we insert expression (17) for g_{123} on the r.h.s. of eq. (6). The result consists of 16 terms:

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}g(1,2,1',2') &= \ldots + \frac{1}{i\hbar}\int_0^{t-t_0} d\tau \int \frac{d3}{(2\pi\hbar)^3}\frac{dq}{(2\pi\hbar)^3}V^2(q) \\ \times\Bigg\{ & e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_{1-q}(\bar{\tau})+\epsilon_2(\bar{\tau})+\epsilon_{3+q}(\bar{\tau})-\epsilon^*_{1'}(\bar{\tau})-\epsilon^*_{2'}(\bar{\tau})-\epsilon^*_3(\bar{\tau})\right)} \\ & \times\Big[f_3\left(g(1,2,1',2')+g(1-q,2+q,1',2')\right) \\ & \quad -f_{3+q}\left(g(1-q,2,1'-q,2')+g(1-q,2,1',2'-q)\right)\Big] \\ & + e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_1(\bar{\tau})+\epsilon_2(\bar{\tau})+\epsilon_{3+q}(\bar{\tau})-\epsilon^*_{1'-q}(\bar{\tau})-\epsilon^*_{2'}(\bar{\tau})-\epsilon^*_{3+q}(\bar{\tau})\right)} \\ & \times\Big[f_3\left(g(1,2,1',2')+g(1,2,1'-q,2'+q)\right) \\ & \quad -f_{3+q}\left(g(1-q,2,1'-q,2')+g(1,2-q,1'-q,2')\right)\Big] \\ & + e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_1(\bar{\tau})+\epsilon_{2-q}(\bar{\tau})+\epsilon_{3+q}(\bar{\tau})-\epsilon^*_{1'}(\bar{\tau})-\epsilon^*_{2'}(\bar{\tau})-\epsilon^*_3(\bar{\tau})\right)} \\ & \times\Big[f_3\left(g(1,2,1',2')+g(1+q,2-q,1',2')\right) \\ & \quad -f_{3+q}\left(g(1,2-q,1'-q,2')+g(1,2-q,1',2'-q)\right)\Big] \\ & + e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_1(\bar{\tau})+\epsilon_2(\bar{\tau})+\epsilon_3(\bar{\tau})-\epsilon^*_{1'}(\bar{\tau})-\epsilon^*_{2'-q}(\bar{\tau})-\epsilon^*_{3+q}(\bar{\tau})\right)} \\ & \times\Big[f_3\left(g(1,2,1',2')+g(1,2,1'+q,2'-q)\right) \\ & \quad -f_{3+q}\left(g(1-q,2,1',2'-q)+g(1,2-q,1',2'-q)\right)\Big] \Bigg\}, \end{aligned} \tag{18}$$

where on the r.h.s., f and g are to be taken at the time $t-\tau$. Of these 16 terms, four (first terms after each exponential) have the same momentum arguments as g on the l.h.s. of the equation, and, therefore, may be taken out of the p_3 and q integrals. The other 12 terms correspond to polarization contributions and have to be neglected in the static second Born approximation. Introducing an operator $\tilde{\Sigma}^{(12)}$, we can rewrite the four remaining terms as

$$\begin{aligned}
&\tilde{\Sigma}^{(12)}(1,2,1',2',t)g(1,2,1',2',t) = \\
&\frac{1}{i\hbar}\int_0^{t-t_0} d\tau g(1,2,1',2',t-\tau)\int \frac{d3}{(2\pi\hbar)^3}\frac{dq}{(2\pi\hbar)^3}V^2(q)f_3(t-\tau) \\
\times\ &\Bigg\{ e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_{1-q}(\bar{\tau})+\epsilon_2(\bar{\tau})+\epsilon_{3+q}(\bar{\tau})-\epsilon^*_{1'}(\bar{\tau})-\epsilon^*_{2'}(\bar{\tau})-\epsilon^*_3(\bar{\tau})\right)} \\
+\ & e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_1(\bar{\tau})+\epsilon_2(\bar{\tau})+\epsilon_3(\bar{\tau})-\epsilon^*_{1'-q}-\epsilon^*_{2'}-\epsilon^*_{3+q}\right)} \\
+\ & e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_1(\bar{\tau})+\epsilon_{2-q}(\bar{\tau})+\epsilon_{3+q}(\bar{\tau})-\epsilon^*_{1'}(\bar{\tau})-\epsilon^*_{2'}(\bar{\tau})-\epsilon^*_3(\bar{\tau})\right)} \\
+\ & e^{-\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_1(\bar{\tau})+\epsilon_2(\bar{\tau})+\epsilon_3(\bar{\tau})-\epsilon^*_{1'}(\bar{\tau})-\epsilon^*_{2'-q}(\bar{\tau})-\epsilon^*_{3+q}(\bar{\tau})\right)} \Bigg\}.
\end{aligned} \tag{19}$$

Due to symmetry in the momentum arguments, $\tilde{\Sigma}^{(12)}$ may be decomposed according to

$$\begin{aligned}
&\tilde{\Sigma}^{(12)}(1,2,1',2',t) = \tilde{\Sigma}_1(t)+\tilde{\Sigma}_2(t)-\tilde{\Sigma}_1'^*(t)-\tilde{\Sigma}_2'^*(t) \qquad \text{with} \\
&\tilde{\Sigma}_1(t)g(1,2,1',2',t) = \tilde{\Sigma}_1^{IC}(t)g(1,2,1',2',t)+\frac{1}{i\hbar}\int_0^{t-t_0} d\tau g(1,2,1',2',t-\tau) \\
\times\ &\int \frac{d3}{(2\pi\hbar)^3}\frac{dq}{(2\pi\hbar)^3}V^2(q)f_3(t-\tau)e^{\frac{i}{\hbar}\int_{t_0}^{\tau} d\bar{\tau}\left(\epsilon_{1-q}(\bar{\tau})+\epsilon_2(\bar{\tau})+\epsilon_{3+q}(\bar{\tau})-\epsilon^*_{1'}(\bar{\tau})-\epsilon^*_{2'}(\bar{\tau})-\epsilon^*_3(\bar{\tau})\right)},
\end{aligned} \tag{20}$$

where the complex conjugation in $\tilde{\Sigma}_1'$ and $\tilde{\Sigma}_2'$ is understood as not to affect g under the integral. Here, $\tilde{\Sigma}_1^{IC}$ contains the initial three–particle correlations. Consistent with approximation (13), they are assumed to be of the form $g^0_{123} \sim [V_{13}+V_{23}, F_3(t_0)g_{12}(t_0)]$+permutations, so $\tilde{\Sigma}^{IC}$ is determined by the initial values of the distribution function and the correlation matrix, $\tilde{\Sigma}_1^{IC}(t)g(t) \sim \int d3dqV^2(q)f_3(t_0)g(t_0)$.

Now, we can write down the equation of motion for g_{12} in momentum representation, including the contributions from the three–particle correlations, eq. (19),

$$\begin{aligned}
&\left\{i\hbar\frac{\partial}{\partial t}-(E^0_1+E^0_2-E^0_{1'}-E^0_{2'})\right\}g(1,2,1',2',t) = \\
&\{V(1-1')\pm V(1-2')\}\{f_1'f_2'(1\pm f_1)(1\pm f_2)-f_1f_2(1\pm f_1')(1\pm f_2')\} - \\
&\left\{\tilde{\Sigma}_1(t)+\tilde{\Sigma}_2(t)-\tilde{\Sigma}_1'^*(t)-\tilde{\Sigma}_2'^*(t)\right\}g(1,2,1',2',t).
\end{aligned} \tag{21}$$

eq. (21) allows to identify the so far unknown renormalized one–particle and two–particle Hamiltonians $\bar{H}_1$ and $\bar{H}_{12}$:

$$\bar{H}_{12} = \bar{H}_1+\bar{H}_2 \tag{22}$$

$$\bar{H}_1\, g(1,2,1',2',t) = \left\{\frac{p_1^2}{2m}+\tilde{\Sigma}_1(t)\right\}g(1,2,1',2',t). \tag{23}$$

eq. (23) shows that $\tilde{\Sigma}_1$ is in fact related to selfenergy effects. Let us briefly comment on this result. The closure relation (13) allows to include selfenergy effects to lowest order (in particular, two–particle selfenergy is neclected). To include spin statistics effects, the closure (13) has to be generalized according to $V_{13}F_3\,g_{12} \longrightarrow (\hat{V}_{13}F_3 + F_1F_3V_{13})\,g_{12}$.

2.3 Non-Markovian Quantum Landau Equation with Selfenergy

Having determined the renormalized one–particle Hamiltonian and its eigenvalue ϵ_1 we now can go back to eq. (16) and calculate the renormalized propagators $U_1^{\pm}$. With these propagators we immediately construct the solution for g_{12} and the collision integral as it was shown in Sec. 2.1. To come to results which can be treated numerically, additional simplifications of the time dependencies on the r.h.s. of eq. (21) are necessary. Taking g under the time integral in the Markov limit, $g(t-\tau) \approx g(t)$ and $g(121'2') \sim \delta(E_1+E_2-E_1'-E_2')$, g can be taken out of the integral and only four energies $\epsilon_{1-q}+\epsilon_{3+q}-\epsilon_{1'}^{*}-\epsilon_3^{*}$ remain in the exponent. Furthermore, the retardation in ϵ in the exponent is neglected. As a result, we obtain the retarded selfenergy in second Born approximation (in local approximation), which is known from Green's functions theory,

$$
\begin{aligned}
\tilde{\Sigma}_1(t) &= \frac{2}{\hbar}\int_0^{t-t_0} d\tau \int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3}(2\pi\hbar)^3\delta(\mathbf{p}_{12}-\bar{\mathbf{p}}_{12}) \\
&\times\; V(\bar{\mathbf{p}}_1-\mathbf{p}_1)\Big(V(\mathbf{p}_1-\bar{\mathbf{p}}_1)\pm V(\mathbf{p}_1-\bar{\mathbf{p}}_2)\Big)\exp\Big\{i\frac{E_{12}-\bar{E}_{12}}{\hbar}\tau\Big\}e^{-(\gamma_{12}+\bar{\gamma}_{12})\tau/\hbar} \\
&\times\; \Big\{\bar{f}_1\bar{f}_2[1\pm f_2] + f_2[1\pm\bar{f}_1][1\pm\bar{f}_2]\Big\}\Big|_{t-\tau},
\end{aligned}
\tag{24}
$$

and damped quasiparticle expressions for the propagators,

$$
U_1^{+}(t-t') = \Theta(t-t')\,e^{-\frac{i}{\hbar}(E_1-i\gamma_1)(t-t')},
\tag{25}
$$

with shifted energy $E_1 = p_1^2/2m_1 + \mathrm{Re}\,\tilde{\Sigma}(p_1,t)$ and the damping $\gamma_1 = -i\mathrm{Im}\,\tilde{\Sigma}(p_1,t)$. Finally, with eq. (25) we obtain the collision integrals of the generalized Landau equation:

$$
\begin{aligned}
I_1(t) &= \frac{2}{\hbar^2}\int_0^{t-t_0} d\tau \int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3}(2\pi\hbar)^3\delta(\mathbf{p}_{12}-\bar{\mathbf{p}}_{12}) \\
&\times\; V(\bar{\mathbf{p}}_1-\mathbf{p}_1)\Big(V(\mathbf{p}_1-\bar{\mathbf{p}}_1)\pm V(\mathbf{p}_1-\bar{\mathbf{p}}_2)\Big)\cos\Big\{\frac{E_{12}-\bar{E}_{12}}{\hbar}\tau\Big\}e^{-(\gamma_{12}+\bar{\gamma}_{12})\tau/\hbar} \\
&\times\; \Big\{\bar{f}_1\bar{f}_2[1\pm f_1][1\pm f_2] - f_1f_2[1\pm\bar{f}_1][1\pm\bar{f}_2]\Big\}\Big|_{t-\tau},
\end{aligned}
\tag{26}
$$

and, the contribution from the initial correlations,

$$
\begin{aligned}
I^{IC}(\mathbf{p}_1,t-t_0) &= \frac{2}{\hbar}\int \frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3}\int \frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3}V(\bar{\mathbf{p}}_1-\mathbf{p}_1) \\
&\times\; (2\pi\hbar)^3\delta(\mathbf{p}_{12}-\bar{\mathbf{p}}_{12})\,e^{-(\gamma_{12}+\bar{\gamma}_{12})(t-t_0)/\hbar} \\
&\times\; \mathrm{Im}\Big\{e^{-\frac{i}{\hbar}(E_{12}-\bar{E}_{12})(t-t_0)}g_0(\mathbf{p}_1,\mathbf{p}_2,\bar{\mathbf{p}}_1,\bar{\mathbf{p}}_2)\Big\},
\end{aligned}
\tag{27}
$$

which are the generalization of eqs. (11), (12). Eq. (26) agrees with the result derived using Green's functions by applying the generalized Kadanoff-Baym ansatz (GKBA) [18] in [16, 17]. Here, we obtained the result without postulating the GKBA based on the BBGKY-hierarchy with a generalized closure relation (13).

Thus, the problem is solved. The generalized Landau equation is given by the non-Markovian collision integral (26), the additional integral (27) and the expression for the selfenergy (24), which are coupled in a complicated way. The energy shift and the damping coefficient are momentum and time dependent and appear under the retardation integral in the collision terms and in $\tilde{\Sigma}$ itself and have to be calculated selfconsistently with the distribution function.

3 Properties of the Generalized Landau Equation

3.1 Memory Effects

Let us discuss some important properties of the generalized kinetic equation. The integral (26) conserves density and momentum. It contains the specific scattering kernel $D = \cos\{\omega\tau\}e^{-\Gamma\tau}$ under the retardation (τ) integral, where we denoted $\omega(1,2,1',2',t) = (E_{12} - E'_{12})/\hbar$ and $\Gamma(1,2,1',2',t) = (\gamma_{12} + \gamma'_{12})/\hbar$. This gives rise to collisional energy broadening and memory effects. The latter are, however, only a formal consequence of the solution for g_{12}. The original differential equations for F_1 and g_{12}, eqs. (5,6), are local in time. As a result of the selfenergy corrections, the initial correlations are being damped and the memory in the collision integrals has a finite duration. Eq. (26) is applicable to times shorter than the correlation time, i.e. beyond the Bogolyubov regime. For $t < \tau_{cor} \sim 1/\Gamma$, it describes the simultaneous relaxation of distribution function and binary correlation function. For $t \sim \tau_{cor}$, initial correlations are damped out, and correlations have reached an equilibrium form, depending on time only via the distribution functions (Bogolyubov's functional hypothesis). In the long-time limit, i.e. $t - t_0 \longrightarrow \infty$, $D \longrightarrow \frac{\hbar\Gamma}{\omega^2 + \Gamma^2}$. If, furthermore, damping is neglected, $D \longrightarrow \hbar\delta(\omega)$, yielding the Markovian Landau collision integral. However, the long-time asymptotics of eq. (26) contains an additional integral

$$\begin{aligned} I^M_{(1)}(t) &= -\frac{2}{\hbar^2}\int\frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\int\frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3}\int\frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3}(2\pi\hbar)^3\delta(\mathbf{p}_{12} - \bar{\mathbf{p}}_{12}) \\ &\times\; V(\bar{\mathbf{p}}_1 - \mathbf{p}_1)\Big(V(\mathbf{p}_1 - \bar{\mathbf{p}}_1) \pm V(\mathbf{p}_1 - \bar{\mathbf{p}}_2)\Big)D^M_1(E_{12} - \bar{E}_{12}, \gamma_{12} + \bar{\gamma}_{12}) \\ &\times\; \frac{d}{dt}\left\{\bar{f}_1\bar{f}_2[1 \pm f_1][1 \pm f_2] - f_1 f_2[1 \pm \bar{f}_1][1 \pm \bar{f}_2]\right\}\Big|_t, \end{aligned} \tag{28}$$

$$\text{with} \quad D^M_1(\omega,\Gamma) = \frac{\hbar^2}{\omega^2 + \Gamma^2}\Big(\frac{2\Gamma^2}{\omega^2 + \Gamma^2} - 1\Big). \tag{29}$$

This additional collision integral (28) is essential to obtain energy conservation in the long-time limit and the correct thermodynamic properties of an interacting many-particle system.

3.2 Correlation Dynamics

It is instructive to consider, instead of the formal solution for the complex correlation matrix element, closed equations for its imaginary and real part. Separating in eq. (21) real and imaginary part and denoting by $\hbar\Psi(1,2,1',2',t)$ the term with the distribution functions on the r.h.s. of eq. (21), we obtain (for fixed momenta)

$$\frac{d}{dt}Im\,g = \omega\,Re\,g - \Gamma\,Im\,g - \Psi \tag{30}$$

$$\frac{d}{dt}Re\,g = -\Gamma\,Re\,g - \omega\,Im\,g. \tag{31}$$

Differentiating eqs.(30) with respect to time, we obtain equations of motion for the real and imaginary part:

$$\begin{aligned}
\frac{d^2}{dt^2} Im\, g + 2\Gamma \frac{d}{dt} Im\, g + \left(\omega^2+\Gamma^2\right) Im\, g &= -\Gamma\Psi + \delta_I, &(32)\\
\frac{d^2}{dt^2} Re\, g + 2\Gamma\, Re\, g + \left(\omega^2+\Gamma^2\right) Re\, g &= \omega\Psi + \delta_R, &(33)\\
\text{with} \quad \delta_I = -\frac{d}{dt}\Gamma\, Im\, g + \frac{d}{dt}\omega Re\, g &- \frac{d}{dt}\Psi,\\
\delta_R = -\frac{d}{dt}\Gamma\, Re\, g - \frac{d}{dt}\omega Im\, g.&
\end{aligned}$$

Eqs. (32) and (33) allow for a clear interpretation of our theoretical model. These equations are fully equivalent to the non-Markovian Landau equation, but they are local in time, i.e. Markovian. If we neglect the, in most cases, weak time dependence of Γ, ω and Ψ, the corrections δ_I and δ_R vanish, and we have two equations of damped quasi-harmonic oscillations. The oscillators are subject to an external force which is defined by the distribution functions and which changes with time weakly. The oscillation freqency is given by $\Omega = [(\omega^2+\Gamma^2) - \Gamma^2]^{1/2} = (E_{12} - \bar{E}_{12})/\hbar$. The damping coefficient is just the sum of the one-particle damping coefficients Γ. Damping coefficient and frequency are weakly time-dependent via their functional dependence on the distribution functions. The solution of eqs. (32), (33) is

$$\begin{aligned}
Re\, g(t,\omega,\Gamma) &= \Psi(t) C_o(\omega,\Gamma,t) + \\
&\quad \{Re\, g(t_o) cos[\omega(t-t_o)] - Im\, g(t_o) sin[\omega(t-t_o)]\}\, e^{-\Gamma(t-t_o)} &(34)\\
Im\, g(t,\omega,\Gamma) &= -\Psi(t) D_o(\omega,\Gamma,t-t_o) + \\
&\quad \{Im\, g(t_o) cos[\omega(t-t_o)] + Re\, g(t_o) sin[\omega(t-t_o)]\}\, e^{-\Gamma(t-t_o)}. &(35)
\end{aligned}$$

D_o and C_o are given by

$$\begin{aligned}
D_o(\omega,\Gamma,t-t_o) &= \frac{\Gamma}{\omega^2+\Gamma^2} + \frac{e^{-\Gamma t}}{\omega^2+\Gamma^2}\left(\omega sin[\omega t] - \Gamma cos[\omega t]\right) &(36)\\
C_o(\omega,\Gamma,t) &= \frac{\omega}{\omega^2+\Gamma^2} - \frac{e^{-\Gamma t}}{\omega^2+\Gamma^2}\left(\Gamma sin[\omega t] + \omega cos[\omega t]\right) &(37)
\end{aligned}$$

and correspond to the approximation where the distribution function does not change over an oscillation period. The next corrections to $\mathrm{Re}\, g$ and $\mathrm{Im}\, g$ follow from assuming $\Psi \sim t^1, t^2$ and so on, resulting in new functions $D_1, D_2, \ldots$ and $C_1, C_2 \ldots$, respectively. This expansion is identical to a retardation expansion of the non-Markovian solution for g_{12}.

The solution (34,35) allows for a transparent discussion of the dynamics of binary correlations: If selfenergy is neglected ($\gamma_{12} = \Delta_{12} = 0$), the oscillations would be undamped, with the frequency $\hbar^2\Omega_o^2 = E_1^o + E_2^o - E_{1'}^o - E_{2'}^o$. This means, the oscillations are more rapid the more the scattering event violates kinetic energy conservation. The matrix element on the energy shell (where kinetic energy is conserved) does not change in time at all. During the relaxation, the oscillations of the off-shell matrix elements become increasingly more rapid. Their contribution to the collision integral which contains a momentum average over $Im\, g$ vanish due to destructive superposition, and only the on-shell terms remain. This means, the relaxation enters the "classical" kinetic stage.

The account of one-particle damping gives rise mainly to damping of the oscillations of the off-shell correlation matrix elements with a characteristic decay time $1/\Gamma$. Furthermore, the functions D_o and C_o obtain a finite spectral width. For the on-shell components we find

$$\begin{aligned}
Re\, g(t,\omega=0,\Gamma) &= Re\, g(t_o,\omega=0,\Gamma)\, e^{-\Gamma(t-t_o)} &(38)\\
Im\, g(t,\omega=0,\Gamma) &= Im\, g(t_o,\omega=0,\Gamma)\, e^{-\Gamma(t-t_o)} - \frac{\Psi(t-t_o)}{\Gamma}[1-e^{-\Gamma(t-t_o)}]. &(39)
\end{aligned}$$

This clearly shows the damping of initial correlations and the correlation build-up. This "on-shell" approximation has been derived in [21] as a relaxation time approximation for g_{12} (correlation time approximation). It was shown that this approximation reproduces basic physical effects of the correlation dynamics qualitatively and even quantitatively correct.

3.3 Energy Conservation and Potential Energy in Second Born Approximation

Energy conservation can be studied in detail for the Landau equation, since one can derive explicit expressions for the potential and kinetic energy (for a classical plasma with weakened initial correlations, cf. [22]). The potential energy density is found to be [20]

$$\langle V\rangle(t) = -\frac{N}{2\hbar}\int\frac{d\mathbf{p}_1}{(2\pi\hbar)^3}\int\frac{d\mathbf{p}_2}{(2\pi\hbar)^3}\int\frac{d\bar{\mathbf{p}}_1}{(2\pi\hbar)^3}\int\frac{d\bar{\mathbf{p}}_2}{(2\pi\hbar)^3}V(\bar{\mathbf{p}}_1-\mathbf{p}_1)\times$$
$$(2\pi\hbar)^3\delta(\mathbf{p}_{12}-\bar{\mathbf{p}}_{12})\Bigg[\int\limits_0^{t-t_0} d\tau e^{-(\gamma_{12}+\bar{\gamma}_{12})\tau/\hbar}\sin\left(\frac{E_{12}-\bar{E}_{12}}{\hbar}\tau\right)\times$$
$$\Big(V(\bar{\mathbf{p}}_1-\mathbf{p}_1)\pm V(\bar{\mathbf{p}}_2-\mathbf{p}_1)\Big)\Big\{2\bar{f}_1\bar{f}_2[1\pm f_1][1\pm f_2]\Big\}\Big|_{t-\tau}$$
$$-\ \hbar\, e^{-(\gamma_{12}+\bar{\gamma}_{12})(t-t_0)/\hbar}\mathrm{Re}\Big\{g_0(\bar{\mathbf{p}}_1,\bar{\mathbf{p}}_2,\mathbf{p}_1,\mathbf{p}_2)e^{-\frac{i}{\hbar}(E_{12}-\bar{E}_{12})(t-t_0)}\Big\}\Bigg], \qquad (40)$$

where N is the particle number. This is the correlation energy density of a quantum system in second Born approximation, including exchange, selfenergy and initial correlations. This expression is valid for all times, including the short-time behavior and the correct asymptotic result. Exact energy conservation can be shown if damping effects are neglected. With selfenergy corrections, the question is essentially more complex. In particular, in local approximation, energy is conserved only approximately. We have to omit the lengthy calculations here [23], and mention only that the error is of the order V^6.

4 Numerical Results and Discussion

We have seen that at short times, $t < \tau_{corr}$, the behavior of correlated many-particle systems is characterized by a coupled dynamics of one-particle and two-particle properties. The formation of binary correlations can be characterized by different quantities. In a one-time theory, such as the density operator formalism, the central quantity is the binary correlation operator g_{12}, Fig. 1. On the other hand, the one-particle energy renormalization $\bar{\Sigma}$ contains the same information, since it is calculated from g_{12} too, cf. eq. (13). Consequently, the short-time behavior of both quantities should be very similar. To confirm this, we have performed numerical studies of relaxation processes in plasmas and semiconductors, e.g. [20]. Figs. 1 and 2 show numerical results for the correlation build-up in a typical femtosecond relaxation process in optically excited semiconductors. In Fig. 1 we plot the matrix element of g_{12} for a typical scattering process of two electrons entering the collision with momenta $\mathbf{p}_1$ and $\mathbf{p}_2$, respectively, as a function of the momentum transfer q and time. Fig. 2 shows $\bar{\Sigma}$ in units of the exciton Rydberg energy as a function of the wave number for different times. Both figures show the initial phase of the relaxation starting from an uncorrelated initial state at $t = 0$. The correlation time in this system is about 50 femtoseconds. After this time, correlations are basically formed, and further changes are only gradual (Bogolyubov regime). Still the one-particle distribution is far from its equilibrium shape.

We have to note further problems related to the local approximation for the selfenergy correction $\bar{\Sigma}$. In the long-time limit it leads to a broadened spectral kernel D which has a finite width Γ rather than to a sharp energy delta function. This does not yield the

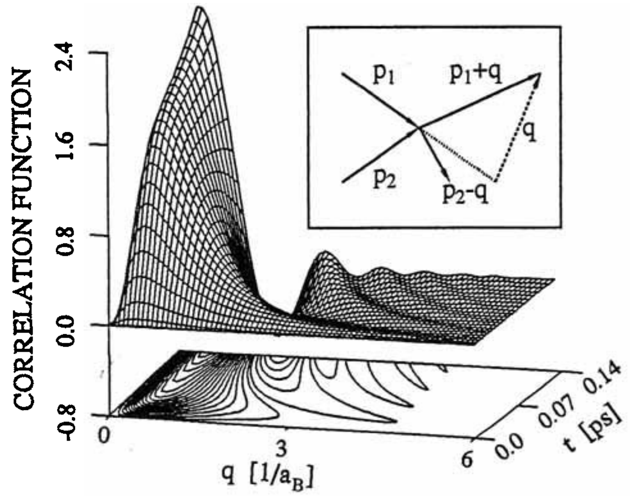

Figure 1: Relaxation of the imaginary part of the binary correlation function for static electron-electron scattering in a bulk semiconductor. The initial distribution is a Gaussian centered at $k = 3a_B^{-1}$, $n = 3.64 \times 10^{17} cm^{-3}, \kappa a_B = 0.2$ in the case of full retardation and no selfenergy. The inset illustrates the two-particle scattering process. The initial momenta of the particle pair are $p_1 = p_2 = 3\hbar/a_B$, $\mathbf{p}_1$ and $\mathbf{p}_2$ are parallel.

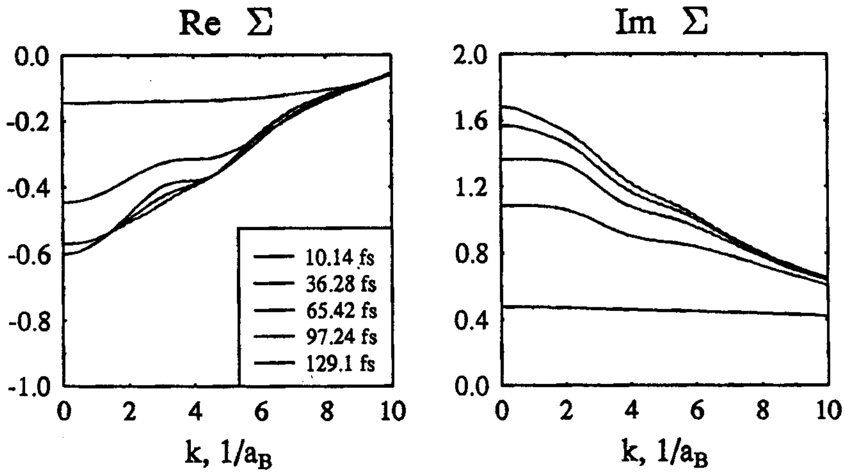

Figure 2: Relaxation of the real and imaginary part of the retarded selfenergy $\tilde{\Sigma}$ as a function of momentum for different times. The results are from a selfconsistent calculation using the local approximation for the selfenergy, eq. (24). Same system parameters as in Fig. 1, except $\kappa a_B = 1.16$.

correct equilibrium distribution of correlated systems and also slows the relaxation down. Therefore, for selfconsistent calculations of the selfenergy which go beyond the correlation time, it is necessary to use improved expressions. One approach is to use phenomenological analytical expressions with non-Lorentzian tails [26]. An exact approach requires to solve the full Dyson equation for the two-time propagators (15) or, alternatively, the two–time Kadanoff-Baym equations [20].

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