Physica **86A** (1977) 25–48 © *North-Holland Publishing Co.*

LINKED CLUSTER EXPANSIONS IN THE EQUATIONS OF MOTION METHOD II

KINETIC EQUATIONS FOR THE SINGLE-PARTICLE DENSITY MATRIX

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Received 15 June 1976

The general method of paper I of this series is applied to derive kinetic equations (KE's), i.e. closed exact equations governing the time evolution of the single-particle density matrix. The short-memory approximation of these non-Markowian equations is formulated in such a way that it is valid even in strongly inhomogeneous systems. The c-number diagram expansion of the integral kernels of the KE's is obtained from the general rules of paper I. It is shown that certain secular divergent terms cancel each other. The diagrams decay into dynamic and correlational parts, the latter being given by cluster functions describing the correlations of the particles in the local equilibrium ensemble $\sigma(t)$ which is formulated in terms of the single-particle density matrix and of the Hamiltonian. The appearance of the cluster functions is the most pronounced difference of our KE's in comparison with other KE's which are formulated in terms of the dynamics of isolated clusters of particles. It is argued that our KE's may be viewed as a highly summed version of these latter KE's and that the ultimate reason for this difference lies in the fact that in our theory the conservation of the average macroscopic energy is taken into account explicitly.

1. Introduction

The use of kinetic equations (KE's), i.e. of closed equations governing the time evolution of the single-particle density matrix which is related to the single-particle Wigner function (or distribution function in the classical case), is an old and very effective method to describe irreversible processes in physical systems. This kind of description lies midway between the full many-body treatment and the description by the use of equations of motion of macroscopic parameters, e.g. the hydrodynamic equations. As in most theories of irreversible processes, at the origin of kinetic theory lies the idea[1]), that with the time evolution of the system the number of parameters needed to describe the system largely reduces.

The single-particle density matrix $\rho^{(1)}$ represents a relatively large set of

parameters. In fact, knowledge of $\rho^{(1)}$ is equivalent to the knowledge of all single particle quantities. Therefore, from the point of view of the many-body theory the derivation of KE's is much simpler than the derivation of the macroscopic equations since the latter correspond to a much more reduced description. Once the KE's are known, macroscopic equations can be obtained from them by well known methods[2]).

However, even in the case of dilute and moderately dense gases, the intuitive concepts which lead to the KE's are based on physically unsatisfying assumptions like the molecular chaos assumption and the more fundamental theories are plagued with divergencies and other difficulties. In recent theories of correlation and memory functions, which are closely linked with linear kinetic theory, these difficulties have been partially solved[3]). These theories, however, rely heavily on the linearity assumption. Thus, the problem of a systematic microscopic derivation of general KE's or, in other words, of the generalization of the Boltzmann equation is far from being solved[4]).

In the present paper we look at this problem from the point of view of the methods for the microscopic treatment of irreversible processes developed in paper I of this series[5]). There, a set of integro-differential equations was derived which are the exact closed evolution equations of a given set P of parameters* of the system. These equations – also called equations of motion – are exactly valid for any system arbitrarily far from equilibrium.

In I it was shown that the equations of motion simplify considerably if the short-memory approximation[5]) (SMA) is valid. For the SMA to be valid we must include all parameters slowly varying in time into the set P. To derive kinetic equations, the relevant set of parameters to be included into P are the matrix elements of $\rho^{(1)}$. However, from the point of view of the SMA this choice is not yet complete. In fact, since the total energy of the system is a conserved quantity it is certainly also a slowly varying quantity and thus has to be included into P, too. In the SMA, this will be seen to change the nature of our KE's considerably.

Except for the parameters in P, in general there might be still other slowly varying parameters forming a parameter set Q. Actually, in this case the SMA is valid only in a set of equations of motion involving the parameters of P and Q. What we do by making the SMA in our KE's is to select from this more general set of equations just that subset which corresponds to the parameters in P. This will be correct as long as the coupling between P and Q is negligible.

If the coupling is strong, the long time tails of the integral kernels in our KE's do not cancel each other and long memory equations result. Apart from physical consequences regarding the sense of such equations this means that the tails have to be calculated by summing the appropriate diagrams.

The numerous works[6]) concerning the ring summation to get the $t^{-3/2}$

*In this paper, we use the word parameter instead of observable as in I because an observable should refer to a macroscopic quantity represented by a hermitean operator whereas a parameter might well be represented by a non-hermitean operator as in (2.5).

behaviour of correlation functions or the investigations in ref. 7 have shown that this is possible but have also revealed the great obstacles which will be encountered in following these lines. The reason, of course, is that here complicated macroscopic processes associated with the variables in Q are treated microscopically.

These considerations quite clearly outline our point of view concerning the practical problem of deriving general KE's. The description of the time evolution of a many-body system by KE's is physically meaning only, if the coupling to the slowly varying parameters in Q is so weak that the short memory approximation is valid. Then, only the rapidly decaying diagrams contribute to the KE's. In other cases one has to refrain from using KE's but instead has to enlarge the space of parameters by including the two-particle density matrix $\rho^{(2)}$.

This approach is inherently free of divergencies and of the need to calculate the long time tails of the kernels. Of course, there always remains the question as to the validity of the short-memory approximation. As a partial confirmation of this approximation, it is explicitly shown in section 5 that in the Markowian limit those parts of the long-time tails of the integral kernels which result from the secular divergent diagrams cancel each other indeed. The proof is carried out indirectly by deriving a new version of the diagram expansion for the KE's, this new version being free of the divergent terms mentioned above. In the Markowian limit both these versions become identical.

2. The kinetic equations

For simplicity of notation, we will consider in this paper a monocomponent fluid of structureless particles interacting via two-body forces only*. The Hamiltonian of the system be given in second quantized form by

$$H = \sum \epsilon_n a_n^+ a_n + \frac{1}{4} \sum \langle \boldsymbol{p}_1 \boldsymbol{p}_2 | W | \boldsymbol{p}_3 \boldsymbol{p}_4 \rangle a_1^+ a_2^+ a_4 a_3 \tag{2.1}$$

where the $a_n^+(a_n)$ are the operators for the creation (annihilation) of a particle having momentum $\boldsymbol{p}_n$ and ϵ_n is the corresponding kinetic energy.

Taking exchange into account explicitly, the matrix elements in (2.1) are given as

$$\begin{aligned} \langle \boldsymbol{p}_1 \boldsymbol{p}_2 | W | \boldsymbol{p}_3 \boldsymbol{p}_4 \rangle &= \langle 1\ 2 | W | 3\ 4 \rangle \\ &= \frac{1}{V} W(\boldsymbol{q}) [\delta(\boldsymbol{p}_1 + \boldsymbol{q} - \boldsymbol{p}_3) \delta(\boldsymbol{p}_2 - \boldsymbol{q} - \boldsymbol{p}_4) \\ &\quad + \kappa \delta(\boldsymbol{p}_2 + \boldsymbol{q} - \boldsymbol{p}_3) \delta(\boldsymbol{p}_1 - \boldsymbol{q} - \boldsymbol{p}_4)], \end{aligned} \tag{2.2}$$

* As should be clear from I, more complicated interactions and the internal degrees of freedom can be included without difficulties.

where

$$W(\boldsymbol{q}) = \int \mathrm{d}^3\boldsymbol{r}\, \mathrm{e}^{-(\mathrm{i}/\hbar)\boldsymbol{q}\boldsymbol{r}} W(\boldsymbol{r}) \tag{2.3}$$

is the Fourier transform of the pair-interaction potential, $\delta(\boldsymbol{p})$ is the Kronecker symbol $\delta_{\boldsymbol{p},0}$ and

$$\kappa = \begin{cases} +1 & \text{for Bosons} \\ -1 & \text{for Fermions.} \end{cases} \tag{2.4}$$

2.1. *Formal structure of the kinetic equations*

The matrix elements $f(i, k; t)$ of the single-particle density matrix $\rho^{(1)}_{(t)}$ are given by

$$\langle k|\rho^{(1)}_{(t)}|i\rangle = f(i, k; t) = \mathrm{Tr}\,\{a_k^+ a_i \rho_{(t)}\}.$$

where $\rho_{(t)}$ is the solution of the Liouville equation of the whole system. The operators corresponding to the $f(i, k; t)$ are thus given by

$$\hat{f}(i, k) = a_k^+ a_i \tag{2.5}$$

The parameters $f(i, k; t)$ are connected with the single-particle Wigner functions $F(\boldsymbol{p}, \boldsymbol{w}, t)$ by the familiar relations[8])

$$F(\boldsymbol{p}, \boldsymbol{r}, t) = \int \mathrm{d}^3\boldsymbol{q}\, \mathrm{e}^{(\mathrm{i}/\hbar)\boldsymbol{q}\boldsymbol{r}} \langle \boldsymbol{p} + \tfrac{1}{2}\boldsymbol{q}|\rho^{(1)}(t)|\boldsymbol{p} - \tfrac{1}{2}\boldsymbol{q}\rangle, \tag{2.6}$$

$$\langle \boldsymbol{p} + \tfrac{1}{2}\boldsymbol{q}|\rho^{(1)}(t)|\boldsymbol{p} - \tfrac{1}{2}\boldsymbol{q}\rangle = \frac{1}{(2\pi t)^3} \int \mathrm{d}^3\boldsymbol{r}\, \mathrm{e}^{(-\mathrm{i}/\hbar)\boldsymbol{q}\boldsymbol{r}} F(\boldsymbol{p}, \boldsymbol{r}, t) \tag{2.7}$$

so that any equation obtained in terms of the f is easily reformulated in terms of the F.

As discussed in section 1 the parameter set P also includes the total energy of the system, which is represented by the Hamiltonian H. For similar reasons we include the total number operator N, too. Thus, our representative ensemble takes the form

$$\sigma(t) = \exp\left\{\lambda_0(t) + \lambda_1(t)H + \lambda_2(t)N + \sum_{ik} \lambda_{i,k}(t)\hat{f}(i, k)\right\}. \tag{2.8}$$

As usual the parameters $\lambda(t)$ are determined from

$$f(i, k, t) = \mathrm{Tr}\,\{\hat{f}(i, k)\sigma(t)\}, \tag{2.9a}$$

$$\langle H\rangle = \mathrm{Tr}\,\{H\sigma(t)\} = \text{const.}, \tag{2.9b}$$

$$\langle N\rangle = \mathrm{Tr}\,\{N\sigma(t)\} = \text{const.}, \tag{2.9c}$$

$$\mathrm{Tr}\,\sigma(t) = 1 \tag{2.9d}$$

and thus may be regarded as functions of $f(i, k; t)$ and $\langle H\rangle$. Since N can be written as a linear combination of $\hat{f}(\alpha)$ we may always put $\lambda_2(t) = \mu$ where μ is the chemical potential of the system in its final equilibrium state. The

concrete functional connection between $\langle H\rangle$, $f(t)$ and $\lambda(t)$ is obtained from the diagram expansion of $\Omega(t,t')$ introduced below by noting that $f(i,k;t)=\Omega_{i,k}(t,t)$. Since $\rho_{(t)}^{(1)}$ is a hermitean operator we find that by virtue of (2.9) $\sigma(t)$ has also to be hermitean wherefrom it follows that $\lambda_{i,k}(t)=\lambda_{k,i}^{*}(t)$ at all times t.

To simplify the notation we introduce greek indices to denote pairs of momenta

$$\alpha=\{i,k\},\qquad \beta=\{l,m\},\ldots,$$

so that

$$f(i,k;t)\equiv f(\alpha,t)\equiv f_\alpha(t);\qquad \hat{f}(i,k)\equiv\hat{f}(\alpha)\equiv\hat{f}_\alpha$$

with the above choice of parameters, the exact KE's are obtained immediately from the equations of motion in I

$$\dot{f}_\alpha(t)=-\mathrm{i}\Omega_\alpha^{(0)}(t)$$
$$-\int_0^t \mathrm{d}t'\left[\Omega_\alpha^{(1)}(t,t')-\mathrm{i}\sum_\beta \dot{f}_\beta(t')\frac{\partial}{\partial f_\beta(t')}\Omega_\alpha^{(2)}(t,t')\right]. \tag{2.10}$$

Introducing the Heisenberg and interaction representation of the operators $\hat{f}_\alpha$

$$\hat{f}_\alpha(t)=\mathrm{e}^{(\mathrm{i}/\hbar)Ht}\hat{f}_\alpha\,\mathrm{e}^{(-\mathrm{i}/\hbar)Ht}, \tag{2.11}$$
$$\hat{f}_\alpha^{\mathrm{i}}(t)=\mathrm{e}^{(\mathrm{i}/\hbar)H_0t}\hat{f}_\alpha\,\mathrm{e}^{(-\mathrm{i}/\hbar)H_0t}, \tag{2.12}$$

the $\Omega^{(i)}$ and the related quantity Ω are written here as

$$\begin{aligned}
&\Omega_\alpha^{(0)}(t)=\mathrm{i}\,\mathrm{Tr}\{\dot{\hat{f}}_\alpha(0)\sigma(t)\},\\
&\Omega_\alpha^{(1)}(t,t')=-\mathrm{Tr}\{\ddot{\hat{f}}_\alpha(\vartheta)\sigma(t')\}=\mathrm{Tr}\{\dot{\hat{f}}_\alpha^{\mathrm{i}}(\vartheta)L(\vartheta)U(\vartheta,0)L\sigma(t')\},\\
&\Omega_\alpha^{(2)}(t,t')=\mathrm{i}\,\mathrm{Tr}\{\dot{\hat{f}}_\alpha(\vartheta)\sigma(t')\}=\mathrm{Tr}\{\dot{\hat{f}}_\alpha^{\mathrm{i}}(\vartheta)L(\vartheta)U(\vartheta,0)\sigma(t')\},\\
&\Omega(t,t')=\mathrm{Tr}\{\hat{f}_\alpha(\vartheta)\sigma(t')\}=\mathrm{Tr}\{\hat{f}_\alpha^{\mathrm{i}}(\vartheta)U(\vartheta,0)\sigma(t')\},
\end{aligned} \tag{2.13}$$

where $L=L_0+L_1$ is the Liouvilleoperator, $L(\vartheta)$ its interaction representation

$$L(\vartheta)=\mathrm{e}^{\mathrm{i}L_0\vartheta}L\,\mathrm{e}^{-\mathrm{i}L_0\vartheta}, \tag{2.14}$$
$$U(\xi,\xi')=\mathrm{e}^{\mathrm{i}L_0\xi}\,\mathrm{e}^{-\mathrm{i}L\cdot(\xi-\xi')}\,\mathrm{e}^{-\mathrm{i}L_0\xi'} \tag{2.15}$$

and $\vartheta=t-t'$.

By virtue of (2.9), the $\Omega^{(i)}$ are functions of the f_α and thus we may consider the equations (2.10) as KE's describing the time evolution of the $f_\alpha(t)$, these equations being written in the form of implicit integrodifferential equations. As demonstrated in I, the $\dot{f}(t')$ on the r.h.s. of (2.10) could be removed by iteration but this proves inconvenient since we focus our attention on the SMA.

2.2. *The short memory approximation*

Before introducing the short-memory assumption (SMA) let us discuss the free-streaming terms occurring in the KE's. As the first step we carry out the L_0 term in $\Omega^{(0)}$. We easily find

$$\mathrm{Tr}\,\{\hat{f}_\alpha L_0 \sigma(t)\} = -\mathrm{Tr}\,\{\sigma(t) L_0 \hat{f}_\alpha\} = \frac{1}{\hbar}(\epsilon_i - \epsilon_k) f_\alpha(t) = \frac{1}{\hbar}\epsilon_\alpha f_\alpha(t). \tag{2.16}$$

Since

$$\mathrm{Tr}\,\{\hat{f}_\alpha \sigma(t)\} = \mathrm{Tr}\,\{\hat{f}_\alpha \rho(t)\}$$

and

$$\rho(t) = \sigma(t) - \int_0^t \mathrm{d}t' \left[\mathrm{i}\, \mathrm{e}^{\mathrm{i}L_0(t-t')} L \sigma(t') + \sum_\beta \dot{f}_\beta(t') \frac{\partial}{\partial f_\beta(t')} \mathrm{e}^{-\mathrm{i}L_0(t-t')} \sigma(t') \right.$$

we may rewrite the KE's as

$$\begin{aligned} \left[\frac{\partial}{\partial t} + \frac{\mathrm{i}}{\hbar}\epsilon_\alpha f_\alpha(t) \right] &= -\mathrm{i}\,\mathrm{Tr}\,\{\hat{f}_\alpha L_1 \sigma(t)\} \\ &\quad - \int_0^t \mathrm{d}\vartheta [\mathrm{Tr}\,\{\hat{f}_\alpha^{\mathrm{i}}(\vartheta) L_1(\vartheta) U(\vartheta, 0) L_1 \mathrm{e}^{\mathrm{i}L_0\vartheta} \tilde{\sigma}(t-\vartheta)\} \\ &\quad + \mathrm{i}\,\mathrm{Tr}\,\{\hat{f}_\alpha^{\mathrm{i}}(\vartheta) L_1(\vartheta) U(\vartheta, 0) \mathrm{e}^{\mathrm{i}L_0\vartheta} \dot{\tilde{\sigma}}(t-\vartheta)\}], \end{aligned} \tag{2.17}$$

where

$$\tilde{\sigma}(t-\vartheta) = \mathrm{e}^{-\mathrm{i}L_0\vartheta} \sigma(t-\vartheta) \tag{2.18}$$

and

$$\dot{\tilde{\sigma}}(t-\vartheta) = \frac{\mathrm{d}}{\mathrm{d}\vartheta} \tilde{\sigma}(t-\vartheta) = \left(-\mathrm{i}L_0 - \sum_\beta \dot{f}_\beta(t-\vartheta) \frac{\partial}{\partial f_\beta(t-\vartheta)} \right) \tilde{\sigma}(t-\vartheta) \tag{2.19}$$

was introduced formally.

To discuss $\tilde{\sigma}(t-\vartheta)$ we assume for the time being that ϑ is a time of the order of the collision time which in turn is of the order of the memory time τ. Assuming τ to be small as compared with the relaxation time $t_{\mathrm{rel.}}$ associated with the dissipative processes, we find that in the interval $\vartheta < \tau$ the time evolution of the system is governed mainly by free streaming, i.e. it is described approximately by (2.17) with the r.h.s. put equal to zero. Since $\exp[-\mathrm{i}L_0\vartheta]$ is the time evolution operator of free streaming we may write approximately

$$\sigma(t-\vartheta) \approx \mathrm{e}^{\mathrm{i}L_0\vartheta} \sigma(t), \quad \vartheta < \tau, \tag{2.20}$$

this approximation being the better, the weaker the interaction and thus the greater $t_{\mathrm{rel.}}$.

In this approximation $\tilde{\sigma}$ is a quantity which in the time interval considered

varies on a time scale given by $t_{\text{rel.}}$ however strong the inhomogeneities in the system might be.

Because of this fact and because of

$$\frac{\mathrm{d}}{\mathrm{d}\vartheta}\,\mathrm{e}^{-\mathrm{i}L\vartheta}\,\mathrm{e}^{\mathrm{i}L_0\vartheta} = -\mathrm{i}\,\mathrm{e}^{-\mathrm{i}L\vartheta}L_1\,\mathrm{e}^{\mathrm{i}L_0\vartheta}$$

we find as in I that in the interval $\vartheta < \tau$ the second term under the intergral sign in (2.17) has a step-function like behaviour if the first term is δ-function like. Therefore, for sufficiently small values of τ the SMA is formulated as

$$\left[\frac{\partial}{\partial t} + \frac{\mathrm{i}}{\hbar}(\epsilon_i - \epsilon_k)\right] f_\alpha(t) = -\mathrm{i}\,\mathrm{Tr}\,\{\hat{f}_\alpha L_1 \sigma(t)\}$$

$$- \int_0^t \mathrm{d}\vartheta\,\mathrm{Tr}\,\{\hat{f}_\alpha^{\mathrm{i}}(\vartheta)L_1(\vartheta)U(\vartheta,0)L_1\sigma(t-\vartheta)\}_{\mathrm{RDP}}, \tag{2.21}$$

where RDP means that only this part of the trace is retained which decays rapidly with time so that its contribution may be neglected after the characteristic time τ. Note that in (2.21) there appear no longer terms containing L_0.

The Markowian limit of this equation is obtained by putting

$$\tilde{\sigma}(t-\vartheta) \approx \tilde{\sigma}(t) = \sigma(t). \tag{2.22}$$

By taking the Markowian limit in this way, the memory effects due to free streaming are accounted for at least approximately, whereas the memory effects with respect to the dissipative processes are neglected.

To assess the physical meaning of the Markowian limit (2.22) let us assume for the moment that the many-particle collision processes contributing to the RDP term in (2.21) are such that they are completed after a very short time $\vartheta < \tau$ so that the index RDP may be dropped. Then, we may assume that the Møller super wave-operator

$$\Omega_L^{(+)} = \lim_{t\to-\infty} \mathrm{e}^{\mathrm{i}Lt}\,\mathrm{e}^{-\mathrm{i}L_0 t}$$

or

$$\Omega_L^{(+)} = 1 - \mathrm{i}\int_{-\infty}^{0} \mathrm{d}t\,\mathrm{e}^{(1/\hbar)\epsilon t}\,\mathrm{e}^{\mathrm{i}Lt}L_1\,\mathrm{e}^{-\mathrm{i}L_0 t}$$

exists[9]). Introducing (2.18), (2.22) into the last term of (2.21) we conclude from the existence of $\Omega_L^{(+)}$ that the lower limit of time integration may be taken to $-\infty$ provided the usual damping factor is introduced. Thus under the above assumptions the Markowian approximation reads

$$\left[\frac{\partial}{\partial t} + \frac{\mathrm{i}}{\hbar}(\epsilon_i - \epsilon_k)\right] f_\alpha(t) = -\mathrm{i}\,\mathrm{Tr}\,\{\hat{f}_\alpha L_1 \Omega_L^{(+)}\sigma(t)\} \tag{2.23}$$

or

$$\left[\frac{\partial}{\partial t}+\frac{\mathrm{i}}{\hbar}(\epsilon_i-\epsilon_k)\right] f_\alpha(t)=-\mathrm{i}\,\mathrm{Tr}\,\{\hat{f}_\alpha L_1 \Omega^{(+)}\sigma(t)\Omega^{(+)+}\}, \tag{2.24}$$

where

$$\Omega_L^{(+)}A=\Omega^{(+)}A\Omega^{(+)+}$$

was used, $\Omega^{(+)}$ being the usual Møller wave operator[10]).

These considerations show that explicitly taking into account the memory effects due to free streaming immediately leads to the occurrence of the many-particle wave operator expressing the scattering properties of a selected number of particles. This would not obtain if we had formulated the short memory approximation and the Markowian limit in the usual way, i.e. in terms of σ instead of $\tilde{\sigma}$. Note also that the reversible term[11,12]) on the r.h.s. of (2.21) is absent in (2.23), (2.24).

2.3. *Correlation functions*

For completeness let us reformulate the KE's (2.10) in terms of non-equilibrium correlation functions and discuss the linear approximation. Using[11])

$$L\sigma(t)=-\mathrm{i}\sum_\beta \lambda_\beta(t)\tilde{\hat{f}}_{\beta,t}\sigma(t), \quad \hat{f}=\hat{f}(0),$$

where the tilde denotes a kind of Kubo transformed

$$\tilde{B}_t=\int_0^1 \mathrm{d}x\,\sigma(t)^{+}B\sigma(t)^{-+} \tag{2.25}$$

and expressing the time derivative $\dot{\sigma}(t)$ as

$$\dot{\sigma}(t)=\left[\sum_\beta \dot{\lambda}_\beta(t)\tilde{\hat{f}}_{\beta,t}+\dot{\lambda}_1(t)\tilde{H}_t\right]\sigma(t)$$

the equations (2.10) are written now

$$\dot{f}_\alpha(t)=-\sum_\beta \langle \hat{f}_\alpha \tilde{\hat{f}}_{\beta,t}\rangle_t \lambda_\beta(t)-\int_0^t \mathrm{d}t'\Big[\sum_\beta \{\langle \dot{\hat{f}}_\alpha(t-t')\tilde{\hat{f}}_{\beta,t}\rangle_{t'}\lambda_\beta(t')$$

$$+\langle \dot{\hat{f}}_\alpha(t-t')\tilde{\hat{f}}_{\beta,t'}\rangle_{t'}\dot{\lambda}_\beta(t')\}+\langle \dot{\hat{f}}_\alpha(t-t')\tilde{H}_{t'}\rangle_{t'}\dot{\lambda}_1(t')\Big], \tag{2.26}$$

where the non-equilibrium correlation functions $\langle AB\rangle_t$ are defined as

$$\langle AB\rangle_t=\mathrm{Tr}\,\{AB\sigma(t)\}. \tag{2.27}$$

In the vicinity of the equilibrium the $\lambda_\beta(t)$ are small so that we may consider the linear approximation of (2.26). This is obtained by replacing in (2.25),

(2.27) $\sigma(t)$ with $\rho_{\text{eq.}}$, the grand canonical ensemble. In this linear approximation the equations (2.26) are

$$\dot{f}_\alpha(t) = -\sum_\beta \langle \hat{f}_\alpha \hat{\bar{f}}_\beta \rangle_{\text{eq.}} \lambda_\beta(t') - \int_0^t \mathrm{d}t' \sum_\beta \{\langle \hat{\dot{f}}_\alpha(t-t') \hat{\bar{f}}_\beta \rangle_{\text{eq.}} \lambda_\beta(t') + \langle \hat{\dot{f}}_\alpha(t-t') \hat{\bar{f}}_\beta \rangle_{\text{eq.}} \dot{\lambda}_\beta(t')\}, \tag{2.28}$$

where

$$|\langle_{\alpha,\beta}(t-t') = \langle \hat{f}_\alpha(t-t') \hat{\bar{f}}_\beta \rangle_{\text{eq.}}$$

is the quantum analog of the van Hove phase-space correlation function[13]).

It is interesting to note that the diagram expansion of $K_{\alpha,\beta}(t-t')$ and its time derivatives appearing in (2.28) are easily obtained from the diagram expansion of $\Omega_\alpha(t-t')$ by using the fact that Ω_α is the generating function (or functional in the case of an infinite system) of the above correlation functions.

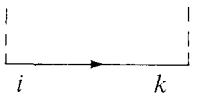
3. The diagrams

We shall now specify the diagrams, given for the general case in I, to the concrete interaction and representation chosen in this paper.

We begin by choosing a concrete form for σ_0, the interaction free ensemble (2.8). We take

$$\sigma_0 = \exp\{\lambda_0^{(0)} - \beta(H_0 - \mu N)\}, \tag{3.1}$$

where β, μ are the inverse temperature and the chemical potential of the system in its final equilibrium state and N is the particle number operator of the whole system. By virtue of its special form σ_0 is independent on time and commutes with H_0. Thus, the free Green functions are diagonal in the momentum representation and we have

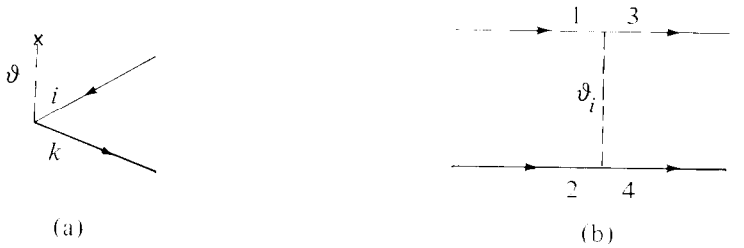


$$= \delta(i,k) g_0^{>}(i) = -\delta(i,k) \operatorname{Tr}\{a_i a_k^+ \sigma_0\}, \tag{3.2}$$

$$= \delta(i,k) g_0^{<}(i) = -\kappa\delta(i,k) \operatorname{Tr}\{a_k^+ a_i \sigma_0\}. \tag{3.3}$$

In I, for the sake of generality, the Hugenholtz notation of the interaction in the diagrams was used. Since we deal only with one- and two-particle interactions here we prefer to use the usual notation by means of interaction

lines. Thus we have two kinds of dashed lines



(3.4)

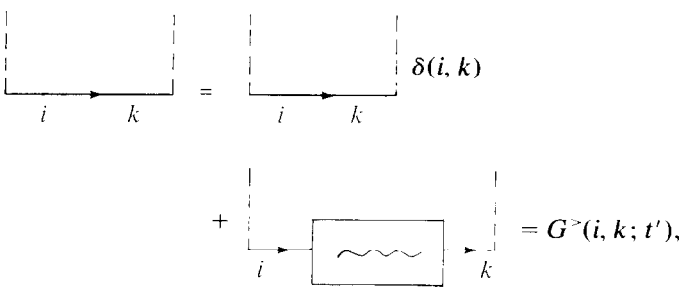
where (3.4a) corresponds to $\hat{f}^{i}_{\alpha}(\vartheta)$ and (3.4b) to the interaction W. Similarly, we have two possibilities for wavy lines occurring in the σ-parts

(3.5)

In the above notation to each Hugenholtz diagram corresponds quite a group of diagrams which differ from each other only in the ways the Green function lines are connected to the vertex points of a given interaction line. We call such a group of diagrams an exchange group. Since the interaction (2.2) contains direct as well as exchange terms all members of an exchange group are taken into account automatically in working with this interaction[14]). Thus only one member of an exchange group has to be considered. As a consequence the equivalent pair of lines rule (A.3) arises.

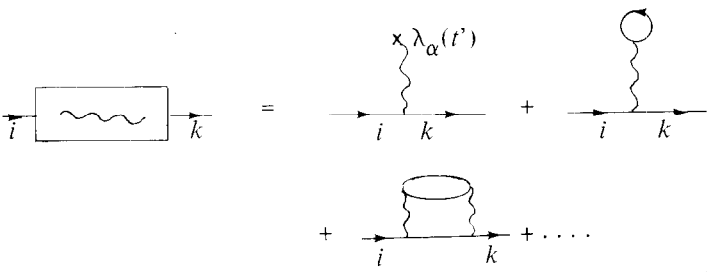
For statistical applications this way of drawing diagrams seems to be especially convenient because at high temperatures exactly one diagram of each exchange group survives (see appendix B).

As usual we may replace free Green functions by exact ones. Consider the diagram series



(3.6a)

where



(3.6b)

Using (3.2) and (3.3) we find immediately

$$G^<(i,k;t') = -\kappa f(i,k;t'),$$
$$G^>(i,k;t') = -[\delta_{i,k} + \kappa f(i,k;t')], \tag{3.7}$$

where the $f(i,k,t')$ are the matrix elements of the single-particle density matrix.

By this procedure, the summing of the σ-part self-energy structures, we introduce the $f(t')$ directly into the diagram expansion. Thus, the $\lambda(t)$ are partly eliminated from the formalism and – apart from the many-particle σ-parts – we never need to worry about the connection between the λ and the f. This is an important simplification and is the main reason why we have favoured the f over the Wigner functions F.

In the following, except for the σ-parts, we will exclusively work with the exact Green functions. For simplicity we shall associate light lines with these exact Green functions. In inhomogeneous systems the line ends carry different momenta. No σ-part self-energy structures must appear between dashed lines. The concrete description for the construction and evaluation of the diagrams is given in appendix A.

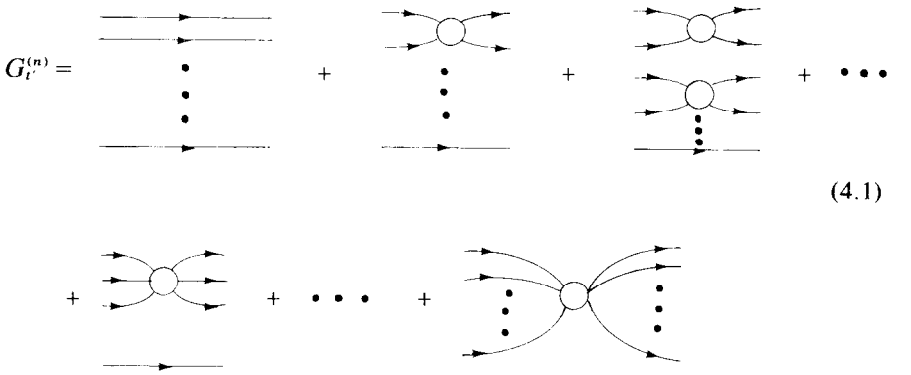
4. Analysis of diagrams

In this section we are going to discuss some of the pecularities of the expansion of the $\Omega^{(n)}(t,t')$. We intend to give qualitative criteria to assess the time dependence of the diagrams and to give a physical interpretation of their different parts. Let us begin with a simple partial summation procedure which leads to the introduction of cluster functions.

4.1. *Cluster functions, dynamic and quasistatic correlations*

Consider the diagram expansion of the n-particle Green function $G_{i'}^{(n)}$

introduced in I. Obviously we may write



(4.1)

not drawing explicitly the exchange diagrams in the single-particle GF's. It is understood that all lines not being connected to circular vertices correspond to exact GF's. The circular vertex having $2m$ external lines denotes the cluster functions g_m and is defined as the sum of all m-particle σ-parts. The expansion (4.1) is analogous to the usual cluster expansion of the m-particle distribution function. The g_m describe the correlations of m particles and have in the case of a short-range potential the property of being zero if the particles are not closely together. From reasons to be made clear below these correlations will be called quasistatic correlations.

The cluster functions can be readily introduced into the diagrams of $\Omega(t, t')$, too. This is easily achieved by replacing any σ-part with the corresponding cluster function. This procedure corresponds to a partial summation of the σ-parts.

Now, consider a diagram containing no cluster functions. From the construction of the diagrams (see I) it follows that this diagram was constructed from the first term on the r.h.s. of (4.1) this term corresponding to the vacuum of quasistatic correlations. We read the diagram in the direction of increasing time, i.e. from right to left. The diagram begins with the interaction line (B.6) describing the dynamical event that two particles in states 1 and 2 collide and go over into the new states 3 and 4, respectively. Thus, starting from the vacuum of correlations, a correlation between the two particles has been created. In the usual language of many-body theory one might also say, that two particle-hole states have been created.

The correlation then propagates in time. Since all lines correspond to exact GFs it is taken into account that the propagation does not take place in free space but in a medium described by $\sigma(t')$. Thus, in the inhomogeneous case the momentum of the propagating particles or holes may change. As time moves on, new correlations are created (B.5) the correlations may change (B.3), (B.4) or may be destroyed (B.2). At time t all correlations are destroyed but for a single particle hole state, the probability of which is "measured" by

the leftmost vertex (3.4a). We find that the diagrams describe the creation, propagation and destruction of dynamical correlations.

Now, consider a diagram containing at least one σ-part or in the resummed form at least one circular vertex corresponding to a cluster function. Actually, this vertex has to be drawn to the right of all LO-vertices since the quasistatic correlations refer to time t'. These diagrams take into account that there are already correlations present before the dynamic correlations are created.

From these considerations qualitative conclusions concerning the time behaviour of the diagrams may be drawn. From a number of papers it is well known[15, 16]) that the short-ranged dynamic correlations decay after a very short time provided the interactions are sufficiently well behaved. Thus it follows, that the dynamic part of the diagrams fitting into the above picture represents very short-lived processes and that these diagrams give a zero contributions if the time difference between the first and last dashed interaction line is greater then a characteristic time which is of the order of the collision time.

Contrarily to this very rapid behaviour of the dynamic correlations, the correlations represented by the cluster functions (or the σ-parts) change only over a time scale which is related to the relaxational behaviour of the $f(t')$. These are the correlations contained in the local equilibrium ensemble $\sigma(t')$, whereas the dynamic correlations are created by the movement of $\rho(t')$ and reflect the fact that $\rho(t')$ is not equal to $\sigma(t')$.

If $\sigma(t')$ changes adiabatically slowly as compared with the characteristic time of the dynamic correlations then we can always assume that the latter are decayed and the cluster functions represent very nearly the real correlations observed in the system at time t'. It is for this reason that we call them quasistatic correlations. In the vicinity of the equilibrium these quasistatic correlations become the static correlations well known from the linear theories[3,17]).

4.2. *Secular divergent diagrams*

From the above rule concerning the time behaviour of diagrams there is an obvious and important exception caused by certain self-energy insertions. Let us call any part of a diagram which is removed from the rest of the diagram considered by cutting two equally (contrarily) directed lines a self-energy structure of type I (II). Thus the diagram of fig. 1b contains a type II self-energy structure (SE II) and the diagram of fig. 3 a self-energy structure of type I (SE I).

Now consider any diagram containing an SE II. From rule (A.2) we could associate with each of the external lines of the SE II an oscillating factor which would cut off the time integration associated with the leftmost dashed line in the SE II. Now, let us consider for the moment a homogeneous system. Because of the momentum conservation the oscillating factors of the two external lines cancel each other this leading to an unrestricted time integration

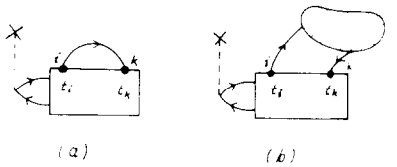


Fig. 1. The dressing procedure. In fig. 1a there is shown an irreducible diagram with a single line running from a dashed line at t_i to another dashed line at t_k drawn explicitly. In fig. 1b this line is replaced by an SE II-insertion having an arbitrary number $n \geq 1$ of dashed and wavy lines. Note that the time integrations associated with the dashed lines in this insertion might well extend to times $t > t_k$.

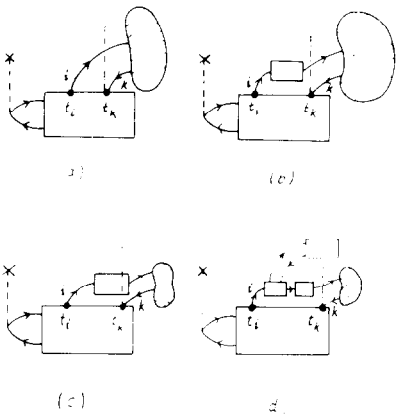


Fig. 2. Some typical diagrams which arise if the time integrations in the SE II-insertion of fig. 1b are split into two regions $t > t_k$ and $t < t_k$. In the figures, these time integrations are restricted by the dash-dotted line. All the dashed lines of the SE II which occur to the left of this line are integrated from t_k onwards and those occurring to the left of it are integrated up to t_k only. Figures 2a to 2c are explained in the text. Figure 2d is an example of a more complicated diagram which is also contained in fig. 1b. In this diagram, the top SE II-insertion is not affected by the dash-dotted line. The latter insertion dresses a line in the SE I-insertion it is connected with.

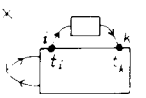


Fig. 3. The diagram of fig. 1a with an SE I-structure inserted. The sum of this diagram and of all the diagrams of fig. 2b is obtained by making the replacement (A.5′) with respect to the line labeled k.

and therefore asymptotically to a factor $(t - t')$. Thus we encounter the secular divergencies well known in all time-dependent perturbation expansions of statistical mechanics.

In inhomogeneous systems the SE II-diagrams are not strictly divergent because the momentum is not conserved. Therefore, the oscillating factors are preserved and the time integrations are cut off, however, for macroscopic times only.

5. Reformulation of the kinetic equations and the short-memory approximation

In the preceding section we found that in the diagram expansion of the $\Omega^{(i)}$ there occur secular divergent terms. As usual[15]) the sum over all of these divergent terms yields part of the long-time tail of the $\Omega^{(i)}$. These diagrams therefore do not contribute to the short-memory form (2.21) of the KE's. From the considerations in section 4.1 one would expect that all the other diagrams of $\Omega^{(i)}(t, t')$ should be taken into account in (2.21). However, if the parameters of the set Q introduced in section 1 play any role in the time evolution of the system then the macroscopic processes associated with these parameters might slow down the formation or decay of the dynamic correlations. In this case, the corresponding diagrams are also slowly decaying or even secular-divergent and have therefore to be excluded from contributing to (2.21).

These considerations show that the application of the SMA allows to exclude from the outset a great number of diagrams from the definition of the integrand in (2.21). Yet there remains always the question as to the validity of the SMA. Partially this important question is answered in the affirmative by showing that those diagrams of $\Omega^{(1)}$ which contain SE II-insertions cancel with certain secular divergent terms of the third term in (2.10), in the Markowian limit and at late times at least.

The proof is sketched briefly as follows. We insert the diagram expansion of the kernels into (2.10) and then we iterate the equations. In doing so one has to notice that the derivative may be written as

$$\frac{\partial}{\partial f(t')} = \frac{\partial^{\mathrm{I}}}{\partial^{\mathrm{I}} f(t')} + \frac{\partial^{\mathrm{c}}}{\partial^{\mathrm{c}} f(t')}, \tag{5.1}$$

where ∂^{I} acts only on the $f(t')$ associated with the lines of the diagrams of $\Omega^{(2)}$ via the line bundle rule and ∂^{c} acts on the cluster functions. The essential point of the proof consists in showing that the terms in ∂^{I} which arise in the course of the iteration are very similar to the SE II diagrams of $\Omega^{(1)}(t, t')$ with the $t_i = 0$ dashed line occurring in an SE II. In the Markowian limit and at sufficiently late times they both become identical and cancel each other because of their opposite sign.

Although conceptually simple the detailed proof is rather involved and will not be given here.

Instead we shall explicitly construct a modified version of the general KE's in which the terms in ∂^{I} and the SE II-diagrams of $\Omega^{(1)}$ are missing altogether. In the Markowian limit the relevant diagrams in the two forms of the KE's become identical and thus the existence of this new version of the KE's may be regarded as an indirect proof of the cancellation procedure alluded to above. In addition, the new version of the KE's is somewhat more compact and allows a more detailed comparison with other existing theories[18, 19, 20]).

To get the new formulation we reverse the way which led us to our

diagrammatical KE's. We diagrammatically express the rate of change of $f(t)$ in terms of the initial conditions first and then remove the initial conditions by partial summation and by applying our partial integration procedure introduced in I.

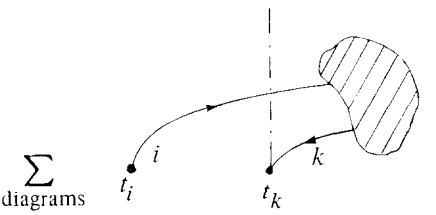
The first step is easily achieved. We introduce

$$f_\alpha(t, t_0) = \Omega_\alpha(t, t_0) = \langle \hat{f}_\alpha(t - t_0) \rangle_{t_0} \tag{5.2}$$

where $f_\alpha(t, t_0)$ is the single-particle density matrix if at time t_0 we had $\sigma(t_0) = \rho(t_0)$. In particular we have $f_\alpha(t, 0) = f_\alpha(t)$. The diagram expansion of $f_\alpha(t, t_0)$ is given by the sum of all the $\Omega_\alpha(t, t_0)$ diagrams. Note that in these diagrams all cluster functions depend on $f_\alpha(t_0)$. Analogously as in ref. 18 the initial conditions given by the $f(t_0)$ are partially removed by summing the SE II insertions.

Consider an irreducible diagram, i.e. a diagram having no self-energy insertions at all. Now let us dress with SE II insertions an arbitrary line of this diagram connecting two dashed lines. The diagrams arising from this procedure are depicted in fig. 1. In fig. 2 some typical diagrams are shown which arise from the diagram of fig. 1b if one splits at the time t_k the time integrations associated with the dashed lines in the insertion. Note that all of the diagram parts in the figures may contain an arbitrary number of wavy lines.

From the diagram rules we find that in fig. 2a the insertion contributes the factor



$$\sum_{\text{diagrams}} = e^{(i/\hbar)\epsilon_\alpha t_k} \Omega_\alpha(t_0 + t_k, t_0) - G^>(i, k; t_0), \tag{5.3}$$

where the box contains any diagram structure having at least one dashed or wavy line and the sum means that all of these diagrams are summed over. From (5.3) and (5.2) it follows that the sum of the diagrams of figs. 1a and 2a is given by the diagram of fig. 1a alone provided in the line bundle rule we replace the Green function associated with this line according to the rule (A.5′) in appendix A.

Similar considerations show that the diagrams of fig. 2b together with the diagrams obtained by dressing the line considered with SE I-insertions (see fig. 3) are taken into account by retaining only the diagrams of fig. 3 provided the replacement (A.5′) is made in the line labeled k.

There appear some anomalous diagrams which result from the diagrams of fig. 2c.

In these diagrams the dash–dotted line is understood to cut through the SE

I-insertion in such a way that the dashed interaction lines the external lines of the insertion are connected with always occur on different sides of the dash–dotted line. Such an insertion we shall call in the following a time restricted self-energy insertion (TRSE).

Carrying out the same dressing procedure with all the lines of a given irreducible diagram and with all the lines of the diagrams thus generated (like those in figs. 4 and 5) we finally find that $\Omega_\alpha(t, t')$ is given by the sum over all

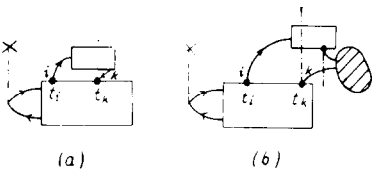


Fig. 4. Some of the diagrams containing TRSE insertions. (a) results directly from fig. 1b whereas (b) results from fig. 2c. The sum of both these diagrams are accounted for by retaining (a) only and making in the line labeled k the replacement (A.5′).

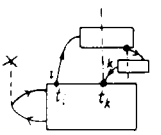


Fig. 5. Another diagram resulting from the diagram of fig. 2c if the time integrations in the SE II are restricted further.

those diagrams which do not contain any SE II and which are evaluated by using rule (A.5′). These diagrams may contain SE I-insertions, TRSE-insertions, TRSE-insertions into TRSE-insertions and so on. A special example is drawn in fig. 5. Considered as a function over the $f(t)$, this new diagram series is an other functional expression than the diagram series of $\Omega(t, t')$ described earlier. To make this difference explicit we denote this new series by $\tilde{\Omega}$ or $\tilde{\Omega}^{(i)}$. Of course, the values of both functionals agree if (and only if) the $f(t)$ are inserted as arguments.

Using the new diagram expansion and (5.2) we may write

$$f_\alpha(t) = \tilde{\Omega}_\alpha(t, 0) = C_\alpha(t) + D_\alpha(t), \tag{5.4a}$$

$$\dot{f}_\alpha(t) = \tilde{\Omega}^{(2)}_\alpha(t, 0) = C^{(2)}_\alpha(t) + D^{(2)}_\alpha(t), \tag{5.4b}$$

the C_α, D_α and $C^{(2)}_\alpha$, $D^{(2)}_\alpha$ denoting the sum of all the diagrams with and without cluster functions (or σ-parts), respectively. Note that the C_α, $C^{(2)}_\alpha$ no longer contain the initial conditions whereas the D_α, $D^{(2)}_\alpha$ depend on the $f(0)$ via the cluster functions.

To remove the dependence on the initial conditions completely we apply the partial integration procedure of I to each of the diagrams of $D_\alpha(t)$, $D^{(2)}_\alpha(t)$

obtaining

$$\left[\frac{\partial}{\partial t}+\frac{\mathrm{i}}{\hbar}\epsilon_\alpha\right] f_\alpha(t) = -\mathrm{i}\,\mathrm{Tr}\,\{\hat{f}_\alpha L_1 \sigma(t)\}$$

$$-\int_0^t \mathrm{d}t'\left[\tilde{\Omega}_\alpha^{(1)}(t,t')+\sum_\beta \dot{f}_\beta(t')\frac{\partial^c}{\partial^c f_\beta(t')}\tilde{\Omega}_\alpha^{(2)}(t,t')\right]. \tag{5.5}$$

As proposed above in (5.5) there are missing all terms containing the derivatives ∂^1 and all those diagrams which contain SE II insertions in which the leftmost dashed line is unrestricted with respect to time integrations.

The short-memory approximation of these equations is formulated as

$$\left[\frac{\partial}{\partial t}+\frac{\mathrm{i}}{\hbar}\epsilon_\alpha\right] f_\alpha(t) = -\mathrm{i}\,\mathrm{Tr}\,\{\hat{f}_\alpha L_1 \sigma(t)\} - \int_0^t \mathrm{d}t'\,\tilde{\Omega}^{(1)}(t,t')\Big|_{\mathrm{RDP}} \tag{5.6}$$

which agrees in the Markowian limit with (2.21).

A detailed discussion of the different forms of KE's shall be attempted in section 6.

6. Conclusions

In the preceding sections we obtained a set of exact closed equations describing the time evolution of the single-particle density matrix. This was achieved by applying the general method developed in I to the concrete set of parameters given in section 2. The diagram expansion of the relevant integral kernels has been discussed in detail.

Some interesting properties of this expansion should be noted. As in the theory of equilibrium and non-equilibrium Green functions[19, 20, 21]), the diagram expansion is a c-number expansion. This results from the fact that the diagrams are written down in terms of the interaction part of the Hamiltonian and not of the Liouvillean. The diagrams have great similarity with the usual many body diagrams for the calculation of the expectation value of a one-body operator starting from a correlated ground state. The most pronounced difference is contained in the line bundle rule. However, from the rules given in appendices A, B it should be obvious that at least in the Maxwell–Boltzmann limit the qualitative behaviour becomes the same as that of the usual many body diagrams. Thus it is felt that all the techniques known from the many body theory in equilibrium or at $T = 0$ may be carried over with minor modifications. Thus, it will be shown in a later paper that the renormalization of the interaction is easily achieved by summing the two-particle ladder diagrams.

The most interesting feature of our diagram expansion consists however in the appearance of the cluster functions in the short-memory form (2.21), (5.6)

of the KE's. To discuss this point further let us consider the KE's (5.4b) first. Since $D_\alpha^{(2)}(t)$ contains the effect of the initial correlations we may neglect $D_\alpha^{(2)}(t)$ after a very short time provided we make the usual assumption of the rapid decay of the initial correlations. This should be valid for sufficiently well behaved potentials, in not too dense systems at least[16]). Then, at sufficiently late times

$$\dot{f}_\alpha(t) = C_\alpha^{(2)}(t). \tag{6.1}$$

are a set of closed KE's describing the time evolution of the system in a very good approximation. As should be clear from the diagram rules, in the Maxwell–Boltzmann limit the diagram expansion of $C_\alpha^{(2)}(t)$ can be regrouped to become an expansion in powers of the density (see also ref. 22). The coefficients of such a virial expansion are given by the dynamics of isolated clusters of particles and are well known to diverge with increasing time[23]). The sum of all slowly decaying and divergent terms yields the long-time tail of $C_\alpha^{(2)}(t)$.

Now compare (5.6) with (6.1) and let us assume for the following discussions the validity of the SMA and the rapid decay of the initial correlations. Then, for sufficiently late times both the equations (5.6) and (6.1) describe the time evolution of the $f(t)$ correctly. Yet they have in common only the rapidly decaying diagrams not containing cluster functions. From the above considerations and from the fact that each cluster function contains arbitrarily high powers of the density it follows, that each cluster function diagram contributing in (5.6) corresponds to the effect of a whole subset of slowly decaying or divergent diagrams of (6.1) or of parts of the contributions of such diagrams*.

These considerations also show that in dense systems where the contribution of the cluster function diagrams is large, the long time tail and thus the long memory behaviour in (6.1) is very important.

To explore this fact further we note that (6.1) would be the exact KE's if we had included the Hamiltonian H into the parameter set Q instead of into P. Then, H is missing in (2.8) and thus there are no diagrams containing cluster functions in the KE's, this yielding also $D(t) = 0$ in (6.1). From the point of view of section 1 we may therefore conclude that the ultimate reason for the difference between the two equations (5.6) and (6.1) lies in the fact, that in the former equations the conservation of total macroscopic energy (2.9b) is taken into account explicitely whereas it is ignored in the latter. This should be expected from physical reasons since isolated clusters of particle cannot "know" about the macroscopic energy of the system, at least if (in classical language) the total potential energy is comparable with or greater than the total kinetic energy.

Of course, the above conclusions hinge on the very probable but as yet

* There is of course the possibility, that the contribution of one diagram of $C^{(2)}(t)$ is represented by several cluster function diagrams of (5.6).

unproven validity of the SMA. It is therefore very satisfying that the cluster function diagram of lowest order contributing to (5.6) yields an Enskog-like equation which reduces in the appropriate limits to the intuitive Enskog equation[2,24]). This will form the subject of a later paper. The Enskog equation is well known to describe the behaviour of rather dense gases and is a good approximation even in simple liquids[25]). At this level of approximation the above general considerations agree completely with the usual reasoning[26,27]) that the Enskog equation represents a highly summed version of those generalized Boltzmann equations which are formulated in terms of isolated clusters of particles.

From the computational point of view the evaluation of the diagrams splits in the problem of the correlations and the problem of dynamics. This is very desirable since the evaluation of the cluster functions is essentially a problem of equilibrium statistics.

It is often argued[28]) that even if the dynamics of the problem is dealt with approximately, the relaxation of the system is described reasonably good provided the cluster functions are calculated correctly. Hopefully, this will be the case in our expansion (5.6), too.

Acknowledgement

We thank S. Fritzsche for reading the manuscript and for discussions.

Appendix A

The diagram rules

In the following the diagram rules for the diagrams of $\Omega(t, t')$ shall be given. Except for rule (A.5) which is to be read together with (A.5') the rules are the same for the diagrams of $\tilde{\Omega}(t, t')$ introduced in section 5. The diagrams of $\Omega^{(i)}$ or $\tilde{\Omega}^{(i)}$ may be obtained either by simple time derivatives or by directly starting from the explicit expressions (2.13) for the $\Omega^{(i)}$. In either way one finds that the diagrams of $\Omega^{(2)}$ are the same as those of Ω except for the fact that the leftmost dashed interaction line carries time $\vartheta = t - t'$. Moreover, in the $\Omega^{(1)}$ diagrams the rightmost interaction line carries time $t_i = 0$.

Additionally, there occur diagrams having a single-particle LO-vertex corresponding to the L_0-terms in $\Omega^{(1)}$, $\Omega^{(2)}$. Since these diagrams are easily obtained from the diagrams of Ω by simply introducing L_0 vertices and since these diagrams should be dropped in the short-memory approximation we do not consider them any further. All the remarks made above carry over immediately to the $\tilde{\Omega}^{(i)}$ diagrams.

The diagram rules read in detail

(A.1) Label the line ends with indices $i, k, l, \ldots$ corresponding to momenta $\boldsymbol{p}_i$,

p_k, p_l, ... and the interaction lines with momenta q_r, q_s, q_t, ... Label the leftmost dashed line with a time $\vartheta = t - t'$ all the other dashed lines with times t_i, $i = 1, 2, \ldots$ and all the wavy lines with imaginary times τ_i, $i = 1, 2, \ldots$.

(A.2) With each dashed interaction line i of the kind (3.4b) associate a factor

$$-(\mathrm{i}/\hbar)\langle 1\,2|W(t_i)|3\,4\rangle = -(\mathrm{i}/\hbar)\exp[(\mathrm{i}/\hbar)(\epsilon_1+\epsilon_2-\epsilon_3-\epsilon_4)t_i]\langle 1\,2|W|3\,4\rangle$$

the latter matrix element being given by (2.2) and $\epsilon_i = p_i^2/2m$. For the $\hat{f}_{i,k}$ vertex include a factor $\exp[-(\mathrm{i}/\hbar)(\epsilon_i - \epsilon_k)\vartheta]$.

(A.3) Include a factor of $\frac{1}{2}$ for each equivalent pair of lines, i.e. for each equally directed pair of two lines which connects any two interaction lines.

(A.4) Associate a step function $\theta(t_i - t_k)$ with each line connecting two dashed lines i, k the dashed line i being situated to the left of k.

(A.5) For each bundle of lines running from a given dashed line to the left include a factor which is given as

$$\prod_{i=1}^{m} G^{>}(i_1, i_2; t') \prod_{k=1}^{n} G^{<}(k_1, k_2; t') - \prod_{i=1}^{m} G^{<}(i_1, i_2; t') \prod_{k=1}^{n} G^{>}(k_1, k_2; t')$$

if the bundle consists of m lines $\overset{i_1}{\longrightarrow}\!\!\!\!\!\!\overset{i_2}{\longrightarrow}$ directed to the right and n lines $\overset{k_2}{\longleftarrow}\!\!\!\!\!\!\overset{k_1}{\longleftarrow}$ directed to the left. We have m, $n = 0, 1, 2$ and $m + n \geqslant 1$. The explicit expressions for $G^{>}$, $G^{<}$ are given in (3.6), (3.7).

(A.5′) In working with $\tilde{\Omega}$ diagrams one has to replace $G(i, k; t')$ by $\mathrm{e}^{(\mathrm{i}/\hbar)(\epsilon_i-\epsilon_k)t_k}G(i, k; t_k + t')$ if $t_i > t_k$ and by $\mathrm{e}^{(\mathrm{i}/\hbar)(\epsilon_i-\epsilon_k)/t_i}G(i, k; t_i + t')$ if $t_i < t_k$.

(A.6) Associate with any interaction line of the kind (3.5b) according to (2.2) a factor $-(\mathrm{i}/\hbar)\langle 1\,2|W|3\,4\rangle$ and with the vertex (3.5a) a factor $\lambda_{i,k}(t') + [\delta(i, k)(\lambda_1(t') + \lambda_2(t') + \beta - \mu)]$.

(A.7) With each line being connected with at least one wavy line associate a free Green function

$$\underset{\tau_i}{\longrightarrow}\!\!\!\!\!\!\overset{p}{\underset{\tau_k}{\longrightarrow}} = G^{(0)}(p, \tau_i - \tau_k) = -\mathrm{Tr}\{T_\tau[a_p(\tau_i)a_p^{+}(\tau_k)]\sigma_0\}.$$

Note that the LO-vertices have imaginary time $\tau_i = 0$.

(A.8) Integrate all real times t_i from 0 to $t - t'$ all imaginary times from 0 to $\lambda_1(t)$ and sum over all momenta. The resulting expression is multiplied by $(-1)^{L+1}$ where L is the number of closed fermion loops.

Appendix B

Explicit expressions for line bundles and the Maxwell–Boltzmann limit

For the practical work with the diagrams it is convenient to have the explicit expressions for the different kinds of line bundles. Since in many practical

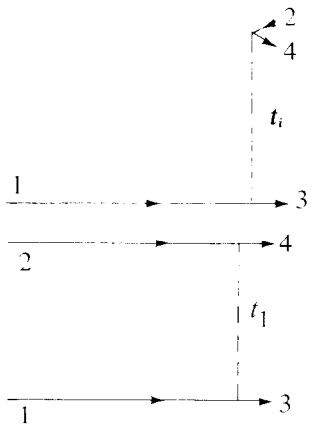
applications it is justified to take the Maxwell–Boltzmann limit, we will consider the corresponding expressions in this limit, too. The formulas shall be given for Ω-diagrams. In the case of $\tilde{\Omega}$ diagrams we have to make the replacements implied by rule (A.5′) in all places where an $f(t')$ occurs.

Introducing for notational purposes the two-particle operators $\hat{F}_2^{(0)}(t')$ and $R(t')$ with matrix elements

$$\langle 1\,2|\hat{F}_2^{(0)}(t')|3\,4\rangle = f(1,3;t')f(2,4;t'),$$

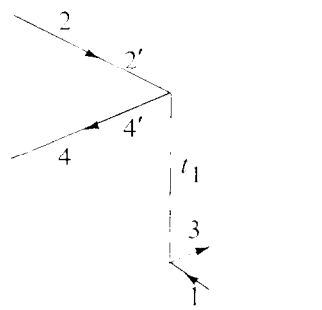
$$\langle 1\,2|R(t')|3\,4\rangle = \delta(1,3)\delta(2,4) + \kappa[\delta(1,3)f(2,4;t') + \delta(2,4)f(1,3;t')] \tag{B.1}$$

the detailed expressions read

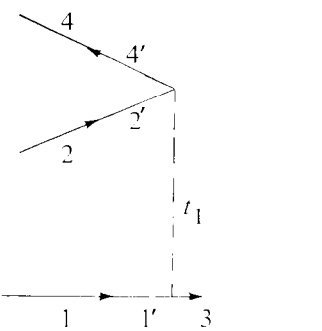


$$= (\mathrm{i}/\hbar)\langle 1\,2|W(t_i)|3\,4\rangle, \tag{B.2}$$

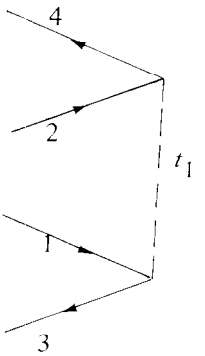
$$= -(\mathrm{i}/\hbar)\langle 1\,2|R(t')W(t_1)|3\,4\rangle \tag{B.3}$$



$$= -(\mathrm{i}\kappa/\hbar)[\delta(2,2')f(4',4;t') - \delta(4,4')f(2,2';t')]\langle 1\,2'|W(t_1)|3\,4'\rangle, \tag{B.4}$$



$$= \kappa(\mathrm{i}/\hbar)[\langle 1\,2|R(t')W(t_2)|3\,4'\rangle f(4',4;t') - \kappa\delta(4,4')\langle 1\,2|\hat{F}_2^{(0)}(t')W(t_1)|3\,4'\rangle \tag{B.5}$$



$$= -(\mathrm{i}/\hbar)\langle 1\,2|[R(t')W(t_2)\hat{F}_2^{(0)}(t') - \hat{F}_2^{(0)}(t')W(t_1)R(t')]|3\,4\rangle. \tag{B.6}$$

In using these rules one has to observe that reversing all the arrow directions in any one of the above diagram elements corresponds to taking the complex conjugate of the corresponding expression and that exchanging lines between vertex points corresponds to a relabeling of the matrix elements.

To get the Maxwell–Boltzmann limit of an arbitrary diagram put in the above expressions $R = 1$ and neglect the term containing $\hat{F}_2^{(0)}(t')$ in (B.5). This is easily verified by noting that in this limit the diagrams must not depend on κ and that each closed loop contributes a factor κ. Exchange interactions and the factors $\frac{1}{2}$ from rule (A.3) have to be neglected, too. Thus, in every line bundle where an even number $n = 0, 2$ of new closed loops begins, in the Maxwell–Boltzmann limit all terms proportional to κ have to be neglected and in any line bundle where one new closed loop begins only the terms in κ survive.

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