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Formal Structure of Kinetic Theory

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We study the Liouville equation in the domain of small deviations from absolute equilibrium. The solution is expressed in terms of amplitudes of n-body additive functions which are orthogonal with respect to the Gibbs weight factor. In the memory operator approach the memory operators are formally exact continued fractions. We show that with the isolation in the Liouville operator of a one-body additive operator L_0, any memory operator can be written alternatively as an exact infinite series, each term of which can be calculated exactly. This yields improvements of the dressed particle approximation. We discuss the choice of L_0, which is in general time dependent. The theory is developed both for smooth potentials and for hard spheres, where we use pseudo-Liouville operators. The theory can be formulated in an equivalent manner by introducing modified cumulant distributions, which are closely related to the amplitudes. The modified cumulants have the same spatial asymptotic properties as ordinary cumulants, but have superior short-time and small-distance behavior.

KEY WORDS: Liouville equation; cumulants; memory function; hierarchy equations.

1. INTRODUCTION

In the present paper we study the formal structure of classical many-body theory. Our considerations are limited to the linear response domain, where there are small amplitude disturbances about an absolute equilibrium state. The object is to derive linearized kinetic equations for time-dependent reduced distribution functions and for time-dependent correlation functions. The approach is one introduced earlier (Ref. 1; hereafter I). Boley[(2)] has analyzed the structure of this theory in detail and has made a number of simplifications and technical improvements. He has also shown that the formulation is

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closely related to the Green's function approach of Mazenko.[3] We will make some further simplifications here. Using a generalization of the idea of "dressed" particle,[4] the relationship to the general theory of Green's functions as well as to numerous other studies of time-dependent correlation functions becomes particularly clear. The formulas needed for explicit computations for smooth potentials will be written down explicitly.

We will do one further thing in this paper. We set down the theory for the case of hard spheres. In that case we deal with pseudo-Liouville operators, and the hierarchy for distribution functions takes a special form.[5] The remarkable feature of the hard-sphere case from the point of view of the general theory is that the "n"-body additive approximation for hard spheres corresponds to the "$n + 1$" approximation for smooth, strong, short-range potentials. The physical reason is that the duration of collisions becomes negligible. For smooth potentials the one-body additive approximation yields a singlet kinetic equation that is a modified Vlasov equation with the direct correlation function replacing the bare potential. It is well known that this is an improvement both at short times and at small distances over the usual Vlasov equation. The latter is derived by neglecting the doublet cumulant in the usual BBGKY hierarchy.[6] In addition the equation remains meaningful (even if inaccurate) for strong, short-range potentials. If the one-body additive approximation is applied to the hard-core case, using a pseudo-Liouville equation, one obtains a modification of the Boltzmann–Enskog equation with superior short-time behavior. This equation was derived by Lebowitz *et al.*,[7] who emphasized very clearly the distinction between the smooth potential and hard-core case. The same equation was derived by Mazenko from his general formalism and the solution of the equation was studied by Mazenko *et al.*[8] Sykes[9] has shown explicitly that the long-time hydrodynamic behavior implicit in the Boltzmann equation is not destroyed by the short-time modification.

The significant point is that for smooth, strong potentials the irreversible velocity relaxation of the Boltzmann equation can only be obtained by going to the two-body additive approximation and by eliminating the doublet function. This is of course much more complicated than the direct use of the one-body additive approximation together with the pseudo-Liouville operator.

In our general approach the next meaningful level of approximation is the dressed particle approximation, which may be thought of roughly as being intermediate between the one-body and two-body additive approximations. It involves the notion of a one-body additive operator and leads to an explicit expression for the memory kernel in the singlet equation. For smooth potentials the structure of the memory kernel is similar to that of Balescu for plasmas.[6] However, again there is the characteristic improvement for short times and small distances for the time correlation approach as compared with the usual cumulant approach to the BBGKY hierarchy. Of course, the ordinary Balescu equation is significant because it gives a description of large-distance phenomena, i.e., the screening of the Coulomb collisions at a Debye length.

Ernst and Dorfman[(10)] have used the pseudo-Liouville operator with the ordinary BBGKY hierarchy of distribution functions. Approximations similar to those of Balescu and Ichikawa[(6)] in plasma physics are made. The triplet cumulant is neglected and the direct binary interaction is treated by iteration. The theory then describes long-time tails in correlation functions and non-analytic contributions to the hydrodynamic equations. These are remarkable results obtained in a very simple way.

It is then quite natural to apply the dressed particle approximation to the hard-sphere problem, using a pseudo-Liouville operator and the time correlation formalism. One expects to find a short-time and small-distance improvement of the Ernst–Dorfman theory analogous to what occurred for smooth potentials. We carry out such a calculation in Section 4.

The two-body additive approximation for the hard-sphere case can be written down easily and corresponds to the three-body additive approximation for smooth, strong, short-range potentials. Furthermore, it is a trivial matter to go a step further, and to write the dressed particle approximation to the two-body memory function. The two-body additive approximation is set down in Section 3 and the dressed particle memory function in Section 4.

The basic ideas of the theory are presented in an elementary way in Section 3. The deviation of the N-body distribution from equilibrium is written as $\Phi F_N(p_1,\cdots, q_N; t)$, where Φ is the Gibbs equilibrium distribution. (Actually, as emphasized by Mazenko and by Boley, a grand canonical formulation is more convenient, and will be used here.) The phase space is supplied with a weight function Φ. The construction starts with the set of one-body additive functions $T(1)$ and an associated projection operator P_1. It is augmented by a set of two-body additive functions made orthogonal to the one-body functions, denoted by $T(12)$, and an associated projection operator P_2. It continues with three-body additive functions orthogonal to the two-body functions, denoted by $T(123)$, and so forth. Then the most elementary procedure is to expand F_N in terms of amplitudes A_n for these functions and to write the Liouville equation in the equivalent form of coupled equations for the amplitudes. The n-body additive approximation corresponds to the obvious procedure of neglecting all amplitudes whose index is greater than n.

There are, however, two nontrivial points. First of all there is no division of the Liouville operator into noninteracting and interacting parts. Only the matrix elements of the total Liouville operator between elements of the function space enter into the theory. For smooth potentials there is an identity (used in the variational formulation of Refs. 11; hereafter II and III) that these matrix elements are equal to the equilibrium average of the Poisson bracket of the two functions. This establishes immediately that the theory is in renormalized form with static correlation functions replacing bare potentials. Second, the time correlation functions constructed as matrix elements of the evolution operator e^{-Lt} with the basis functions are the same as Mazenko's correlation functions. They have the same large-separation behavior as ordinary time-dependent cumulant distribution functions. Since isolation of appropriate asymptotic behavior is the chief reason for introducing cumulants, the theory may be thought of in terms of the introduction of a new type of cumulant with superior short-time and small-distance behavior. The definition is almost forced on us by the requirement of orthogonalization with the Gibbs weight factor.

In Section 2 we express the theory in an abstract algebraic form, using projection operators, and find the continued fraction form for memory operators.[2] In addition we use the notion of a one-body additive operator to write a formal exact expression for the residual operator $\tilde{M}_{nn}$ belonging to the n-body additive approximation (different from the residual infinite continued fraction). Here we encounter a separation of the Liouville operator into an "unperturbed" one-body additive part L_0 and a perturbed part L_1. So the question arises as to how to choose L_0 and what to do about evaluating the residual $\tilde{M}_{nn}$. Existing theories differ in treatments of these points.

The primitive dressed particle theory stops at the one-body additive level, and keeps only the first term in the expression for $\tilde{M}_{11}$. For both smooth potentials and hard spheres L_0 is chosen by the condition

$$P_1 L_0 P_1 = P_1 L P_1$$

The best choice of L_0 is, however, that suggested by the general theory of Green's functions,[12] viz.,

$$P_1 L_0 P_1 = P_1 L P_1 + \tilde{M}_{11} \tag{1}$$

Then, one-body excitations propagate in a "finally dressed" way. Since $\tilde{M}_{11}$ is evaluated to some approximation using L_0, this leads to a difficult nonlinear self-consistent problem. On the other hand, comparison of the two-body additive approximation for smooth potentials with the one-body additive theory for hard spheres points to a simple recipe. At the n-body additive approximation compute $\tilde{M}_{11}$ neglecting $\tilde{M}_{nn}$. This leads to a revised $\tilde{M}_{11}$, which is the dressed particle improvement of the n-body additive approximation. This can also be written in a fully renormalized form.

In the body of the text and in the appendices we give relatively complete and explicit expressions for the static correlation functions, projection operators, and matrix elements of the Liouville operators.

2. ALGEBRAIC ASPECTS OF THE GENERAL THEORY

We wish to solve the Liouville equation[2]

$$\left(\frac{\partial}{\partial t} + L\right)\hat{F}_N(p_1,\ldots, q_N; t) = 0 \tag{2}$$

given the initial condition $F_N(t = 0) = F_N{}^0$. Here $\hat{F}_N\Phi$ is the deviation from absolute equilibrium. We use the time correlation point of view and introduce the evolution operator $\hat{G}(t) = e^{-Lt}$ and the Laplace transform, i.e., the resolvent operator $\tilde{G}(S) \equiv (S + L)^{-1}$. Then $\hat{F}_N(t) = e^{-Lt}F_N{}^0$ and $\tilde{F}_N(S) = \tilde{G}(S)F_N{}^0$

$$(S + L)\tilde{G}(S) = 1 \tag{3}$$

where 1 is the identity operator in N-body space.

Using a projection operator P and its complement Q, $P + Q = 1$, the basic formulas are

$$(S + PLP)P\tilde{G} + PLQ\cdot Q\tilde{G} = P, \qquad (S + QLQ)Q\tilde{G} + QLP\cdot P\tilde{G} = Q \tag{4}$$

We refer to $P\tilde{G}F_N{}^0$ and $Q\tilde{G}F_N{}^0$ as "amplitudes," and the concrete version of the theory is formulated in terms of amplitudes in Section 3. From these formulas, taking right-hand projections, we find

$$(S + PLP + \tilde{M})P\tilde{G}P = P, \qquad \tilde{M} = -PLQ(S + QLQ)^{-1}QLP \tag{5}$$

Here M is the memory operator associated with P. In particular we first take P_1 to be a projection operator onto one-body additive functions. Thus we have

$$(S + P_1LP_1 + \tilde{M}_{11})P_1\tilde{G}P_1 = P_1, \qquad \tilde{M}_{11} = -P_1LQ_1(S + Q_1LQ_1)^{-1}Q_1LP_1 \tag{6}$$

Now introduce a sequence of projection operators $P_2, P_3,\ldots$ with complements such that Q_2 is orthogonal to both P_1 and P_2, Q_3 is orthogonal to $P_1 + P_2 + P_3$, etc. Then let

$$\mathscr{L}_1 = Q_1LQ_1, \qquad \mathscr{G}_1 = (S + Q_1LQ_1)^{-1} \tag{7}$$

$$\tilde{M}_{11} = -P_1LQ_1\tilde{\mathscr{G}}_1Q_1LP_1, \qquad (S + \mathscr{L}_1)\tilde{\mathscr{G}}_1 = Q_1 \tag{8}$$

Treat this in the same way, noting that ($Q_1Q_2 = Q_2$, $Q_1 - Q_2 = P_2$)

$$P_2\mathscr{L}_1P_2 = P_2Q_1LQ_1P_2 = P_2LP_2, \qquad P_2\mathscr{L}_1Q_2 = P_2LQ_2 \tag{9}$$

Then

$$\{S + P_2LP_2 - P_2LQ_2(S + Q_2LQ_2)^{-1}Q_2LP_2\}P_2\tilde{\mathscr{G}}_1P_2 = P_2 \tag{10}$$

Hence, for the case that L connects only successive spaces (pairwise interactions),

$$\tilde{M}_{11} = -P_1LP_2\{S + P_2LP_2 + \tilde{M}_{22}\}^{-1}P_2LP_1 \tag{11}$$

[2] We use the caret to denote time-dependent quantities and the tilde to denote Laplace transforms.

with $\tilde{M}_{22} = -P_2LQ_2(S + Q_2LQ_2)^{-1}Q_2LP_2$. We thus have a continued fraction generated by the recursion relation

$$\tilde{M}_{nn} \equiv P_n\tilde{M}P_n = -P_nLP_{n+1}\{S + P_{n+1}LP_{n+1} + \tilde{M}_{n+1,n+1}\}P_{n+1}LP_n \quad (12)$$

and

$$\{S + P_nLP_n + \tilde{M}_{nn}\}P_n\tilde{G}P_n = P_n. \quad (13)$$

This is a formally exact reformulation of the problem.[2]

Now let L_0 be a one-body additive operator. This notion will be defined more precisely later. The relevant property for the present argument is that

$$P_mL_0P_n = 0 \qquad \text{for} \quad m \neq n \quad (14)$$

Since L_0P_1 belongs to P_1, we have $Q_1f(L_0)P_1 = 0$. From the identities

$$\begin{aligned}(S + Q_1L_0)^{-1} &= (S + L_0)^{-1}\{1 + P_1L_0(S + Q_1L_0)^{-1}\}\\ &= \{1 + (S + Q_1L_0)^{-1}P_1L_0\}(S + L_0)^{-1} \quad (15)\end{aligned}$$

we find

$$Q_1(S + Q_1L_0)^{-1} = Q_1(S + L_0)^{-1} \quad (16)$$

In addition, with $L = L_0 + L_1$ and the definitions

$$\tilde{G}_0 = (S + L_0)^{-1}, \qquad \tilde{I}_1 = [S + Q_1(L_0 + L_1)]^{-1} \quad (17)$$

we have the identities

$$\tilde{I}_1 = (S + Q_1L_0)^{-1}\{1 - Q_1L_1\tilde{I}_1\} = \{1 - \tilde{I}_1Q_1L_1\}(S + Q_1L_0)^{-1} \quad (18)$$

with the formal solution

$$Q_1\tilde{I}_1Q_1 = Q_1[1 + \tilde{G}_0Q_1L_1Q_1]^{-1}\tilde{G}_0Q_1 = Q_1\tilde{G}_0Q_1[1 + Q_1L_1Q_1\tilde{G}_0]^{-1}Q_1 \quad (19)$$

We therefore find the formally exact expressions for the first memory operator

$$\begin{aligned}\tilde{M}_{11} &= -P_1LQ_1[1 + \tilde{G}_0Q_1L_1Q_1]^{-1}Q_1\tilde{G}_0Q_1LP_1\\ &= -P_1LQ_1\tilde{G}_0Q_1[1 + \tilde{G}_0Q_1L_1Q_1]^{-1}Q_1LP_1 \quad (20)\end{aligned}$$

This type of expression can be established at any level. For example, for $\tilde{M}_{22}$, we have $Q_2(S + Q_2L_0)^{-1} = Q_2(S + L_0)^{-1}$, resting on the fact that $Q_2L_0P_1 = 0$, $Q_2L_0P_2 = 0$. With

$$\tilde{I}_2 \equiv [S + Q_2(L_0 + L_1)]^{-1} \quad (21)$$

we again have

$$Q_2\tilde{I}_2Q_2 = Q_2\tilde{G}_0Q_2\{1 - Q_2L_1Q_2I_2\}Q_2 = [1 - \tilde{I}_2Q_2L_1Q_2]Q_2\tilde{G}_0Q_2 \quad (22)$$

and

$$\begin{aligned}M_{22} &= -P_2LQ_2[1 + \tilde{G}_0Q_2L_1Q_2]^{-1}\tilde{G}_0Q_2LP_2\\ &= -P_2LQ_2\tilde{G}_0[1 + Q_2L_1Q_2\tilde{G}_0]^{-1}Q_2LP_2 \quad (23)\end{aligned}$$

The analogous expression holds for any value of n, viz.

$$\begin{aligned}\tilde{M}_{nn} &= -P_nLQ_n[1 + \tilde{G}_0Q_nL_1Q_n]^{-1}\tilde{G}_0Q_nLP_n \\ &= -P_nLQ_n\tilde{G}_0[1 + Q_nL_1Q_n\tilde{G}_0]^{-1}Q_nLP_n \end{aligned} \tag{24}$$

A number of existing theories fit naturally into this framework. The one-body additive theory entirely neglects $\tilde{M}_{11}$. It leads to a modified Vlasov equation because the term P_1LP_1 involves the direct correlation function rather than the bare potential (cf. Section 4). The Forster–Martin weak coupling theory[13] uses only the first term of the geometric series for $\tilde{M}_{11}$, namely $\tilde{M}_{11} \cong -P_1LP_2\tilde{G}_0P_2LP_1$, and takes L_0 equal to the free-particle streaming one-body additive operator. The work of the Brussels school[14] involves a diagrammatic analysis of the higher order terms of the series. The primitive dressed particle theory[4] also uses only the first term for $\tilde{M}_{11}$. But L_0 is chosen to be a one-body additive extension of the relation $P_1L_0P_1 = P_1LP_1$. As a result the theory can be written in renormalized form.

The two-body additive theory[1] sets $\tilde{M}_{22} = 0$, leading to an expression for $\tilde{M}_{11}$ where close binary collisions in the presence of the medium are taken into account. It is more convenient to do this than to make a partial summation of terms in the closed-form expression for $\tilde{M}_{11}$. When L_0 is chosen in one of the two ways just discussed, the dressed particle theory appears as a further approximation to the two-body additive theory. This is of course no longer the case when more terms in the geometric series for $\tilde{M}_{11}$ are taken into account. It is also not the case when L_0 is chosen in a different way. For example, the most attractive choice for L_0 is as the one-body additive extension based on Eq. (1). Then $\tilde{G}_0$ is a resolvent operator giving exact propagation in the P_1 space. It is of course dependent on $\tilde{M}_{11}$, which in turn is evaluated using the series involving L_0. This then gives rise to a difficult self-consistent type problem. This procedure is precisely the one used in quantum field theory based on Green's functions.

In classical liquid and plasma theory the use of clusters is physically compelling, at least in treatment of the small-distance aspects of the problem. Our algebraic reformulation shows that one can proceed to an n-body additive approximation with the continued fraction. This takes into account elementary collisions of various types occurring in a medium and does not involve any division of the Liouville operator. However, one has the same type of expression for the residual memory operator $\tilde{M}_{nn}$. Again one is tempted to use the "exact" L_0, leading to a self-consistent problem. But it is more practical to use an L_0 based on the $\tilde{M}_{11}$ computed in the n-body additive approximation, thus avoiding the self-consistency problem. At the $\tilde{M}_{22}$ this procedure is closely related to Mazenko's main working approximation. We will discuss this point in more detail later.

As an illustration we describe a cruder theory. Let $L_0{}^D$ be the primitive dressed L_0 chosen from $P_1 L_0{}^D P_1$. Then an improved L_0 can be chosen as

$$P_1 L_0 P_1 = P_1 L P_1 - P_1 L P_2 \frac{1}{S + L_0{}^D} P_2 L P_1 \tag{25}$$

This expression on the right-hand side has been explicitly evaluated.[4] The improved L_0 is no longer anti-Hermitian, as was $L_0{}^D$. It therefore has an eigenvalue spectrum describing velocity relaxation (as well as Landau damping). So the improved $\tilde{M}_{11} \approx -P_1 L Q_1 (S + \tilde{G}_0) Q_1 L P_1$ has a different behavior in the hydrodynamic regime.

It should be noted that all of the results of this section hold when L is a pseudo-Liouville operator.

3. FUNCTION SPACE AND PROJECTION OPERATORS

We now make the formal scheme more concrete. We have the one-body additive functions

$$N(1) = \sum_{\alpha=1}^{N} \delta(p_\alpha - p_1)\, \delta(q_\alpha - x_1) \tag{26}$$

and the deviations from equilibrium

$$T(1) \equiv \delta N(1) = N(1) - \langle N(1) \rangle, \qquad \langle N(1) \rangle = \rho_0 \phi(p_1) \equiv \rho_0 \phi_1 \tag{27}$$

where $\phi(p_1)$ is a Maxwellian distribution. Actually, one should use the grand ensemble for defining averages. We use the inner product

$$\langle A \mid B \rangle = \int \Phi \, d\Gamma \, A^* B \tag{28}$$

However, in the spatial form with which we work, A and B are real functions.

The projection operator for the functions $T(1)$ is written as

$$P_1 = |T(\bar{1})\rangle\langle T(\bar{1})|T(\bar{1}')\rangle^{-1}\langle T(\bar{1}')| \equiv |T(\bar{1})\rangle\langle \bar{1}|Z_1|\bar{1}'\rangle\langle T(\bar{1}') \tag{29}$$

The bars over variables mean integrations. The inverse Z_1 is defined by the equations

$$\begin{aligned} \langle T(1)|T(\bar{2})\rangle\langle \bar{2}|Z_1|3\rangle &= \delta(1-3) \\ \langle 1|Z_1|\bar{2}\rangle\langle T(\bar{2})|Z_1|T(3)\rangle &= \delta(1-3) \end{aligned} \tag{30}$$

Using

$$\begin{aligned} \langle T(1) \mid T(2) \rangle &= \langle N(12) \rangle - \langle N(1) \rangle \langle N(2) \rangle + \delta(1-2) \langle N(1) \rangle \\ &= \{\rho_2(x_1 x_2) - \rho_0{}^2\} \phi_1 \phi_2 + \delta(1-2)\rho_0 \end{aligned} \tag{31}$$

where $\rho_2(x_1 x_2)$ is the static pair distribution, we have the well-known result[15]

$$\langle 1|Z_1|2\rangle = [\delta(1-2)/\rho_0 \phi_1] - C(x_1 - x_3) \tag{32}$$

Here $C(x)$ is the direct correlation function, defined by the integral equation

$$h(x) = C(x) + \rho_0 \int C(|x - x'|)h(x')\,dx' \qquad (33)$$
$$h(x) = [\rho_2(x)/\rho_0^2] - 1$$

The next step is to introduce two-body additive functions

$$N(12) = \sum_{\alpha \neq \beta} \delta(p_\alpha - p_1)\,\delta(p_\beta - p_2)\,\delta(q_\alpha - x_1)\,\delta(q_\beta - x_2) \qquad (34)$$

and deviations $\delta N(12) = N(12) - \langle N(12)\rangle$. In order to define P_2, we want the two-body functions that are orthogonal to the one-body additive functions. Let

$$T(12) = \delta N(12) - \Delta(12\bar{3})\,\delta N(\bar{3}) \qquad (35)$$

Since $T(12)$ is defined in terms of deviations, its equilibrium average is zero. To fix $\Lambda(123)$ we require, for all values of p_3, x_3,

$$\langle T(12)|\delta N(3)\rangle = 0 \qquad (36)$$

Hence

$$\begin{aligned}\Lambda(123) &= \langle \delta N(12)|\delta N(\bar{4})\rangle\langle\bar{4}|Z_1|3\rangle \\ &= \{\langle N(12\bar{4})\rangle - \langle N(12)\rangle\langle N(\bar{4})\rangle\}\langle\bar{4}|Z_1|3\rangle \\ &\quad + \langle N(12)\rangle\{\langle 1|Z_1|3\rangle + \langle 2|Z_1|3\rangle\}\end{aligned} \qquad (37)$$

Explicitly,

$$\Lambda(123) = K(x_1x_2x_3)\phi_1\phi_2 + [\rho_2(x_1x_2)/\rho_0][\phi_2\delta(1-3) + \phi_1\delta(2-3)] \qquad (38)$$

where

$$\begin{aligned}K(x_1x_2x_3) &= [\rho_3(x_1x_2x_3)/\rho_0] - \rho_2(x_1x_2) - \int \rho_3(x_1x_2x_4)C(x_4 - x_3)\,dx_4 \\ &\quad + \rho_2(x_1x_2)\rho_0 \int C(x_4 - x_3)\,dx_4 \\ &\quad - \rho_2(x_1x_2)[C(x_3 - x_1) + C(x_3 - x_2)]\end{aligned} \qquad (39)$$

Before going on to the three-body space, we first find the four-point static correlation function $\langle T(12)|T(34)\rangle$ and the two-body projection operator P_2. The four-point static correlation has a simple structure. We write it as the sum of three parts A, B, and C, with different momentum dependences:

$$\langle T(12)|T(34)\rangle_A = \phi_1\phi_2\rho_2(x_1, x_2)[\delta(3-1)\delta(4-2) + \delta(3-2)\delta(4-1)] \qquad (40)$$

$$\begin{aligned}\langle T(12)|T(34)\rangle_B &= \phi_1\phi_2\phi_3[\delta(4-1) + \delta(4-2)] \\ &\quad \times \left[\rho_3(x_1x_2x_3)\frac{-\rho_2(x_1x_2)\rho_2(x_3x_4)}{\rho_0}\right] + 3 \rightleftarrows 4\end{aligned} \qquad (41)$$

$$\langle T(12)|T(34)\rangle_C = \phi_1\phi_2\phi_3\phi_4\mathcal{S}(x_1x_2x_3x_4) \qquad (42)$$

where $\mathscr{S}(x_1x_2x_3x_4)$ is given in Appendix A as Eq. (A.7). The A sector is of order ρ_0^2, the B sector is of order ρ_0^3, and the C sector is of order ρ_0^4. The four-point static correlation function is all that we need for the calculation of the IBA dressed particle memory function.

The next step is to introduce a set of three-body additive functions orthogonal to $N(1)$ and $T(12)$. Thus

$$T(123) = \delta N(123) - \Lambda(123|\bar{4}\bar{5})T(\bar{4}\bar{5}) - \Lambda(123|\bar{4})\,\delta N(\bar{4}) \tag{43}$$

Here

$$\Lambda(123|4) = \langle \delta N 123)|\delta N(\bar{5})\rangle\langle \delta N(\bar{5})|\delta N(4)\rangle^{-1} \tag{44}$$

and

$$\Lambda(123|45) = \langle \delta N(123)|T(\bar{6}\bar{7})\rangle\langle T(\bar{6}\bar{7})|T(45)\rangle^{-1} \tag{45}$$

This requires a knowledge of the two-body inverse that occurs in the projector

$$P_2 = |T(\bar{1}\bar{2})\rangle\langle T(\bar{1}\bar{2})|T(\bar{3}\bar{4})\rangle^{-1}\langle T(\bar{3}\bar{4})| \tag{46}$$

$$\langle 12|Z_2|34\rangle \equiv \langle T(12)|T(34)\rangle^{-1} \tag{47}$$

It obeys the equation

$$\langle 12|Z_2|\bar{3}\bar{4}\rangle\langle T(\bar{3}\bar{4})|T(56)\rangle = \tfrac{1}{2}[\delta(5-1)\delta(6-2) + \delta(5-2)\delta(6-1)] \tag{48}$$

The two-body projection operator is determined from the equation

$$\begin{aligned}\langle 12|Z_2|78\rangle &+ [1 + P(12)]F(x_1 - x_2\|x_1 - \bar{x}_3)\phi_3\rho_2(x_1\bar{x}_3)\langle \bar{3}1|Z_2|78\rangle \\ &+ \phi_3\phi_4\frac{\mathscr{S}(x_1x_2\bar{x}_3\bar{x}_4)}{2\rho_2(x_1x_2)}\langle 34|Z_2|78\rangle \\ &= \frac{\delta(7-1)\delta(8-2) + \delta(7-2)\delta(8-1)}{4\rho_2(x_1x_2)\phi_1\phi_2}\end{aligned} \tag{49}$$

where

$$F(x_1 - x_2\|x_1 - x_3) = \frac{\rho_3(x_1x_2x_3)}{\rho_2(x_1x_2)\rho_2(x_1x_3)} - \frac{1}{\rho_0} \tag{50}$$

and $P(12)$ is a permutation operator.

Z_2 has A, B, C parts with momentum structure like the parts of $\langle T(12)|T(34)\rangle$. We have

$$\langle 12|Z_2|34\rangle_{\rm A} = \frac{\delta(3-1)\delta(4-2) + \delta(3-2)\delta(4-1)}{4\rho_2(x_1x_2)\phi_1\phi_2} \tag{51}$$

$$\langle 12|Z_2|34\rangle_{\rm B} = [1 + P(12)][1 + P(34)]B(x_1 - x_2\|x_1 - x_3)[\delta(1-4)/\phi_1] \tag{52}$$

where B obeys the integral equation

$$B(y_2\|y_5) = -(1/4)F(y_2\|y_5) + \int F(y_2\|y_3)\rho_2(y_3)B(y_3\|y_5)\,dy_3 \tag{53}$$

The quantity B has the low-density behavior ρ_0^{-1} for hard spheres. Finally,

$$\langle 12|Z_2|34\rangle_C \equiv \langle x_1x_2|U|x_3x_4) \tag{54}$$

The purely spatial function U obeys the integral equation

$$\begin{aligned}
&\langle x_1x_2|U|x_7x_8\rangle + \frac{\mathscr{S}(x_1x_2\bar{x}_3\bar{x}_4)}{2\rho_2(x_1x_2)}\langle \bar{x}_3\bar{x}_4|U|x_7x_8\rangle \\
&\quad + 2[1 + P(12)]F(x_1 - x_2\|x_1 - \bar{x}_3)\rho_2(x_1x_2)\langle \bar{x}_3x_1|U|x_7x_8\rangle \\
&= \frac{-\mathscr{S}(x_1x_2x_7x_8)}{4\rho_2(x_1x_2)\rho_2(x_7x_8)} - [1 + P(\bar{3}\bar{4})][1 + P(78)] \\
&\quad \times \frac{\mathscr{S}(x_1x_2x_8\bar{x}_4)}{2\rho_2(x_1x_2)} B(x_8 - \bar{x}_4\|x_8 - x_7) \\
&\quad -2\,[1 + P(12)]F(x_1 - x_2\|x_1 - \bar{x}_3)\rho_2(x_1\bar{x}_3)B(\bar{x}_3 - x_1\|\bar{x}_3 - x_7)
\end{aligned} \tag{55}$$

Since $\mathscr{S}$ is proportional to ρ_0^4, the quantity U has $\rho_0^0 \sim 1$ behavior at low density.

An expression for $\Lambda(123|45)$ and thus for $T(123)$ can be obtained by combining the above relations with the expression for $\langle \delta N(123)|T(67)\rangle$ given in Appendix A.

4. AMPLITUDES AND DISTRIBUTION FUNCTIONS

We now develop the theory along the elementary line of thought of *I*, i.e., from a "Schrödinger" picture. We write the N-body distribution function $\hat{F}_N(t)$ as

$$\hat{F}_N(t) = |T(\bar{1})\rangle\hat{A}_1(1;t) + |T(\bar{1}\bar{2})\rangle\hat{A}_2(\bar{1}\bar{2};t) + |T(\bar{1}\bar{2}\bar{3})\rangle\hat{A}_3(\bar{1}\bar{2}\bar{3};t)\rangle + \cdots \tag{56}$$

with initial condition $A_n(t = 0) \equiv A_n^0$.

The amplitudes $\hat{A}_1(1;t)$, $\hat{A}_2(12;t)$,... have the properties

$$\begin{aligned}
&\langle T(1)|T(\bar{1}')\rangle\hat{A}_1(\bar{1}';t) \\
&\quad = \langle T(1)|P_1\hat{F}_N(t)\rangle = \langle T(1)|e^{-Lt}F_N^0 \\
&\quad = \langle T(1)|e^{-Lt}|T(\bar{1}')\rangle A_1^0(\bar{1}') + \langle T(1)|e^{-Lt}|T(\bar{1}'\bar{2}')\rangle A_2^0(\bar{1}'\bar{2}') + \cdots
\end{aligned} \tag{57}$$

$$\begin{aligned}
&\langle T(12)|T(\bar{1}'\bar{2}')\rangle\hat{A}_2(\bar{1}'\bar{2}';t) \\
&\quad = \langle T(12)|\hat{F}_N(t)\rangle \\
&\quad = \langle T(12)|e^{-Lt}|T(\bar{1}')\rangle A_1^0(\bar{1}') + \langle T(12)|e^{-Lt}|T(\bar{1}'\bar{2}')\rangle A_2^0(\bar{1}'\bar{2}') + \cdots
\end{aligned} \tag{58}$$

Thus the amplitudes involve superpositions of correlation functions with weights depending on the initial distribution $F_N{}^0$. The correlation functions $\langle T(12)|e^{-Lt}|T(1'2')\rangle$ are just Mazenko's correlation functions.

The theory is most easily expressed in terms of these amplitudes. We will use the notation

$$\langle T(12)|L|T(34)\rangle \equiv \langle 12|L|34\rangle, \quad \text{etc.} \tag{59}$$

For clarity we underline with a wiggle arguments that are not summed over. In that case, bars indicating summation are omitted. From the Laplace transform of the Liouville equation we have

$$S\langle T(\underset{\sim}{1})|T(1')\rangle\tilde{A}_1(1') + \langle\underset{\sim}{1}|L|1'\rangle\tilde{A}_1(1') + \langle\underset{\sim}{1}|L|1'2'\rangle\tilde{A}_2(1'2') = \langle T(1)|T(\underset{\sim}{1'})\rangle A_1{}^0(1') \tag{60}$$

$$\langle\underset{\sim}{12}|S+L|1'2'\rangle\tilde{A}_2(1'2') + \langle\underset{\sim}{12}|L|1'2'3'\rangle\tilde{A}_3(1'2'3') = \langle T(\underset{\sim}{12})|T(1'2')\rangle A_2{}^0(1'2') - \langle\underset{\sim}{12}|L|1'\rangle\tilde{A}_1(1') \tag{61}$$

etc. Using the inverses, we have the explicit forms

$$\begin{aligned} &S\tilde{A}_1(\underset{\sim}{1^*}) + \langle T(\underset{\sim}{1^*})|T(1)\rangle^{-1}\langle 1|L|1'\rangle\tilde{A}_1(1') \\ &\quad + \langle T(\underset{\sim}{1^*})|T(1)\rangle^{-1}\langle 1|L|1'2'\rangle\tilde{A}_2(1'2') = A_1{}^0(\underset{\sim}{1^*}) \end{aligned} \tag{62}$$

$$\begin{aligned} &S\tilde{A}_2(\underset{\sim}{1^*}\underset{\sim}{2^*}) + \langle T(\underset{\sim}{1^*}\underset{\sim}{2^*})|T(12)\rangle^{-1}\langle 12|L|1'2'\rangle\tilde{A}_2(1'2') \\ &\quad + \langle T(\underset{\sim}{1^*}\underset{\sim}{2^*})|T(12)\rangle^{-1}\langle 12|L|1'2'3'\rangle\tilde{A}_3(1'2'3') \\ &\quad = A_2{}^0(\underset{\sim}{1^*}\underset{\sim}{2^*}) - \langle T(\underset{\sim}{1^*}\underset{\sim}{2^*})|T(12)\rangle^{-1}\langle 12|L|1'\rangle\tilde{A}_1(1') \end{aligned} \tag{63}$$

We now introduce one-body operators L_0 by the definition

$$L_0|N(\underset{\sim}{1})\rangle = |N(1')\rangle\langle 1'|R|\underset{\sim}{1}\rangle \tag{64}$$

i.e., operating on a one-body additive function, it produces a sum of one-body additive functions. In the two-body space its action is

$$L_0|N(\underset{\sim}{1})N(\underset{\sim}{2})\rangle = |N(1')N(\underset{\sim}{2})\rangle\langle 1'|R|\underset{\sim}{1}\rangle + |N(\underset{\sim}{1})N(2')\rangle\langle 2'|R|\underset{\sim}{2}\rangle \tag{65}$$

with an obvious extension to the n-body space. In V we defined[4] such operators in a functional notation. This is not convenient for the hard-sphere case. We thus have the matrix elements

$$\begin{aligned} \langle T(1)|L_0|T(1')\rangle &= \langle T(1)|T(\bar{2})\rangle\langle\bar{2}|R|1'\rangle \\ \langle T(12)|L_0|T(1'2')\rangle &= \langle T(12)|T(\bar{3}2')\rangle\langle\bar{3}|R|1'\rangle \\ &\quad + \langle T(12)|T(1'\bar{3})\rangle\langle\bar{3}|R|2'\rangle \end{aligned} \tag{66}$$

etc.

We now write down the amplitude equations when we have made the separation $L = L_0 + L_1$. We have

$$\begin{aligned} &S\tilde{A}_1(\underset{\sim}{1}^*) + \langle \underset{\sim}{1}^*|R|1'\rangle \tilde{A}_1(1') + \langle T(\underset{\sim}{1}^*)|T(1)\rangle^{-1}\langle 1|L_1|1'\rangle \tilde{A}_1(1') \\ &\quad + \langle T(\underset{\sim}{1}^*)|T(1)\rangle^{-1}\langle 1|L|1'2'\rangle \tilde{A}_2(1'2') = A_1{}^0(\underset{\sim}{1}^*) \end{aligned} \tag{67}$$

$$\begin{aligned} &S\tilde{A}_2(\underset{\sim}{1}^*\underset{\sim}{2}^*) + \langle \underset{\sim}{1}^*|R|1'\rangle \tilde{A}_2(1'\underset{\sim}{2}^*) + \langle \underset{\sim}{2}^*|R|1'\rangle \tilde{A}_2(1'\underset{\sim}{1}^*) \\ &\quad + \langle T(\underset{\sim}{1}^*\underset{\sim}{2}^*)|T(12)\rangle^{-1}\langle 12|L_1|1'2'\rangle \tilde{A}_2(1'2') \\ &\quad + \langle T(\underset{\sim}{1}^*\underset{\sim}{2}^*)|T(12)\rangle^{-1}\langle 12|L|1'2'3'\rangle \tilde{A}_3(1'2'3') \\ &\quad = A_2{}^0(\underset{\sim}{1}^*\underset{\sim}{2}^*) - \langle T(\underset{\sim}{1}^*\underset{\sim}{2}^*)|T(12)\rangle^{-1}\langle 12|L|3\rangle \tilde{A}_1(3) \end{aligned} \tag{68}$$

The n-body additive approximation effects a truncation to a closed set of equations by neglecting the amplitude $\tilde{A}_{n+1}$ entirely. The dressed particle correction to the one-body additive theory calculates $\tilde{A}_2$ by neglecting the term involving $\langle 12|L_1|1'2'\rangle$ after neglecting $\tilde{A}_3$. The equation for $\tilde{A}_2$ then involves the sum of operators that act separately on the two arguments of $\tilde{A}_2(1'2')$. This is precisely what happens in the ordinary BBGKY hierarchy when it is written in terms of cumulant distribution functions.[6] Here it is a consequence of the introduction of a one-body additive part of L. In both cases the doublet equation is explicitly soluble in the time domain in terms of the solution of the singlet equation. The $\hat{A}_2(1'2'; t)$ can be inserted into the equation for $\hat{A}_1(1^*; t)$ to yield a Balescu-type singlet equation.

In the primitive dressed particle approximation L_0 is chosen so that

$$\langle 1|L|1'\rangle = \langle 1|L_0|1'\rangle, \qquad R(1^*|1') = \langle T(1^*)|T(\bar{1})\rangle^{-1}\langle \bar{1}|L|1'\rangle \tag{69}$$

and

$$\langle 1^*|L_1|1'\rangle = 0 \tag{70}$$

To obtain the dressed particle correction to the two-body additive approximation, we write an equation for $\tilde{A}_3$ and neglect the $\tilde{A}_4$ amplitude together with the term $\langle T(1^*2^*3^*)|T(123)\rangle^{-1}\langle 123|L_1|1'2'3'\rangle \tilde{A}_3(1'2'3')$. Again this is an explicitly soluble equation for $\hat{A}_3(t)$, involving the R operators. At this level the R operator is chosen so that

$$\langle 1|R|2\rangle \tilde{A}_1(2) = \langle 1|L|2\rangle \tilde{A}_1(2) + \langle 1|L|1'2'\rangle \tilde{B}_2(1'2') \tag{71}$$

where $\tilde{B}_2(1'2')$ is the two-body additive $\tilde{A}_2(1'2')$ with $A_2{}^0(1'2')$ set equal to zero. This procedure is more conveniently expressed in the projection formalism.

We now discuss the relation of this approach to one involving ordinary singlet, doublet, etc., time distributions and ordinary cumulants.[6] These distributions (i.e., deviations from equilibrium) are defined as

$$\begin{aligned} \hat{F}_1(1) &= \langle \delta N(1)|\hat{F}_N(t)\rangle \\ \hat{F}_2(12) &= \langle \delta N(12)|\hat{F}_N(t)\rangle \\ \hat{F}_3(123) &= \langle \delta N(123)|\hat{F}_N(t)\rangle \end{aligned} \tag{72}$$

We thus have the connections

$$\begin{aligned} \hat{F}_1(\underset{\sim}{1}) &= \langle \delta N(\underset{\sim}{1}) | \delta N(1') \rangle \hat{A}_1(1') \\ \hat{F}_2(\underset{\sim}{12}) &= \langle \delta N(\underset{\sim}{12}) | \delta(\hat{N}1') \rangle \hat{A}_1(1') + \langle T(\underset{\sim}{12}) | T(1'2') \rangle \hat{A}_2(1'2') \\ \hat{F}_3(\underset{\sim}{123}) &= \langle \delta N(\underset{\sim}{123}) | \delta N(1') \rangle \hat{A}_1(1') + \langle \delta N(\underset{\sim}{123}) | T(1'2') \rangle \hat{A}_2(1'2') \\ &\quad + \langle T(\underset{\sim}{123}) | T(1'2'3') \rangle \hat{A}_3(1'2'3') \end{aligned} \tag{73}$$

These equations terminate because $\delta N(12)$ is orthogonal to $\bar{T}(123)$, etc. We can invert the relations to find

$$\begin{aligned} \hat{A}_1(\underset{\sim}{1}) &= \langle \delta N(\underset{\sim}{1}) | \delta N(1') \rangle^{-1} \hat{F}_1(1') \\ \hat{A}_2(\underset{\sim}{12}) &= \langle T(\underset{\sim}{12}) | T(1'2') \rangle^{-1} [\hat{F}_2(1'2') - \langle \delta N(1'2') | \delta N(3) \rangle \\ &\quad \times \langle \delta N(3) | \delta N(4) \rangle^{-1} \hat{F}_1(4)] \\ \hat{A}_3(\underset{\sim}{123}) &= \langle T(\underset{\sim}{123}) | T(1'2'3') \rangle^{-1} [\hat{F}_3(1'2'3') - \langle \delta N(1'2'3') | T(45) \rangle \hat{A}_2(45) \\ &\quad - \langle \delta N(1'2'3') | \delta N(4) \rangle \hat{A}_1(4)] \end{aligned} \tag{74}$$

For the usual distribution functions we have the time-dependent BBGKY hierarchy

$$\begin{aligned} S\hat{F}_1(1) + \langle \delta N(1) | LF_N \rangle &= F_1{}^0(1) \\ S\hat{F}_2(12) + \langle \delta N(12) | L\tilde{F}_N \rangle &= F_2{}^0(12) \end{aligned} \tag{75}$$

When written out in detail using

$$L = \sum_\alpha \frac{p_\alpha}{m} \frac{\partial}{\partial q_\alpha} - \sum \frac{\partial V}{\partial q_\alpha} \frac{\partial}{\partial p_\alpha} \tag{76}$$

the hierarchy involves the bare potentials.

To establish the meaning of our truncation schemes in the context of this hierarchy most directly, one can use the inversion relations [Eq. (74)]. Thus the one-body additive approximation corresponds to taking the first equation of the hierarchy and to putting

$$\hat{F}_2(1'2') \simeq \langle \delta N(1'2') | \delta N(3) \rangle \langle \delta N(3) | \delta N(4) \rangle^{-1} \hat{F}_1(4) \tag{77}$$

In this form the bare potential occurs, and a use of the equilibrium hierarchy is required to establish a fully renormalized form. In higher approximations a similar procedure is followed. This was the point of view in I and IV. At the two-body additive level, we exhibited in IV[17] the self-contained equation for $\hat{F}_2(12)$ involving $\hat{F}_1(1)$ in inhomogeneous terms.

The most effective treatment of the BBGKY hierarchy involves introduction of cumulants. These are needed to treat clearly the asymptotic properties of the distribution functions at large separations. When one rewrites the hierarchy in terms of cumulants, one-body additive operators similar to our $\langle 1 | R | 1' \rangle$ appear naturally. This is the key to the treatments of Balescu[6,14] for plasmas and of Ernst and Dorfman[10] and Pomeau[16] for the hard-sphere chain.

Some characteristic features are already present at the one-body additive level. Neglect of the ordinary cumulant $\hat{D}(12)$ gives the ordinary Vlasov equation, but there is already a difficulty with the initial conditions. The assumption involves putting $\hat{D}(12)$ equal to zero at all times including at $t = 0$. But the initial preparation in a light scattering or external field experiment involves a microscopic preparation of the Liouville distribution in which, for example, $A_1{}^0 \neq 0$, $A_2{}^0 = A_3{}^0 = \cdots = 0$. The one-body additive approximation requires a $\hat{D}(12)$ that is nonzero at $t = 0$ to fit the initial conditions. This relation between $\hat{D}(12)$ and $\hat{F}_1(1)$ is taken to be the same for all t as $\hat{F}_1(1)$ varies with time. At large spatial separations $\hat{D}(12)$ vanishes. So the truncation improves the short-time, short-distance behavior without violating the long-time, large-separation behavior. This gives rise to the modified Vlasov equation.[15]

In the theory that works with the usual hierarchy one frequently argues that a suitable initial condition implying "prior chaos" is to take $\hat{D}(12, t = 0) = 0$. Apart from the lack of clarity of the meaning of this condition in operational terms, one obtains the Vlasov kernel in place of the modified term involving the direct correlation function in the singlet equation. Thus the short-distance as well as short-time behavior is defective. It should be noted that this trouble persists at higher levels of approximation. Thus if one keeps two equations in the BBGKY chain and takes $\hat{D}(123, t) = 0$, one again violates a microscopic preparation since for such a preparation $\hat{D}(123, t = 0) \neq 0$ even if only $A_1{}^0 \neq 0$. One obtains a doublet equation which is badly behaved at small particle separations for strong short-range potentials. After solving for the doublet cumulant and inserting it into the singlet equation we obtain a collision kernel. This does not correct the Vlasov mean field term. In addition the one-body additive part of the doublet operator involves the Vlasov operators, so that the kernel itself is defective at small times and distances. We conclude that the time correlation formulation is superior at all levels, and that there is a one to one correspondence between the two formulations. The differences are intrinsic, and the defects of the BBGKY treatments are not remedied by standard improved truncations of the Kirkwood type. As was shown in IV,[17] the truncations needed in the usual hierarchy to get good short-time behavior (e.g., $A_3 = 0$) are nonlocal and unnatural from the BBGKY point of view. However, we are not here arguing against the usual treatment for the study of large-distance and long-time behavior.

In this connection it should be noted that $\hat{A}_2(12)$ has the same spatial asymptotic behavior as the cumulant $\hat{D}(12)$ (i.e., goes to zero for large separations). So the amplitude method may be thought of as the introduction of a new type of cumulant, better suited to the treatment of small distances.

5. KINETIC EQUATIONS

Equations based on the time correlation point of view take somewhat different forms for smooth potentials and for hard cores. For smooth potentials we find forms in which the bare potential is eliminated. This is immediate by noting the identity,[11] for any two phase-space functions,

$$\int \Phi\, d\Gamma\, A^*(p_1,\ldots,q_N) L B(p_1,\ldots,q_N) = \kappa T \int \Phi\, d\Gamma \sum_{\alpha=1}^{N} \left(\frac{\partial A^*}{\partial p_\alpha}\frac{\partial B}{\partial q_\alpha} - \frac{\partial A^*}{\partial q_\alpha}\frac{\partial B}{\partial p_\alpha}\right) \tag{78}$$

Thus it is not advisable to split L into a free streaming part $L_0{}^0$ and an interaction term. The matrix elements of L between the basic functions of phase space are simpler, and only involve static correlation functions (cf. Appendix B). This makes it unnecessary to use the equilibrium hierarchy explicitly. Thus the one-body additive approximation uses

$$\begin{aligned} \langle 1^*|L|1\rangle &= \rho_0\phi(p_1{}^*)\frac{p_1{}^*}{m}\,\delta(1-1^*)\frac{\partial}{\partial x_1} \\ \langle 1^*|L|\bar{1}'\rangle\langle\bar{1}'|Z_1|2\rangle &= \rho_0\phi(p_1{}^*)\frac{p_1{}^*}{m}\frac{\partial}{\partial x_1{}^*}\langle 1^*|Z_1|2\rangle \end{aligned} \tag{79}$$

We find the well-known singlet equation[15] from

$$\begin{aligned} &\left(S + \frac{p_1{}^*}{m}\frac{\partial}{\partial x_1{}^*}\right)\tilde{F}_1(1^*) - \rho_0\phi(p_1{}^*)\frac{p_1{}^*}{m}\frac{\partial}{\partial x_1{}^*}\,C(x_1{}^* - \bar{x}_2)\tilde{F}_1(\bar{2}) \\ &\quad + \langle 1^*|\tilde{M}_{11}|\bar{1}'\rangle\langle\bar{1}'|Z_1|\bar{2}\rangle\tilde{F}_1(\bar{2}) = F_1{}^0 \end{aligned} \tag{80}$$

when we neglect the memory function $\tilde{M}_{11}$.

For hard cores we use the separation $L_- = L_0{}^0 - L_-^{(1)}$, where $L_+^{(1)}$ is a pseudo-Liouville operator (cf. Appendix C). The contribution of $L_0{}^0$ to the singlet is

$$\begin{aligned} &\langle 1^*|L_0{}^0|\bar{1}\rangle\langle\bar{1}|Z_1|\bar{2}\rangle\tilde{F}_1(\bar{2}) \\ &\qquad = \frac{p_1{}^*}{m}\frac{\partial\tilde{F}_1(1^*)}{\partial x_1{}^*} + \frac{\rho_2(x_1{}^*\bar{x}_1)}{\rho_0}\frac{\bar{p}_1}{m}\frac{\partial\tilde{F}_1(\bar{1})}{\partial x_1}\phi(p_1{}^*) \\ &\qquad\quad - \rho_0\frac{p_1{}^*\phi(p_1{}^*)}{m}\,C(x_1{}^* - \bar{x}_2)\frac{\partial\tilde{F}_1(\bar{2})}{\partial x_2} \end{aligned} \tag{81}$$

The second term cancels against part of the interaction, when one uses the equilibrium hierarchy. To calculate the interaction, we note that

$$\begin{aligned} &-\langle \underset{\sim}{1}{}^*|L_-^{(1)}|\bar{1}\rangle\langle\bar{1}|Z_1|\bar{2}\rangle\tilde{F}_1(\bar{2}) \\ &\quad = [\langle N_3(\underset{\sim}{1}{}^*2'3')\rangle - \langle N(\underset{\sim}{1}{}^*)\rangle\langle N(2'3')\rangle]\langle 2'3'|W_{\bar{2}1}|1'\rangle\langle 1'|Z_1|2\rangle\tilde{F}_1(2) \\ &\qquad + 2\langle N_2(\underset{\sim}{1}{}^*3')\rangle\langle \underset{\sim}{1}{}^*3'|W_{\bar{2}1}|1'\rangle\langle 1'|Z_1|2\rangle\tilde{F}_1(2) \end{aligned} \tag{82}$$

The one-body inverse has a delta-function part and a purely spatial part involving the direct correlation function. Since $\int \langle 2'3'|W_{21}|1'\rangle\, dp_1' = 0$, the direct-correlation-function part does not contribute and $\langle 1|Z_1|\bar{2}\rangle\tilde{F}_1(\bar{2})$ may be replaced by $\tilde{F}_1(1)/\rho_0\phi(p_1)$. The first term involves the three-point static function and the quantity $\langle x_2x_3|H|1'\rangle = \iint dp_2'\,dp_3'\phi(p_2')\phi(p_3')\langle 2'3'|W_{\bar{2}1}|1'\rangle$. This quantity is given in Appendix C. We then find for the first term

$$\phi(\underset{\sim}{p_1}^*)\frac{p_1'}{m}\int \frac{\rho_3(x_1^*, x_1', x_3')}{\rho_0}\,\delta(|x_{13}'| - \sigma)\hat{x}_{13}'\,dx_3'\,\tilde{F}_1(1') \tag{83}$$

It combines with the free streaming term and the two terms are eliminated using the equilibrium hierarchy equation

$$\frac{\partial \rho_2(x_1x_3)}{\partial x_1} - \int d\hat{x}_2\delta(|x_{12}| - \sigma)\hat{x}_{12}\rho_3(x_1x_2x_3) = \rho_2(\sigma)\frac{\partial}{\partial x_1}\,\theta(|x_{13}| - \sigma) \tag{84}$$

The second term in Eq. (82) contains the Boltzmann–Enskog operator plus a term arising from the θ functions (cf. Appendixes C and E). We find the LPS–Mazenko[7,8] equation

$$\begin{aligned}\left(S + \frac{p_1^*}{m}\frac{\partial}{\partial x_1^*}\right)\tilde{F}_1(1^*) - \rho_0\frac{p_1^*}{m}\phi(p_1^*)\left[C(x_1^* - \bar{x}_2) + \frac{\rho_2(\sigma)\theta(\sigma - x_{1\bar{2}}^*)}{\rho_0}\right]\\ \times\frac{\partial\tilde{F}(\bar{2})}{\partial x_2} - \rho_2(\sigma)\langle 1^*|\mathscr{B}|2\rangle\frac{\tilde{F}_1(\bar{2})}{\rho_0\phi_2} + \langle 1^*|\tilde{M}_{11}|\bar{2}\rangle\frac{\tilde{F}_1(\bar{2})}{\rho_0\phi(p_2)} = F_1^0(1^*)\end{aligned} \tag{85}$$

The memory function $\tilde{M}_{11}$ will be evaluated in the dressed particle approximation in the next section. The relation between the smooth-potential and hard-sphere cases is discussed by Blum and Lebowitz.[7]

We now write down the explicit form of the equation for the two-particle amplitude $\tilde{A}_2$ for the hard-sphere case. In Eq. (63) we need to evaluate $\langle 1^*2^*|Z_2|\bar{1}\bar{2}\rangle\langle\bar{1}\bar{2}|L|1'2'\rangle$. We use

$$L_-^{(1)}|N(\underset{\sim}{12})\rangle = [1 + P(\underset{\sim}{12})]|N(\underset{\sim}{1}45)\rangle\langle 45|W_{\bar{2}1}|\underset{\sim}{2}\rangle + |N(34)\rangle\langle 34|W_{\bar{2}2}|\underset{\sim}{12}\rangle \tag{86}$$

Furthermore, note that

$$\langle\underset{\sim}{1}^*\underset{\sim}{2}^*|W_{\bar{2}1}|3\rangle\Lambda(123)\tilde{A}_2(12) = [1 + P(12)]\langle\underset{\sim}{1}^*\underset{\sim}{2}^*|W_{\bar{2}1}|1\rangle\frac{\rho_2(x_1x_2)}{\rho_0}\phi(p_2)\tilde{A}_2(12) \tag{87}$$

This gives

$$\begin{aligned}&\left(S + \frac{p_1^*}{m}\frac{\partial}{\partial x_1^*} + \frac{p_2^*}{m}\frac{\partial}{\partial x_2^*}\right)\tilde{A}_2(\underset{\sim}{1}^*\underset{\sim}{2}^*)\\ &\quad - \left\{\langle\underset{\sim}{1}^*\underset{\sim}{2}^*|W_{\bar{2}2}|12\rangle - [1 + P(12)]\langle\underset{\sim}{1}^*\underset{\sim}{2}^*|W_{\bar{2}1}|1\rangle\frac{\rho_2(x_1x_2)}{\rho_0}\phi(p_2)\right\}\tilde{A}_2(12)\\ &\quad - \langle\underset{\sim}{1}^*\underset{\sim}{2}^*|K_{22}|12\rangle\tilde{A}_2(12) - \langle\underset{\sim}{1}^*\underset{\sim}{2}^*|K_{23}|123\rangle\tilde{A}_3(123)\\ &\quad = A_2^0(\underset{\sim}{1}^*\underset{\sim}{2}^*) - \langle\underset{\sim}{1}^*\underset{\sim}{2}^*|Z_2|12\rangle\langle 12|L_-|1'\rangle\tilde{A}_1(1')\end{aligned} \tag{88}$$

Here

$$\langle \underset{\sim}{1}^*\underset{\sim}{2}^*|K_{22}|\underset{\sim}{12}\rangle = \langle \underset{\sim}{1}^*\underset{\sim}{2}^*|Z_2|3^*4^*\rangle[1 + P(\underset{\sim}{12})] \times \langle T(3^*4^*)|N(\underset{\sim}{2}45)\rangle\langle 45|W_{21}^-|\underset{\sim}{1}\rangle \tag{89}$$

$$\langle \underset{\sim}{1}^*\underset{\sim}{2}^*|K_{23}|\underset{\sim}{123}\rangle = \langle \underset{\sim}{1}^*\underset{\sim}{2}^*|Z_2|1'2'\rangle\langle 1'2'|L_-|\underset{\sim}{123}\rangle \tag{90}$$

In the two-body additive approximation we neglect $\tilde{A}_3$. The term W_{22}^- describes isolated encounters, while the W_{21}^- term involves a medium effect ($\sim \rho_0$). However, since we have been forced into a division of L into $L_0{}^0$ and $-L_-^{(1)}$, the term K_{22} contains additional medium effects (and in particular another term of order ρ_0). To simplify these, we need to use the equilibrium hierarchy explicitly.

We now discuss the contributions to the doublet kernel K_{22} according to powers of the density. In $\langle T(12)|N(345)\rangle$ there is a set of terms of order $\rho_0{}^3$. These come from

$$[1 + P(12)][1 + P(34) + P(35)]\ \delta(3 - 1)\ \delta(4 - 2)\langle N_3(125)\rangle$$

Thus the contribution of this type of term to K_{22} (without the premultiplying two-body inverse) is

$$2[1 + P(\underset{\sim}{3}^*\underset{\sim}{4}^*)]\phi(\underset{\sim}{p_3}^*)\phi(p_4^*)\rho_3(\underset{\sim}{x_3}^*\underset{\sim}{x_4}^*x_2)\langle \underset{\sim}{3}^*\underset{\sim}{4}^*|W_{21}^-|1\rangle\phi_2\tilde{A}_2(12) + \rho_3(\underset{\sim}{x_3}^*\underset{\sim}{x_4}^*x_4)\phi_4[\langle 4\underset{\sim}{4}^*|W_{21}^-|1\rangle + \langle 4\underset{\sim}{4}^*|W_{21}^-|\underset{\sim}{3}^*\rangle]\tilde{A}_2(1\underset{\sim}{3}^*) \tag{91}$$

When we premultiply by $\langle 1^*2^*|Z_2|3^*4^*\rangle$ to find K_{22}, the leading term arising from the A sector yields a contribution of order ρ_0, i.e., of the same order as the W_{21}^- term already isolated. Thus to order ρ_0 in the doublet amplitude, just replace 3* by 1* and 4* by 2* and divide by $2\rho_2(x_1{}^*x_2{}^*)\phi(p_1{}^*)\phi H(p_2{}^*)_j$ Note that the analytic structure of the three terms differs. The first involves $\int \phi_2\tilde{A}_2(12)\,dp_2$. The second has a collision operator acting on the full $\tilde{A}_2\,(13^*)$, and the third has a collision operator acting on the function of one argument $\int\int \phi_1 A_2(13^*)\,dp_1\,dx_1$.

The terms of order $\rho_0{}^2$ are of two types. First, there is a contribution from the B part of the two-body inverse acting on the terms just discussed. Second, there is a part involving the $[1 + P(12)][1 + P(34) + P(35)] \times \delta(3\text{–}1)\langle N_4(1245)\rangle$ part of $\langle T(12|N(345)\rangle$. Explicit expressions can be found in Appendix D. We also note in the next section that the leading term in the two-body memory kernel in dressed particle approximation is of order $\rho_0{}^4$. Hence, when premultiplied by the two-body inverse it also yields a term of order $\rho_0{}^2$ in the equation for the two-body amplitude.

For the case of smooth potentials, Eq. (63) for the two-body amplitude $\tilde{A}_2(1^*2^*)$ involves only the kernel $\langle 1^*2^*|Z_2|\bar{1}\bar{2}\rangle\langle\bar{1}\bar{2}|L|1'2'\rangle$, after neglecting the three-particle amplitude. The matrix element $\langle 12|L|1'2'\rangle$ may be determined from the equations in Appendix B, namely (B.13) and (B.14). The A part of the two-body inversion then yields

$$\langle 1^*2^*|Z_2|\bar{1}\bar{2}\rangle_A\langle\bar{1}\bar{2}|L|\bar{1}'\bar{2}'\rangle\tilde{A}_2(\bar{1}'\bar{2}')$$
$$= [L(1^*|2^*) + L(2^*|1^*)]\tilde{A}(1^*2^*) + \frac{1 + P(1^*2^*)}{\rho_2(x_1{}^*x_2{}^*)}$$
$$\times \left[R_3(x_1{}^*x_2{}^*\bar{x}_4)\frac{p_1{}^*}{m}\frac{\partial}{\partial x_1{}^*} + \kappa T\frac{\partial R_3(x_1{}^*x_2{}^*\bar{x}_4)}{\partial x_1{}^*}\frac{\partial}{\partial p_1{}^*}\right]\bar{\phi}_4\tilde{A}_2(1\bar{4}) \tag{92}$$

This is similar to the result of Eq. (40), with the potential of mean field $-\kappa T \ln \rho_2(x_1x_2)$ replacing the bare interaction. The C part contributes

$$\langle \underset{\sim}{1}^*\underset{\sim}{2}^*|Z_2|12\rangle_C\langle 12|L|1'2'\rangle\tilde{A}_2(1'2')$$
$$= -[1 + P(12)]\frac{\partial[U(\underset{\sim}{x}_1{}^*\underset{\sim}{x}_2{}^*x_1x_2)\rho_2^{-1}(x_1x_2)]}{\partial x_1}2\rho_2(x_1x_2)\phi_1\phi_2\frac{p_1}{m}\tilde{A}(12)$$
$$-4\frac{\partial U(\underset{\sim}{x}_1{}^*\underset{\sim}{x}_2{}^*x_1x_2)}{\partial x_1}R_3(x_1x_2x_4)\phi_1\phi_4\frac{p_1}{m}\tilde{A}(14) \tag{93}$$

Finally the B contribution is

$$\langle \underset{\sim}{1}^*\underset{\sim}{2}^*|Z_2|12\rangle_B\langle 12|L|1'2'\rangle\tilde{A}_2(1'2')$$
$$= [1 + P(\underset{\sim}{1}^*\underset{\sim}{2}^*)]2\frac{B(\underset{\sim}{x}_1{}^* - \underset{\sim}{x}_2{}^*\|\underset{\sim}{x}_1{}^* - x_1)}{\phi(\underset{\sim}{p}_1{}^*)}\langle 1\underset{\sim}{1}^*|L|1'2'\rangle\tilde{A}_2(1'2') \tag{94}$$

6. DRESSED-PARTICLE MEMORY OPERATORS

In the dressed particle approximation we have

$$\hat{M}_{nn}(t) = -P_nLQ_ne^{-L_0t}Q_nL_1P_n \tag{95}$$

For the case of hard spheres, L stands for L_-, L_1 for $-L_-^{(1)}$.

There are a number of equivalent but distinct ways of expressing $\hat{M}_{nn}$. We start with the matrix elements of the one-body memory operator

$$\langle \underset{\sim}{1}^*|\hat{M}_{11}|\underset{\sim}{1}\rangle = -\langle \underset{\sim}{1}^*|LQ_1e^{-L_0t}Q_1L_1|\underset{\sim}{1}\rangle \tag{96}$$

since $Q_1L_0|1\rangle = 0$.

We write (cf. Appendix C)

$$L_1|N(\underset{\sim}{1}) = |N(23)\rangle\langle 23|W_{21}|\underset{\sim}{1}\rangle \tag{97}$$

Now e^{-L_0t} acting on an n-body function yields at most an n-body part. The subsequent action of Q_1 rejects lower order parts. Using

$$|N(23)\rangle = |N(2)N(3)\rangle - \delta(2-3)|N(2)\rangle$$
$$e^{-L_0t}|N(\underset{\sim}{1})\rangle \equiv |N(1')\rangle\langle 1'|\hat{\Gamma}|\underset{\sim}{1}\rangle \tag{98}$$
$$e^{-L_0t}|N(\underset{\sim}{2})N(\underset{\sim}{3})\rangle = |N(2')N(3')\rangle\langle 2'|\hat{\Gamma}|\underset{\sim}{2}\rangle\langle 3'|\hat{\Gamma}|\underset{\sim}{3}\rangle$$

we find

$$\langle \underset{\sim}{1}^*|M_{11}|\underset{\sim}{1}\rangle = -\langle \underset{\sim}{1}^*|L|2'3'\rangle\langle 2'|\hat{\Gamma}|2\rangle\langle 3'|\hat{\Gamma}|3\rangle\langle 23|W_{21}|\underset{\sim}{1}\rangle \tag{99}$$

This "mixed" form involves the bare potential once through W_{21}. The factor $\langle 1^*|L|2'3'\rangle$ is expressed in terms of correlation functions for the case of smooth potentials (cf. Appendix B). It involves the one-body inverse, i.e., the direct correlation function.

A second form of $\hat{M}_{11}$ is particularly useful for the case of hard spheres. Here the adjoint $L_+{}^+ = -L_-$ and L_- has the property

$$\langle L_+^{(1)}N(\underset{\sim}{1}^*)| = \langle \underset{\sim}{1}^*|W_{21}^{(+)}|2^*3^*\rangle\langle N(2^*3^*)| \tag{100}$$

Hence

$$\begin{aligned}\langle \underset{\sim}{1}^*|\hat{M}_{11}|\underset{\sim}{1}\rangle = &+\langle \underset{\sim}{1}^*|W_{21}^{(+)}|2^*3^*\rangle\langle N(2^*3^*)|T(2'3')\rangle \\ &\times \langle 2'|\hat{\Gamma}|2\rangle\langle 3'|\hat{\Gamma}|3\rangle\langle 23|W_{21}^{-}|\underset{\sim}{1}\rangle\end{aligned} \tag{101}$$

This involves two factors containing the bare potential. It also involves the one-body inverse in the factor $\langle N(2^*3^*)|T(2'3')\rangle$.

Finally, there is a third, more complicated form, involving only correlation functions, for the case of smooth potentials. We write

$$\begin{aligned}\langle \underset{\sim}{1}^*|\hat{M}_{11}|\underset{\sim}{1}\rangle = &-\langle \underset{\sim}{1}^*|L|2^*3^*\rangle\langle 2^*3^*|Z_2|4^*5^*\rangle\langle 4^*5^*|e^{-L_0 t}|45\rangle \\ &\times \langle 45|Z_2|23\rangle\langle 23|L|\underset{\sim}{1}\rangle\end{aligned} \tag{102}$$

This involves the two-body inverse twice. Using the relation

$$\langle 4^*5^*|e^{-L_0 t}|45\rangle = \langle T(4^*5^*)|T(\bar{4}'\bar{5}')\rangle\langle \bar{4}'|\hat{\Gamma}|4\rangle\langle \bar{5}'|\hat{\Gamma}|5\rangle \tag{103}$$

and the defining relation for the two-body inverse, we find

$$\begin{aligned}&\langle \underset{\sim}{1}^*|\hat{M}_{11}|\underset{\sim}{1}\rangle \\ &\quad = -\tfrac{1}{2}\langle \underset{\sim}{1}^*|L|2'3'\rangle[\langle 2^*|\hat{\Gamma}|4\rangle\langle 3^*|\hat{\Gamma}|5\rangle + \langle 2^*|\hat{\Gamma}|5\rangle\langle 3^*|\hat{\Gamma}|4\rangle] \\ &\qquad \times \langle 45|Z_2|23\rangle\langle 23|L|\underset{\sim}{1}\rangle\end{aligned} \tag{104}$$

For smooth potentials this involves no bare potentials and serves to show that the theory can always be written in renormalized form. The same thing is true of higher order memory functions. However, the price paid here is the introduction of the two-body inverse. These forms are unnecessarily complicated, and we use the first two forms in the calculation of memory functions.

We now turn to the evaluation of the two-body memory function in the dressed particle approximation. The action of L on a two-body additive function produces a three-body and a two-body additive part. Q_2 rejects the two-body part. We can write

$$Q_2 L|T(12)\rangle = Q_2[1 + P(12)]|N(2)N(\bar{3})N(\bar{4})\rangle\langle \bar{3}\bar{4}|W_{21}|1\rangle \tag{105}$$

The action of $e^{-L_0 t}$ produces a part involving the product of three $\hat{\Gamma}$ at the same time. Hence

$$\begin{aligned}\langle \underset{\sim}{1}^*\underset{\sim}{2}^*|\hat{M}_{22}|\underset{\sim}{12}\rangle = &-\langle \underset{\sim}{1}^*\underset{\sim}{2}^*|L|3'4'5'\rangle[1 + P(\underset{\sim}{12})]\langle 3'|\hat{\Gamma}|\underset{\sim}{2}\rangle\langle 4'|\hat{\Gamma}|3\rangle \\ &\times \langle 5'|\hat{\Gamma}|4\rangle\langle 34|W_{21}|\underset{\sim}{1}\rangle\end{aligned} \tag{106}$$

The second form is

$$\begin{aligned}\langle \underset{\sim}{1}^*\underset{\sim}{2}^*|\hat{M}_{22}|\underset{\sim}{12}\rangle &= [1 + P(\underset{\sim}{1}^*\underset{\sim}{2}^*)][1 + P(\underset{\sim}{12})]\langle \underset{\sim}{1}^*|W_{21}^{(+)}|3^*4^*\rangle \\ &\quad \times \langle N(\underset{\sim}{2}^*3^*4^*)T(3'4'5')\rangle\langle 3'|\Gamma|\underset{\sim}{2}\rangle\langle 4'|\Gamma|3\rangle\langle 5'|\Gamma|4\rangle\langle 34|W_{21}^{-}|\underset{\sim}{1}\rangle \qquad (107)\end{aligned}$$

This involves the two-body inverse because of the presence of $T(3'4'5')$.

It is clear that the n-body memory function in the dressed particle approximation can be written down immediately.

The hard-sphere memory function $\hat{M}_{11}$ can be put into an explicit form using the A, B, C separation of the four-point static correlation function according to the momentum. We have

$$\begin{aligned}\langle \underset{\sim}{1}^*|\hat{M}_{11}|\underset{\sim}{1}\rangle_{\rm A} &= 2\langle \underset{\sim}{1}^*|W_{21}^{(+)}|2^*3^*\rangle\phi(p_2^*)\phi(p_3^*)\rho_2(x_2^*x_3^*) \\ &\quad \times \langle 2^*|\Gamma|2\rangle\langle 3^*|\hat{\Gamma}|3\rangle\langle 23|W_{21}^{-}|\underset{\sim}{1}\rangle \qquad (108)\end{aligned}$$

$$\begin{aligned}\langle \underset{\sim}{1}^*|\hat{M}_{11}|\underset{\sim}{1}\rangle_{\rm B} &= 4\langle \underset{\sim}{1}^*|W_{21}^{(+)}|2^*3^*\rangle\phi(p_2^*)\phi(p_3^*)\hat{I}(p_2|x_2' - x_2)\langle 2^*|\Gamma|3\rangle \\ &\quad \times \left[\frac{\rho_3(x_2^*x_3^*x_2') - \rho_2(x_2^*x_3^*)\rho_2(x_2'x_3')}{\rho_0}\right]\langle 23|W_{21}^{-}|\underset{\sim}{1}\rangle \qquad (109)\end{aligned}$$

where

$$\hat{I}(p_2|x_2' - x_2) = \int \langle 2'|\hat{\Gamma}|2\rangle\phi(p_2')\,dp_2' \qquad (110)$$

$$\begin{aligned}\langle \underset{\sim}{1}^*|M_{11}|\underset{\sim}{1}\rangle_{\rm C} &= \langle \underset{\sim}{1}^*|H_+|x_2^*x_3^*\rangle\mathscr{S}(x_2^*x_3^*x_2'x_3') \\ &\quad \times \hat{I}(p_2|x_2' - x_2)\hat{I}(p_3|x_3' - x_3)\langle 23|W_{21}^{-}|\underset{\sim}{1}\rangle \qquad (111)\end{aligned}$$

where

$$\langle 1^*|H_+|x_2^*x_3^*\rangle = \iint \langle 1^*|W_{21}^{(+)}|2^*3^*\rangle\phi(p_2^*)\phi(p_3^*)\,dp_2^*\,dp_3^* \qquad (112)$$

The A contribution is of order ρ_0^2 and that of B is of order ρ_0^3, apart from the density dependence contained in the propagators $\hat{\Gamma}$. The C contributions are of order ρ_0^4 and ρ_0^5. In order to have the kernel acting on the singlet distribution function [cf. Eq. (63)], we must postmultiply by $\langle T(1)|T(\bar{5})\rangle^{-1}F_1(\bar{5})$. The delta-function contribution to the one-body inverse just supplies a multiplicative factor $(1/\rho_0)\bar{F}_1(1)/\phi_1$. The direct correlation function contribution is purely spatial, viz., $-C(\bar{x}_1 - \bar{x}_5)\bar{F}_1(\bar{5})$. Since $\int \langle \dot{2}3|W_{21}|1\rangle\,dp_1 = 0$, there is no contribution from the direct correlation term. Thus the A part of the memory operator contributes a term of order ρ_0, i.e., of the same order as the other terms in the singlet equation.

A key point is of course the choice of the one-body operator L_0. Since it is one-body additive, it is fully defined by the matrix element $\langle 1'|R|1\rangle$ in Eq. (64). The most attractive choice for R is the implicit form, Eq. (1). Thus in the limit of large n, M_{11} evaluated in n-body approximation approaches the exact one-body memory function

$$\langle 1^*|R|1\rangle = \langle 1^*|L|1\rangle + \langle 1^*|M_{11}|1\rangle \tag{113}$$

If M_{11} is evaluated in an approximation where the last memory function is neglected (n-body attractive approximation), the operator L_0 never occurs. This approximation involves only the matrix elements of the full Liouville operator and decomposition is called for. We then have an explicit form for $\langle 1^*|R|1\rangle$ and thus for the propagator $\langle 1^*|\hat{\Gamma}|1\rangle$.

On the other hand, if R is defined as above, using the unknown exact M_{11}, we have a series of exact reformulations of the problem. With $\tilde{G}_0 = (S + L_0)^{-1}$ and Eqs. (12) and (13), i.e., the continued fraction form, together with Eq. (24), namely

$$\tilde{M}_{nn} = -P_n L Q_n \frac{1}{1 + \tilde{G}_0 Q_n L_1 Q_n} \tilde{G}_0 Q_n L P_n$$

an approximation to $\tilde{M}_{nn}$ leads to a self-consistent evaluation of $\tilde{M}_{11}$.

A scheme involving, for example, the determination of $\langle 1^*|R|1\rangle$ from

$$P_1 L_0 P_1 \cong P_1 L P_1 - P_1 L Q_1 \frac{1}{S + L_0} Q_1 L P_1 \tag{114}$$

leads to an improvement over the simple one-body dressed particle theory since L_0 will have collisional damping properties. However, even with the self-consistent evaluation of R, not enough attention is paid to binary collisions. Thus to make the smooth potential case approach the hard-sphere results, $\tilde{M}_{11}$ must be evaluated in at least two-body additive approximation and the resulting $\tilde{R}$ used to evaluate $\tilde{M}_{22}$ in dressed particle approximation. This leads to an improved $\tilde{M}_{11}$. The self-consistent approach appears to be impracticable, although it may play a role in general arguments.

This line of argument leads to the suggestion that for the hard-sphere case the two-body memory function should also be evaluated with an L_0 that is determined by an $\tilde{M}_{11}$ evaluated in the two-body additive approximation.

Finally, we discuss the relationship between $\langle 1|\hat{\Gamma}|2\rangle \equiv \langle 1|e^{-L_0 t}|2\rangle$ and $\langle 1|\tilde{R}|2\rangle = \langle T(1)|T(\bar{1}')\rangle^{-1}\langle \bar{1}'|L_0|2\rangle$. The argument is the same as in our dressed particle paper.[4] We have the differential equation

$$d\hat{\Gamma}/dt = -L_0\hat{\Gamma}(t) \qquad \text{with} \quad \hat{\Gamma}(0) = 1 \tag{115}$$

The Laplace transform is

$$(S + L_0)\tilde{\Gamma}(S) = 1 \tag{116}$$

For smooth potentials, with L_0 the modified Vlasov operator, the equation is exactly soluble. For hard spheres when L_0 is the LPS operator, one needs to know the Green's function for the linearized Boltzmann–Enskog equation. The additional mean field term in L_0 has a separable character, so that, as shown by LPS[7] and Sykes,[9] the Green's function for L_0 can be written explicitly in terms of the Green's function for the Boltzmann–Enskog equation. In more sophisticated choices of L_0 the only simplifying features are translational invariance and the requirement that L_0 have suitable hydrodynamic consequences.

7. SUMMARY AND CONCLUSIONS

We would like to stress the extreme simplicity of the theory from the methodological point of view. Classical many-body theory for processes occurring near absolute equilibrium is analyzed by constructing a symmetric function basis for phase space. The key point is that orthogonality of the functions is defined with respect to the exact Gibbs equilibrium distribution. The construction is made by a Gram Schmidt process, based on the notion of n-body additive functions as the way to choose successive functions. Orthogonalization is explicitly achieved for functions in different spaces. No attempt is made to make the functions belonging to a given space P_n orthogonal to each other. One then sets up the amplitude representation of the Liouville equation. The solution of these equations is equivalent to a diagonalization problem, which in fact would yield an orthogonal, complete basis for P_n. For example at the one-body additive level, Zwanzig[15] analyzed the modified Vlasov equation in terms of van Kampen eigenfunctions. However, in practice, it is not necessary to do this explicitly. The inverses in the projection operators maintain consistency.

This is all completely in accord with the most standard procedures of mathematical physics, and the theory then "plays itself." At first sight it is disturbing that the equations appear unavoidably complicated because of the appearance of high-order static correlation functions, even after simplifications have been effected by using the equilibrium hierarchy. The main reason for this is that the theory is accurate at short times. One uses precise, microscopic initial conditions needed to analyze time-dependent correlation functions. Then, already at $t = 0$, all of the higher order normal distribution functions and ordinary cumulants are nonzero. While one can simplify equations by neglecting these cumulants (within the context of some parameter expansion), the results are limited by the $t = 0$ inaccuracy.

We have set down the theory in terms of integrodifferential equations, retaining all terms. In the solution of problems, for example, in the low-density limit, it is tempting to neglect most of the terms. Caution is required, however, for there are terms of different analytic structure. They play different roles in determining the behavior of phenomena in different time, space, or momentum domains. A safer procedure is to retain the leading terms for each distinct analytic structure. We have adopted the traditional viewpoint toward the computation of observable quantities. One first sets up (perhaps very complicated) integrodifferential equations governing the quantities, which may include other quantities not of immediate interest. Then one focuses on suitable approximation schemes for solving the equations. This is of course the situation with the ordinary Boltzmann equation. The equations are equivalent to the summation of classes of diagrams in methods that aim directly at the computation of the observable quantities.

It seems that for low to moderate densities the three-body additive approximation contains almost all known results regarding short-time, hydrodynamic and long-time behavior. Naturally, to the extent that, for example, "irreducible" three- or four-body collision sequences (cf. Sengers[(18)]) are important, one must keep amplitudes $\tilde{A}_n$ of requisite order. The medium effects that are taken into account in the present treatment can at best diminish, without ever annulling the effects of such collision sequences.

The treatment of the hard-sphere problem using pseudo-Liouville[(19)] operators has enabled us to see clearly into the structure of the theory, since the two-body additive theory is on the same level as the three-body additive theory for smooth potentials. The use of a one-body additive operator L_0 yields an alternative, formally exact expression for the residual memory function associated with the size of the cluster at which one stops. To treat certain long-range screening and long-time tail effects, a dressed particle type of approximation avoids going to the next order cluster. Fortunately the expressions for the dressed particle memory functions can be written down explicitly. The hard-sphere case shows, already at the one-body additive level, that a satisfactory L_0 should have, for example, hydrodynamic eigenfunctions for long wavelength. This fits in with both the general theory of Green's function and with specific kinetic theory analysis of critical phenomena[(20)] and of long time tails.[(21)]

In the general theory of Green's functions,[(12)] other, more sophisticated but more complicated methods of treating the "last" memory operator have been discussed. The dressed particle point of view emphasizes interaction of each member of a cluster with the medium via fluctuations. With attractive forces, members of a cluster might form bound states which then interact with fluctuations. Mazenko has discussed some of these decompositions by analyzing connected and disconnected parts of the residual memory operator. However, it does not seem to us that the use of ordinary or Kubo cumulants to make this distinction is in the spirit of the general formulation of the theory.

To a large extent, differences between current theories are more a matter of language and formalism than of point of view. Thus (aided by Boley's work) the author believes that the theory is closely related to that of Mazenko, who has gone further in a number of directions. Likewise, recent work by Dorfman and Cohen[22] and Lebowitz and Résibois[23] (which has appeared too recently for us to study and evaluate here) may "do the same job." We feel that an advantage of this present formulation is its elementary character—in fact, its simple-minded character. Given the few initial ideas, the rest of the steps are obvious.

APPENDIX A. STATIC CORRELATION FUNCTIONS

$$\langle\delta N(1)|\delta N(2)\rangle = [\rho_2(x_1x_2) - \rho_0{}^2]\phi_1\phi_2 + \delta(1-2)\rho_0\phi_1 \tag{A.1}$$

$$\begin{aligned}\langle\delta N(12)|\delta N(3)\rangle = {} & [\rho_3(x_1x_2x_3) - \rho_0\rho_2(x_1x_2)]\phi_1\phi_2\phi_3 \\ & + [\delta(3-1) + \delta(3-2)]\phi_1\phi_2\rho_2(x_1x_2)\end{aligned} \tag{A.2}$$

$$\begin{aligned}\langle\delta N(123)|\delta N(4)\rangle = {} & [\rho_+(x_1x_2x_3x_4) - \rho_0\rho_3(x_1x_2x_3)]\phi_1\phi_2\phi_3\phi_4 \\ & + [\delta(4-1) + \delta(4-2) + \delta(4-3)]\phi_1\phi_2\phi_3\rho_3(x_1x_2x_3)\end{aligned} \tag{A.3}$$

$$\begin{aligned}\langle\delta N(12)|\delta N(34)\rangle = {} & [\rho_+(x_1x_2x_3x_4) - \rho_2(x_1x_2)\rho_2(x_3x_4)]\phi_1\phi_2\phi_3\phi_4 \\ & + [1 + P(34)][\delta(3-1) + \delta(3-2)]\phi_1\phi_2\phi_4\rho_3(x_1x_2x_4)\end{aligned} \tag{A.4}$$

$$\begin{aligned}\langle\delta N(123)|\delta N(45)\rangle = {} & [\rho_5(x_1x_2x_3x_4x_5) - \rho_3(x_1x_2x_3)\rho_2(x_4x_5)]\phi_1\phi_2\phi_3\phi_4\phi_5 \\ & + [1 + P(45)][\delta(4-1) + \delta(4-2) + \delta(4-3)] \\ & \times \phi_1\phi_2\phi_3\phi_5\rho_4(x_1x_2x_3x_5) + [1 + P(45)] \\ & \times [\delta(4-1)\delta(5-2) + \delta(4-1)\delta(5-3) \\ & + \delta(4-2)\delta(5-3)]\phi_1\phi_2\phi_3\rho_3(x_1x_2x_3)\end{aligned} \tag{A.5}$$

$$\begin{aligned}\langle T(12)|T(34)\rangle = {} & \phi_1\phi_2\phi_3\phi_4\mathscr{S}(x_1x_2x_3x_4) \\ & + [1 + P(34)][1 + P(12)]\rho_3(x_1x_2x_3) \\ & \times [-\rho_2(x_1x_2)\rho_2(x_3x_4)/\rho_0]\phi_1\phi_2\phi_3\,\delta(4-1) \\ & + \phi_1\phi_2\rho_2(x_1x_2)[\delta(3-1)\delta(4-2) + \delta(3-2)\delta(4-1)]\end{aligned} \tag{A.6}$$

Here

$$\begin{aligned}\mathscr{S}(x_1x_2x_3x_4) = {} & \rho_4(x_1x_2x_3x_4) - \rho_2(x_1x_2)\rho_2(x_3x_4) \\ & - K(x_3x_4\bar{x}_5)[\rho_3(x_1x_2\bar{x}_5) - \rho_0\rho_2(x_1x_2)] \\ & - [K(x_3x_4x_1) + K(x_3x_4x_2)]\rho_2(x_1x_2) \\ & - [\rho_2(x_3x_4)/\rho_0][1 + P(34)][\rho_3(x_1x_2x_3) - \rho_0\rho_2(x_1x_2)]\end{aligned} \tag{A.7}$$

and

$$\begin{aligned} K(x_1x_2x_3) = {} & [\rho_3(x_1x_2x_3)/\rho_0] - \rho_2(x_1x_2) \\ & - \int \rho_3(x_1x_2x_4)C(x_4 - x_3)\,dx_4 \\ & - \rho_2(x_1x_2)[C(x_3 - x_1) + C(x_3 - x_2)] \\ & + \rho_2(x_1x_2)\rho_0 \int C(x_4 - x_3)\,dx_4 \end{aligned} \tag{A.8}$$

$$\begin{aligned} \langle T(12)|N(345)\rangle = {} & [1 + P(12|][1 + P(35) + P(45)] \\ & \times \delta(3 - 1)\delta(4 - 2)\langle N_3(125)\rangle \\ & + [1 + P(12)][1 + P(34) + P(35)] \\ & \times \delta(3 - 1)\langle N_4(1245)\rangle \\ & + [\langle N_5(12345)\rangle - \langle N_2(12)\rangle\langle N_3(345)\rangle] \\ & - [\Lambda(123) + \Lambda(124) + \Lambda(125)]\langle N_3(345)\rangle \\ & - \Lambda(12\bar{6})[\langle N_4(345\bar{6})\rangle - \langle N(\bar{6})\rangle\langle N_3(345)\rangle] \end{aligned} \tag{A.9}$$

A more explicit form, ordered in powers of the density, is

$$\begin{aligned} \langle T(12)|N(345)\rangle = {} & \rho_0^3[1 + P(12)][1 + P(35) + P(45)] \\ & \times \delta(3 - 1)\delta(4 - 2)\langle N_3(125)\rangle/\rho_0^3 \\ & + \rho_0^4[1 + P(12)][1 + P(34) + P(35)] \\ & \times \delta(3 - 1)\langle N_4(1245)\rangle/\rho_0^4 \\ & - \rho_0^4[1 + P(34) + P(35)][1 + P(12)] \\ & \times [\delta(3 - 1)/\phi_1]\langle N_2(12)\rangle\langle N_3(345)\rangle/\rho_0^5 \\ & + \phi_1\phi_2\phi_3\phi_4\phi_5(\mathscr{D}_5 + \mathscr{D}_6) \end{aligned} \tag{A.10}$$

Here

$$\begin{aligned} \mathscr{D}_5(x_1x_2x_3x_4x_5) = {} & \rho_5(x_1x_2x_3x_4x_5) - \rho_2(x_1x_2)\rho_3(x_3x_4x_5) \\ & - \rho_3(x_3x_4x_5)[K(x_1x_2x_3) + K(x_1x_2x_4) + K(x_1x_2x_5)] \\ & - [\rho_2(x_1x_2)/\rho_0][\rho_4(x_1x_3x_4x_5) \\ & + \rho_4(x_2x_3x_4x_5) - 2\rho_0\rho_3(x_3x_4x_5)] \end{aligned} \tag{A.11}$$

$$\mathscr{D}_6(x_1x_2x_3x_4x_5) = -K(x_1x_2\bar{x}_6)[\rho_4(\bar{x}_6x_3x_4x_5) - \rho_0\rho_3(x_3x_4x_5)] \tag{A.12}$$

and we set

$$\mathscr{M}(x_1x_2x_3x_4x_5) = \mathscr{D}_5 + \mathscr{D}_6 \tag{A.13}$$

APPENDIX B. MATRIX ELEMENTS OF L FOR SMOOTH POTENTIALS

We use the basic formula

$$\langle A(\Gamma)LB(\Gamma)\rangle = \kappa T\langle\{A, B\}_{\mathrm{PB}}\rangle \tag{B.1}$$

where

$$\{A, B\}_{\mathrm{PB}} = \sum_{\alpha}\left(\frac{\partial A}{\partial p_\alpha}\frac{\partial B}{\partial q_\alpha} - \frac{\partial A}{\partial q_\alpha}\frac{\partial B}{\partial p_\alpha}\right)$$

In order to avoid errors arising from the singular nature of the phase-space functions, we use real, smooth, symmetric support functions on the left- and right-hand sides of matrix elements. We also use the notation

$$L(1|2) = \frac{p_1}{m}\frac{\partial}{\partial x_1} + \kappa T\,\frac{\partial \ln \rho_2(x_1x_2)}{\partial x_1}\frac{\partial}{\partial p_1} \tag{B.2}$$

$$L(1|23) = \frac{p_1}{m}\frac{\partial}{\partial x_1} + \kappa T\,\frac{\partial \ln \rho_3(x_1x_2x_3)}{\partial x_1}\frac{\partial}{\partial p_1} \tag{B.3}$$

etc., and note that $L(1|2)\langle N(12)\rangle = 0$, $L(1|23)\langle N(123)\rangle = 0$. We then have the tabulation

$$J_{11} \equiv A(1)\langle N(1)|L|N(2)\rangle B(2) = \rho_0 A(1)\phi(p_1)\frac{p_1}{m}\frac{\partial B(1)}{\partial x_1} \tag{B.4}$$

$$J_{21} \equiv C(12)\langle N(12)|L|N(3)\rangle B(3) = 2C(12)\langle N(12)\rangle L(1|2)B(1) \tag{B.5}$$

$$J_{12} \equiv B(1)\langle N(1)|L|N(23)\rangle C(23) = -2B(1)\langle N(12)\rangle L(1|2)C(12) \tag{B.6}$$

$$\begin{aligned} J_{22} &\equiv C(12)\langle N(12)|L|N(34)\rangle D(34) \\ &= 4C(12)\langle N(123)\rangle L(1|23)D(13) \\ &\quad + 2C(12)\langle N(12)\rangle[L(1|2) + L(2|1)]D(12) \end{aligned} \tag{B.7}$$

$$\begin{aligned} J_{23} &\equiv C(12)\langle N(12)|L|N(345)\rangle E(345) \\ &= 3C(12)\langle N_4(234)\rangle[1 + P(12)]L(1|234)E(134) \\ &\quad + 6C(12)\langle N_4(123)\rangle[1 + P(12)]L(1|23)E(123) \end{aligned} \tag{B.8}$$

The theory requires the matrix elements of L with the basis functions,

$$j_{11} \equiv A(1)\langle T(1)|L|T(2)\rangle B(2) = J_{11} \tag{B.9}$$

$$\begin{aligned} j_{21} &\equiv C(12)\langle T(12)|L|T(3)\rangle B(3) \\ &= 2C(12)\frac{\partial \rho_2(x_1x_2)}{\partial x_1}\phi(p_1)\phi(p_2)\frac{\partial B(1)}{\partial p_1} \\ &\quad - C(12)\phi(p_1)\phi(p_2)S(x_1x_2x_4)\frac{p_4\phi_4}{m}\frac{\partial B(4)}{\partial x_4} \end{aligned} \tag{B.10}$$

where

$$S(x_1x_2x_4) = \rho_3(x_1x_2x_4) - \rho_0{}^2\int \rho_3(x_1x_2x_3)C(x_3 - x_4)\,dx_3$$
$$- \rho_0\rho_2(x_1x_2)[C(x_1 - x_4) + C(x_2 - x_4)] \qquad \text{(B.11)}$$

$$j_{12} \equiv \langle B(3)\langle T(3)|L|T(12)\rangle C(12) = -j_{21} \qquad \text{(B.12)}$$

$$j_{22} \equiv C(12)\langle T(12)|L|T(34)\rangle D(34)$$
$$= C(12)[\langle N(12)\rangle[L(1|2) + L(2|1)]D(12)$$
$$+ 4C(12)\phi_1\phi_2\phi_4\left[R_3(x_1x_2x_4)\frac{p_1}{m}\frac{\partial}{\partial x_1} + \kappa T\frac{\partial R_3(x_1x_2x_4)}{\partial x_1}\frac{\partial}{\partial p_1}\right]D(14)$$
$$\text{(B.13)}$$

with

$$R_3(x_1x_2x_4) = \rho_3(x_1x_2x_4) - [\rho_2(x_1x_2)\rho_2(x_1x_4)/\rho_0] \qquad \text{(B.14)}$$

APPENDIX C. MATRIX ELEMENTS OF THE PSEUDO-LIOUVILLE OPERATORS

We use the formulation of Refs. 5 and 19. The latter paper gives the derivation of the one-body additive equation of LPS[7] and Mazenko[8] in a form close to the notation of this paper. The pseudo-Liouville operators are

$$L_\pm = L_0{}^0 \pm \tfrac{1}{2}\sum_{i\neq j}\mathscr{T}_\pm(ij) = L_0{}^0 \pm L_\pm^{(1)} \qquad \text{(C.1)}$$

$$\mathscr{T}_\pm(ij) = (1/m)|\mathbf{p}_{ij}\cdot\hat{\mathbf{q}}_{ij}|\,\theta(\mp\mathbf{p}_{ij}\cdot\mathbf{q}_{ij})\delta(|q_{ij}| - \sigma)(b_{ij} - 1) \qquad \text{(C.2)}$$

Here σ is diameter of the hard spheres, $\theta(x)$ is the step function, $\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x > 0$. Also,

$$\mathbf{p}_{ij} = \mathbf{p}_i - \mathbf{p}_j, \qquad \hat{\mathbf{q}}_{ij} = \mathbf{q}_{ij}/|\mathbf{q}_{ij}| \qquad \text{(C.3)}$$

The exchange operator b_{ij} operates according to the rule

$$b_{ij}f(\mathbf{p}_1,\ldots,\mathbf{p}_i,\mathbf{q}_i,\ldots,\mathbf{p}_j,\mathbf{q}_j,\ldots,\mathbf{q}_N) = f(\mathbf{p}_1,\ldots,\mathbf{p}_i{}^F,\mathbf{q}_i,\mathbf{p}_j{}^F,\ldots,\mathbf{q}_j,\ldots,\mathbf{q}_N) \qquad \text{(C.4)}$$

where the final momenta $\mathbf{p}_i{}^F$, $\mathbf{p}_j{}^F$ obey

$$\mathbf{p}_i{}^F = \mathbf{p}_i - (\mathbf{p}_{ij}\cdot\hat{\mathbf{q}}_{ij})\hat{\mathbf{q}}_{ij}, \qquad \mathbf{p}_j{}^F = \mathbf{p}_j + (\mathbf{p}_{ij}\cdot\hat{\mathbf{q}}_{ij})\hat{\mathbf{q}}_{ij} \qquad \text{(C.5)}$$

The evolution operator is e^{-tL_+} for $t > 0$ and e^{-tL_-} for $t < 0$. With inner products defined with a Gibbs weight factor Φ, we have

$$\langle A|B\rangle = \int \Phi A^*B\,d\Gamma$$

$$\langle A|L_+|B\rangle = -\langle L_-A|B\rangle, \qquad \langle A|L_-B\rangle = -\langle L_+A|B\rangle \qquad \text{(C.6)}$$

in contrast to the smooth potential case, where the same anti-Hermitian operator L occurs in both sides. It should be noted that even in the smooth potential case the free streaming operator $L_0{}^0$ is not anti-Hermitian, since it does not have the Gibbs function as an eigenfunction with eigenvalue zero. The above pseudo operators are to be used in time-dependent correlation functions, where they operate on functions to the right. The multiplication by Φ is put to the left and then one integrates over phase space. Let

$$\alpha_\pm(34) = (1/m)|\mathbf{p}_{34}\cdot\hat{\mathbf{x}}_{34}|\,\theta(\mp\mathbf{p}_{34}\cdot\hat{\mathbf{x}}_{34})\,\delta(|x_{34}| - \sigma) \tag{C.7}$$

$$\langle 1|V|34\rangle = \tfrac{1}{2}[1 + P(34)]\,\delta(\mathbf{x}_3 - \mathbf{x}_1)[\delta(\mathbf{p}_3 - \mathbf{p}_{34}\cdot\hat{\mathbf{x}}_{34}\hat{\mathbf{x}}_{34} - \mathbf{p}_1) - \delta(\mathbf{p}_3 - \mathbf{p}_1)] \tag{C.8}$$

and

$$\langle 34|W_{21}^{\pm}|1\rangle = \alpha_\pm(34)\langle 1V|34\rangle \tag{C.9}$$

Then

$$L_\pm^{(1)}N(1) = N_2(\bar{3}\bar{4})\langle\bar{3}\bar{4}|W_{21}^{\pm}|1\rangle \tag{C.10}$$

$$L_\pm^{(1)}N_2(12) = [1 + P(12)]N_3(2\bar{3}\bar{4})\langle\bar{3}\bar{4}|W_{21}^{\pm}|1\rangle + N_2(\bar{3}\bar{4})\langle\bar{3}\bar{4}|W_{22}^{\pm}|12\rangle \tag{C.11}$$

Here

$$\begin{aligned}\langle 34|W_{22}^{\pm}|12\rangle = {} & [1 + P(12)]\alpha_\pm(34)\,\delta(\mathbf{x}_3 - \mathbf{x}_1)\,\delta(\mathbf{x}_4 - \mathbf{x}_2)\\ & \times [\delta(\mathbf{p}_3 - \mathbf{p}_{34}\hat{\mathbf{x}}_{34}\hat{\mathbf{x}}_{34} - \mathbf{p}_1)\,\delta(\mathbf{p}_4 + \mathbf{p}_{34}\hat{\mathbf{x}}_{34}\hat{\mathbf{x}}_{34} - \mathbf{p}_2)\\ & - \delta(\mathbf{p}_3 - \mathbf{p}_1)\,\delta(\mathbf{p}_4 - \mathbf{p}_2)]\end{aligned}$$

We encounter

$$\langle x_3x_4|H_\pm|1\rangle \equiv \int\!\!\int \phi(p_3)\phi(p_4)\langle 34|W_{21}^{\pm}|1\rangle \tag{C.12}$$

This is evaluated by going to final momenta and using

$$\phi(p_3{}^F)\phi(p_4{}^F) = \phi(p_3)\phi(p_4) \tag{C.13}$$

We have

$$\begin{aligned}\langle x_3x_4|H_\pm|1\rangle &= \pm\frac{\mathbf{p}_1\phi(p_1)}{2m}[\delta(|x_{14}| - \sigma)\,\delta(\mathbf{x}_3 - \mathbf{x}_1)\hat{\mathbf{x}}_{14}\\ &\quad + \delta(|x_{13}| - \sigma)\,\delta(\mathbf{x}_4 - \mathbf{x}_1)\hat{\mathbf{x}}_{13}]\\ &\equiv \pm\frac{\mathbf{p}_1\phi(p_1)}{m}\langle x_3x_4|\mathbf{U}_+|x_1\rangle\end{aligned} \tag{C.14}$$

The matrix elements are

$$\langle 2|L_0{}^0|1\rangle = \rho_0 \frac{\mathbf{p}_1}{m}\phi_1 \frac{\partial\delta(1-2)}{\partial \mathbf{x}_1} - \frac{\mathbf{p}_1\phi_1\phi_2}{m}\frac{\partial\rho_2(x_1x_2)}{\partial \mathbf{x}_1} \tag{C.15}$$

$$\langle 2|L_\pm^{(1)}|1\rangle = \pm \frac{\mathbf{p}_1\phi_1\phi_2}{m}\int \rho_3(\mathbf{x}_1\mathbf{x}_2\mathbf{x}_4)\cdot\delta(|x_{14}|-\sigma)\hat{\mathbf{x}}_{14}\,d\mathbf{x}_4$$
$$+\, 2\phi_2\bar{\phi}_4\rho_2(\sigma)\langle 2\bar{4}|W_{21}^{\pm}|1\rangle \tag{C.16}$$

Using the equilibrium relations,

$$\langle 1|L_\pm|2\rangle = \rho_0\phi_1\frac{\mathbf{p}_1}{m}\frac{\partial\delta(1-2)}{\partial\mathbf{x}_1} + \rho_2(\sigma)\phi_1\phi_2\frac{\mathbf{p}_2\cdot\hat{\mathbf{x}}_{12}}{m}\delta(|x_{12}|-\sigma)$$
$$\pm\, 2\rho_2(\sigma)\phi_1\bar{\phi}_4\langle 1\bar{4}|W_{21}^{\pm}|2\rangle \tag{C.17}$$

We also have

$$\langle 1|L_-|\bar{2}\rangle\langle\bar{2}|Z_1|3\rangle = \rho_0\frac{\mathbf{p}_1}{m}\phi_1\frac{\partial\langle 1|Z_1|3\rangle}{\partial\mathbf{x}_1} + \frac{\rho_2(\sigma)\phi_1}{\rho_0}\frac{\mathbf{p}_3\cdot\hat{\mathbf{x}}_{13}}{m}\delta(|x_{13}|-\sigma)$$
$$-\, 2\frac{\rho_2(\sigma)\phi_1\bar{\phi}_4}{\rho_0}\langle 1\bar{4}|W_{21}^{-}|3\rangle\frac{1}{\phi_3} \tag{C.18}$$

The Boltzmann–Enskog operator $\mathscr{B}$ involves a different combination of θ functions than is contained in W_{21}^{-}. We introduce

$$\langle 1|\mathscr{B}|2\rangle = 2\phi_1\bar{\phi}_4\langle 1\bar{4}|W_{21}^{-}|2\rangle + \frac{\mathbf{p}_{12}\cdot\hat{\mathbf{x}}_{12}}{m}\phi_1\phi_2\,\delta(|x_{12}|-\sigma) \tag{C.19}$$

Then

$$\langle 1|\mathscr{B}|2\rangle = \iint \alpha_-(14)\phi_1\phi_4[\delta(\mathbf{x}_1-\mathbf{x}_2)\,\delta(\mathbf{p}_1-\mathbf{p}_{14}\hat{\mathbf{x}}_{14}\hat{\mathbf{x}}_{14}-\mathbf{p}_2)$$
$$+\,\delta(\mathbf{x}_4-\mathbf{x}_2)\,\delta(\mathbf{p}_4+\mathbf{p}_{14}\hat{\mathbf{x}}_{14}\hat{\mathbf{x}}_{14}-\mathbf{p}_2]\,d\hat{\mathbf{p}}_4\,d\mathbf{x}_4$$
$$-\iint \alpha_+(14)\phi_1\phi_4[\delta(\mathbf{x}_1-\mathbf{x}_2)\,\delta(\mathbf{p}_1-\mathbf{p}_2)$$
$$+\,\delta(\mathbf{x}_4-\mathbf{x}_2)\,\delta(\mathbf{p}_4-\mathbf{p}_2)]\,d\mathbf{x}_4\,d\mathbf{p}_4 \tag{C.20}$$

and

$$\langle 1|L_-|2\rangle = \rho_0\frac{\mathbf{p}_1\phi_1}{m}\frac{\partial\delta(1-2)}{\partial\mathbf{x}_1} + \frac{\mathbf{p}_1\rho_2(\sigma)}{m}\phi_1\phi_2\hat{\mathbf{x}}_{12}\,\delta(|x_{12}|-\sigma)$$
$$-\,\rho_2(\sigma)\langle 1|\mathscr{B}|2\rangle \tag{C.21}$$

APPENDIX D. TWO-BODY COLLISION KERNEL FOR HARD SPHERES

The kernel operating on the two-body amplitude $\tilde{A}_2$ consists of the two body inverse multiplied by the quantity

$$[1 + P(1'2')]\langle T(\underset{\sim}{3}^*\underset{\sim}{4}^*)|N_3(1'4'5')\rangle\langle 4'5'|W_{\bar{2}1}|2'\rangle\tilde{A}_2(1'2')$$

We write down the contributions to this quantity here. There are three parts. The term of order ρ_0^3 is

$$\begin{aligned}2\phi(p_3^*)\phi(p_4^*)[1 + P(3^*4^*)][&\rho_3(x_3^*x_4^*\bar{x}_2)\langle 3^*4^*|W_{\bar{2}1}|\bar{1}'\rangle\phi(\bar{p}_2')\tilde{A}_2(\bar{1}'\bar{2}')\\ &+ \rho_3(x_3^*x_4^*\bar{x}_4')[\phi(\bar{p}_4')\langle\bar{4}'4^*|W_{\bar{2}1}|\bar{1}'\rangle\tilde{A}_2(\bar{1}'3^*)\\ &+ \phi(\bar{p}_4')\langle\bar{4}'4^*|W_{\bar{2}1}|3^*\rangle\tilde{A}_2(\bar{1}'\bar{3}^*)]\end{aligned} \tag{D.1}$$

The term of order ρ_0^4 contains the spatial kernels

$$\begin{aligned}\langle x_3^*|\boldsymbol{\lambda}_3|x_2'\rangle &= \rho_3(x_3^*\bar{x}_4'\bar{x}_5')\langle\bar{x}_4'\bar{x}_5'|\mathbf{U}_+|x_2'\rangle\\ \langle x_3^*x_4^*|\boldsymbol{\lambda}_4|x_2'\rangle &= \rho_4(x_3^*x_4^*\bar{x}_4'\bar{x}_5')\langle\bar{x}_4'\bar{x}_5'|\mathbf{U}_+|x_2'\rangle\end{aligned} \tag{D.2}$$

where

$$\langle x_3x_4|\mathbf{U}_+|x_1\rangle = \tfrac{1}{2}[\delta(|x_{14}| - \sigma)\,\delta(\mathbf{x}_3 - \mathbf{x}_1)\hat{\mathbf{x}}_{14} + \delta(|x_{13}| - \sigma)\,\delta(\mathbf{x}_4 - \mathbf{x}_1)\hat{\mathbf{x}}_{13}] \tag{D.3}$$

It is

$$\begin{aligned}2\phi(p_3^*)\phi(p_4^*)[1 + P(3^*4^*)]\{&[\langle x_3^*x_4^*|\lambda_4|\bar{x}'\rangle\\ &- \frac{\rho_2(x_3^*x_4^*)}{\rho_0}\langle x_3^*|\lambda_3|\bar{x}'\rangle]\bar{p}_2'\,\frac{\phi(\bar{p}_2')}{m}\,\tilde{A}_2(3^*\bar{2}')\\ &+ \begin{bmatrix}[1 + P(\bar{1}'\bar{2}')]\rho_4(x_3^*x_4^*\bar{x}_1'\bar{x}_5')\\ - \dfrac{\rho_2(_3^*x_4^*)}{\rho_0}\,\rho_3(x_3^*, \bar{x}_1', \bar{x}_5')\end{bmatrix}\phi(\bar{p}_5')\langle 3^*\bar{5}'|W_{21}|\bar{2}'\rangle\phi(\bar{p}_1')\tilde{A}_2(\bar{1}'\bar{2}')\}\end{aligned} \tag{D.4}$$

Finally, the terms of order ρ_0^5 and ρ_0^6 are

$$\begin{aligned}&\phi(p_3^*)\phi(p_4^*)[1 + P(\bar{1}'\bar{2}')]\mathscr{M}(x_3^*x_4^*\bar{x}_1'\bar{x}_4'\bar{x}_5')\langle\bar{x}_4'\bar{x}_5'|U_+|x_2'\rangle\\ &\iint\phi(\bar{p}_1')(\bar{p}_2'/m)\phi(\bar{p}_2')\tilde{A}_2(\bar{1}'\bar{2}')\end{aligned} \tag{D.5}$$

Here $\mathscr{M} = \mathscr{D}_5 + \mathscr{D}_6$ is written in the appendix dealing with static correlation functions.

APPENDIX E. MODIFIED CUMULANTS

Our starting point for the hard-sphere case is the Liouville equation

$$[(\partial/\partial t) + L_0{}^0 - \tfrac{1}{2} \sum_{i \neq j} \bar{T}(ij)]\Phi \hat{F}_N = 0 \tag{E.1}$$

Here

$$\bar{T}(ij) = \mathscr{T}_-(ij) + Q(ij), \qquad Q(ij) = \frac{\mathbf{p}_{ij}\cdot\hat{\mathbf{q}}_{ij}}{m}\,\delta(|q_{ij}| - \sigma) \tag{E.2}$$

i.e.,

$$\bar{T}(ij) = \delta(|q_{ij}| - \sigma)\,\frac{|\mathbf{p}_{ij}\cdot\hat{\mathbf{q}}_{ij}|}{j}\,[\theta(\mathbf{p}_{ij}\cdot\hat{\mathbf{q}}_{ij})b_{ij} - \theta(-\mathbf{p}_{ij}\cdot\hat{\mathbf{q}}_{ij})] \tag{E.3}$$

We also note that because of the discontinuous functions in Φ,

$$L_0{}^0\Phi = \tfrac{1}{2} \sum_{i \neq j} Q(ij)\Phi \tag{E.4}$$

From this equation, by multiplying by $N(1)$, $N(12)$,..., we find the equilibrium hierarchy

$$\begin{aligned} L_0{}^0(1)\langle N(1)\rangle &= Q(1\bar{2})\langle N(1\bar{2})\rangle \\ [L_0{}^0(1) + L_0{}^0(2)]\langle N(12)\rangle &= [Q(1\bar{3}) + Q(2\bar{3})]\langle N(12\bar{3})\rangle \end{aligned} \tag{E.5}$$

For the nonequilibrium case we find the hierarchy used by Ernst and Dorfman:

$$\begin{aligned} [(\partial/\partial t) + L_0{}^0(1)]\hat{F}_1(1) &= \bar{T}(1\bar{2})\hat{F}_2(1\bar{2}) \\ [(\partial/\partial t) + L_0{}^0(1) + L_0{}^0(2) - \bar{T}(12)]\hat{F}_2(12) &= [\bar{T}(1\bar{3}) + \bar{T}(2\bar{3})]\hat{F}_3(12\bar{3}) \end{aligned} \tag{E.6}$$

Note that our $\hat{F}_n$ are $\rho_0{}^n$ times the ones used by the cited authors.

The modified cumulants Δ_n are simply the amplitudes multiplied by correlation functions.

Thus the quantities in brackets in Eq. (74) are cumulants,

$$\begin{aligned} \hat{\Delta}_1(1) &\equiv \hat{F}_1(1) = \langle T(1)|T(\bar{2})\rangle\tilde{A}_1(\bar{2}) = \langle T(1)|\hat{F}_N\rangle \\ \hat{\Delta}_2(12) &= \langle T(12)|T(\bar{3}\bar{4})\rangle\hat{A}_2(\bar{3}\bar{4}) = \langle T(12)|\hat{F}_N \\ &= \hat{F}_2(12) - \Lambda(12\bar{3})\hat{F}_1(\bar{3}) \\ \hat{\Delta}_3(123) &= \langle T(123)|\hat{F}_N\rangle = \langle T(123)|T(\bar{4}\bar{5}\bar{6})\rangle\hat{A}_3(\bar{4}\bar{5}\bar{6}) \\ &= \hat{F}_3(123) - \Lambda(123|\bar{4}5)\hat{\Delta}_2(\bar{4}\bar{5}) - \Lambda(123|\bar{4})\hat{F}_1(\bar{4}) \end{aligned} \tag{E.7}$$

We call the Δ_n modified cumulants. To justify the name, note that

$$\hat{\Delta}_2(12) = \hat{F}_2(12) - K(x_1x_2\bar{x}_3)\phi_1\phi_2\hat{F}_1(\bar{3}) - [\rho_2(x_1x_2)/\rho_0][\phi_1\hat{F}_1(2) + \phi_2\hat{F}_1(1)] \tag{E.8}$$

Asymptotically, there is agreement with the usual time-dependent linearized cumulant $D_2(12)$,

$$D_2(12) \equiv F_2(12) - \rho_0[\phi_1 F_1(2) + \phi_2 F_1(1)] \tag{E.9}$$

The equations for Δ_n may be formed by taking combinations of Eqs. (E.6). Thus

$$(\partial/\partial t)_1 \hat{\Delta}(1) + L_0{}^0(1)\hat{\Delta}_1(1) - \bar{T}(12)\Lambda(12\bar{3})\hat{\Delta}_1(\bar{3}) = \bar{T}(1\bar{2})\hat{\Delta}_2(1\bar{2}) \tag{E.10}$$

$$\begin{aligned}
&[(\partial/\partial t) + L_0{}^0(1) + L_0{}^0(2) - \bar{T}(12)]\hat{\Delta}_2(12) + \Lambda(12\bar{3})\bar{T}(\bar{3}\bar{4})\hat{\Delta}_2(1\bar{2}) \\
&\quad - \bar{T}(1\bar{3}) + \bar{T}(2\bar{3})][\Lambda(123|\bar{4}\bar{5})\hat{\Delta}_2(\bar{4}\bar{5}) + \hat{\Delta}_3(12\bar{3})] \\
&= -[L_0{}^0(1) + L_0{}^0(2) - \bar{T}(12)]\Lambda(12\bar{3})\hat{\Delta}_1(3) + \Lambda(12\bar{3})L_0(\bar{3})\hat{\Delta}_1(\bar{3}) \\
&\quad + [\bar{T}(1\bar{3}) + \bar{T}(2\bar{3})]\Lambda(12\bar{3}|\bar{4})\hat{\Delta}_1(\bar{4}) - \Delta(12\bar{3})\bar{T}(\bar{3}\bar{4})\Lambda(\bar{3}\bar{4}\bar{5})\hat{\Delta}_1(\bar{5})
\end{aligned} \tag{E.11}$$

Considerable simplification may be achieved in these equations, which are an alternative form of the theory. The work needed is similar to what was outlined in the body of the paper. One technical difference lies in the position of the inverses, which are here embedded in the $\Lambda(123)$, etc. The second difference lies in the different combinations of θ functions in $\bar{T}(ij)$ and in $L_-^{(1)}$. The $\bar{T}$ combination is more satisfactory since it isolates directly the Boltzmann–Enskog operator. Thus in the one-body additive approximation the key terms are

$$\begin{aligned}
\bar{T}(1\bar{2})\Lambda(12\bar{3})\hat{\Delta}_1(\bar{3}) &= \bar{T}(1\bar{2})\phi_1\bar{\phi}_2 K(x_1 x_2 \bar{x}_3)\hat{\Delta}_1(\bar{3}) \\
&\quad + \bar{T}(1\bar{2})[\rho_2(\sigma)/\rho_0][\bar{\phi}_2\hat{\Delta}_1(1) + \phi_1\hat{\Delta}_1(\bar{2})]
\end{aligned} \tag{E.12}$$

The first term, involving $K(x_1 x_2 x_3)$, contains the LPS mean field term, while the second term is the Boltzmann–Enskog collision term.

The time correlation point of view is convenient in general arguments involving memory functions in Section 2, as well as in the evaluation of memory functions in the dressed particle and related approximations in Section 5. To establish the connection, we must move Φ in Eq. (E.1) to the left of the operators. We have

$$\Phi[(\partial/\partial t) + L_0{}^0 + \tfrac{1}{2}\sum_{i\neq j} Q(ij) - \sum \bar{T}(ij)]\hat{F}_N = 0 \tag{E.13}$$

or

$$\Phi[(\partial/\partial t) + L_0{}^0 - \tfrac{1}{2}\sum_{i\neq j} \mathscr{T}_-(ij)]\hat{F}_N = 0 \tag{E.14}$$

Since

$$L_0{}^0 - \tfrac{1}{2}\sum \mathscr{T}_-(ij) \equiv L_0{}^0 - L_-^{(1)} \equiv L_-$$

we see that L_- is the pseudo-Liouville operator needed and the starting point for the time correlation point of view is

$$[(\partial/\partial t) + L_-]\hat{F}_N = 0 \tag{E.15}$$

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