

## Projection-operator approach to a renormalized kinetic theory\*

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(Received 24 June 1974)

A renormalized kinetic theory is developed for the classical phase-space density correlation function by means of the projection-operator formalism. The technique consists of introducing a sequence of projection operators which project onto spaces involving successively larger numbers of particles. The first such operator is the Akcasu-Duderstadt projection operator, which yields a generalized Langevin equation (kinetic equation) for the correlation function. The structure of the memory function in this equation suggests a second projection operator, which is shown to lead to a two-body kinetic equation for one factor in the memory function. Further projection operators proceed similarly, and the result is a continued-fraction expansion of the correlation function. This expansion is renormalized in the sense that the interparticle potential always drops out in favor of static correlation functions. The expansion is shown to be equivalent to the result of the kinetic theory formulated by Gross. The analogous development for self-correlations is also given.

### I. INTRODUCTION

In most formulations of classical kinetic theory, the interparticle potential appears explicitly. Because collision processes are considered in the long-time limit, the Boltzmann equation itself contains only the two-body cross section; but to account for the noninstantaneous nature of a binary collision, the collision operator must be made time dependent. Such generalizations of the linearized Boltzmann equation<sup>1-5</sup> contain the potential explicitly. The potential is not directly measurable, however, so it seems useful to "renormalize" kinetic theory so that the final equations contain only measurable quantities such as correlation functions.

One such formulation, valid in the linear regime, was introduced some years ago by Gross.<sup>6</sup> In this approach, the deviation from equilibrium of the Liouville distribution function is taken to be successively one-body additive, two-body additive, and so forth. These constraints lead to corresponding truncations of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy, and in the resulting kinetic equations the potential appears only implicitly via static equilibrium correlation functions. Many of the properties of this renormalized theory were worked out by Gross, and several further consequences have recently been explored by the present author.<sup>7</sup> The final theory also has important points in common with the work of Mazenko.<sup>8</sup>

As one would hope, the Gross theory contains as special cases the above-mentioned generalizations of the linearized Boltzmann equation. Specifically, the collision kernel of the second approximation gives, after expansion to first order in the density, the space-time extension of the Boltzmann ker-

nel,<sup>1-3</sup> which is valid at all wavelengths and frequencies for which quantum effects can be ignored. When the collision kernel of the third approximation is expanded to second order in the density, one recovers the space-time extension of the triple-collision kernel.<sup>4,5</sup>

In the last decade or so, a great deal of attention has been given to another, independent approach to time-dependent statistical mechanics. This is the use of projection operators, along the lines initiated by Zwanzig<sup>9,10</sup> and Mori.<sup>11</sup> Aside from its successes in general problems<sup>12</sup> this approach has led to a number of useful results in linear kinetic theory.<sup>13-20</sup> In one of the first applications to kinetic theory, Akcasu and Duderstadt<sup>13</sup> introduced an operator which projects onto the local phase-space density at a point  $\vec{r}_1, \vec{p}_1$  and which was shown to yield a generalized Langevin equation for the phase-space density correlation function. The static part of the collision kernel, or memory function, in this equation was shown to be of the linearized Vlasov form with the potential replaced by the direct correlation function,  $v(r) \rightarrow -\beta^{-1}c(r)$ . This result, which had earlier been deduced from other considerations,<sup>21,22</sup> can be regarded as the first step toward a potential-independent theory. The Akcasu-Duderstadt formulation also gave a compact expression for the dynamical part of the memory function, in terms of the well-known modified propagator. A great deal has been learned about this function via expansions in the potential<sup>13,17,23</sup> and density.<sup>1-5,17</sup> As regards nonperturbative advances beyond this point, however, the projection-operator method has largely lain dormant. In particular, it has not been applied to the problem of continuing the potential-independent expansion beyond the Vlasov level.

In this paper we use the projection-operator

method to derive a completely potential-independent kinetic theory which, in fact, will be shown to be equivalent to the Gross theory. As in the earlier references, the basic quantity in the theory is the phase-space density correlation function,<sup>23-26</sup> written in the form

$$F(\vec{r}_1\vec{p}_1, \vec{r}'_1\vec{p}'_1; t_1 - t'_1) = \langle [f(\vec{r}_1\vec{p}_1 t_1) - \langle f(\vec{r}_1\vec{p}_1 t_1) \rangle] \times [f(\vec{r}'_1\vec{p}'_1 t'_1) - \langle f(\vec{r}'_1\vec{p}'_1 t'_1) \rangle] \rangle, \quad (1)$$

where  $f(\vec{r}\vec{p}t)$  is the local density,

$$f(\vec{r}\vec{p}t) = \sum_{\alpha} \delta(\vec{r} - \vec{r}_{\alpha}(t)) \delta(\vec{p} - \vec{p}_{\alpha}(t)).$$

Our method of treating this correlation function [abbreviated to  $F(1, 1'; t)$ ] consists of introducing a sequence of projection operators, the first of which is equivalent to the Akcasu-Duderstadt operator. We write the kinetic equation which follows from consideration of the first operator in the form

$$[z + i(\vec{p}_1/m) \cdot (\partial/\partial \vec{r}_1)] F(1, 1'; z) = F(1, 1') + \int d2 \Sigma(1, 2; z) F(2, 1'; z), \quad (2)$$

where we have used the Laplace-transform convention

$$F(1, 1'; z) = -i \int_0^{\infty} dt e^{izt} F(1, 1'; t), \quad (3)$$

and  $F(1, 1')$  is the initial condition. The memory function breaks up into two terms

$$\Sigma(1, 2; z) = \Sigma^{(s)}(1, 2) + \Sigma^{(d)}(1, 2; z), \quad (4)$$

corresponding to its static and dynamic (collisional) parts.

We begin the analysis by turning to  $\Sigma^{(d)}(1, 2; z)$ , written as the correlation function of the appropriate random force evolving according to the modified propagator.<sup>13,26</sup> We note that an interaction operator can be factored out of each random-force term, thereby exposing a four-point correlation function  $G(12, 1'2'; t)$  which describes two particles at time  $t$  and two particles at the initial time. While this function still evolves according to the modified propagator, it is in many ways a more tractable quantity than the memory function itself. To study its time dependence we introduce a new projection operator which involves the joint density at two points  $(\vec{r}_1\vec{p}_1, \vec{r}_2\vec{p}_2)$ , in generalization of the Akcasu-Duderstadt operator. This operator leads to a kinetic equation for  $G(12, 1'2'; t)$  in which the streaming terms contain two-body dynamics. The memory function appropriate to the new equation

again has two parts, static and dynamic. An important point here is that the static part can be expressed in potential-independent form; thus, if we momentarily drop the dynamic part, we see that  $G(12, 1'2'; t)$  obeys a mean-field equation which is a two-body generalization of the modified Vlasov equation.<sup>27</sup>

The dynamical part of the new memory function again has the form of a random force evolving according to a modified propagator, and we apply to it the same sort of considerations which were applied to  $\Sigma^{(d)}(1, 2; z)$ . Thus we factor out interaction operators and introduce a three-body projection operator which leads to a renormalizable three-body kinetic equation, and so forth.

When this procedure is carried out to general order, the result is a continued-fraction expansion of  $F(1, 1'; z)$ , or equivalently of each of the dynamical memory functions. Each term is potential independent, and each successive level involves the dynamics of one more particle. In Ref. 7 it was shown that the Gross theory<sup>6</sup> could be cast into precisely this form. We recover the successive approximations of Gross by truncation of the continued fraction, which means omission of the dynamical effects associated with successive projection operators.

The idea of developing a continued-fraction representation of correlation functions via a sequence of projection operators is attributed to Mori.<sup>28</sup> A straightforward application of his procedure to  $F(1, 1'; z)$  would lead to an expansion different from the one discussed here, however, as it would remain in the one-particle space.

These results are developed in Secs. II and III. In an appendix we extend the projection-operator methods to the case of self-diffusion, in which the basic correlation function is

$$F_s(\vec{r}_1\vec{p}_1, \vec{r}'_1\vec{p}'_1; t) = \left\langle \sum_{\alpha} \delta(\vec{r}_1 - \vec{r}_{\alpha}(t)) \delta(\vec{p}_1 - \vec{p}_{\alpha}(t)) \times \delta(\vec{r}'_1 - \vec{r}_{\alpha}(0)) \delta(\vec{p}'_1 - \vec{p}_{\alpha}(0)) \right\rangle. \quad (5)$$

In this case the Boltzmann-like description is, of course, the neutron transport equation. The space- and time-dependent generalization of this equation appears to have been given first by Stecki and Wojnar<sup>19</sup> and the corresponding result at next order in the density is also known.<sup>4</sup> We obtain a potential-independent theory by introducing an appropriate sequence of projection operators, and the result again has a continued-fraction structure. At the first level of truncation the tagged particle streams freely. At the next level of truncation we make contact with an approximation due to Mazen-

ko,<sup>29</sup> which serves as a potential-independent generalization of the Stecki-Wojnar equation. Further truncations proceed similarly.

## II. PROJECTION-OPERATOR FORMULATION

The inner product of two dynamical variables  $A(1 \cdots N)$  and  $B(1 \cdots N)$  is taken to be  $(A, B) = \langle AB^* \rangle$ , with  $\langle \cdots \rangle$  the grand canonical average. In the  $N$ -particle system we denote the phase-space density at point  $1'$  (i.e., at  $r'_1, p'_1$ ) by

$$f(1', 1 \cdots N) = \sum_{\alpha=1}^N \delta(1' - \alpha), \quad (6)$$

and the joint density at points  $1'$  and  $2'$  by

$$f(1'2', 1 \cdots N) = \sum_{\alpha \neq \beta}^N \delta(1' - \alpha) \delta(2' - \beta), \quad (7)$$

which is taken to vanish when  $N=1$ . We often drop the internal coordinates  $1 \cdots N$  on the  $f$ 's. These "fields" and their higher-order generalizations give rise to a set of time-dependent equilibrium correlation functions defined schematically by

$$F(1 \cdots l, 1' \cdots m'; t) = (e^{itL} f(1 \cdots l), f(1' \cdots m')) - \langle f(1 \cdots l) \rangle \langle f(1' \cdots m') \rangle, \quad (8)$$

or in more detail by, for example,

$$F(1', 1''; t) = \Xi^{-1} \sum_{N=1}^{\infty} \frac{\xi^N}{N! h^{3N}} \int d1 \cdots dN e^{-\beta H(1 \cdots N)} \times [e^{itL(1 \cdots N)} f(1', 1 \cdots N)] \times f(1'', 1 \cdots N) - \langle f(1') \rangle \langle f(1'') \rangle. \quad (9)$$

In Eq. (9) and below we use the notational conventions of Ref. 7, unless otherwise indicated.

The quantity  $F(1, 1'; t)$ , which is the object of primary interest, has the familiar initial condition

$$F(1, 1') \equiv F(1, 1'; t=0) = n\phi(p_1) \delta(1-1') + n^2 \phi(p_1) \phi(p'_1) h(\tilde{r}_1 - \tilde{r}'_1), \quad (10)$$

where  $\phi(p)$  is the Maxwellian and  $h(r)+1=g(r)$  is the radial distribution function. Of course in the grand canonical ensemble the density is  $n = V^{-1} \xi \partial (\ln \Xi) / \partial \xi$ . We adopt the convention that when the time variable does not appear explicitly in a correlation function, as in  $F(1, 1')$ , the initial value is meant. We often make use of one particular property of  $F(1, 1')$ , namely that it has a matrix inverse in the sense that

$$\int d2 F(1, 2) F^{-1}(2, 1') = \int d2 F^{-1}(1, 2) F(2, 1') = \delta(1-1'), \quad (11)$$

with  $F^{-1}$  given in terms of the direct correlation function by

$$F^{-1}(1, 1') = \delta(1-1') / [n\phi(p_1)] - c(\tilde{r}_1 - \tilde{r}'_1). \quad (12)$$

This inverse is well behaved in the grand canonical ensemble with finite  $V$ . On the other hand, Eq. (11) cannot be solved in the canonical ensemble with finite  $N$  and  $V$ , because of the anomalous behavior at long wavelengths.

The natural projection operator for  $F(1, 1'; t)$  is the grand canonical analog of the Akcasu-Duderstadt operator.<sup>13</sup> Thus we define a projection operator  $P_N^{(1)}$  in each  $N$ -body system according to

$$P_N^{(1)} a(1 \cdots N) = \int d1' d2' (a, \delta f(1')) \times F^{-1}(1', 2') \delta f(2', 1 \cdots N), \quad (13)$$

where  $\delta f$  is the deviation from equilibrium:

$$\delta f(1', 1 \cdots N) = f(1', 1 \cdots N) - \langle f(1') \rangle,$$

and all the averages are still in the grand canonical ensemble. This operator projects onto the  $\delta f(1)$  axis, and it also depends on the thermodynamic parameters  $\beta, \xi, V$ . The kinetic equation which follows from consideration of  $P^{(1)}$  has the form of the generalized Langevin equation (2), with the two contributions to the memory function given by

$$\Sigma^{(s)}(1, 1') = - \int d2 (L f(1), f(2)) F^{-1}(2, 1') - L(1) \delta(1-1') = in\phi(p_1) (\tilde{p}_1/m) \cdot (\partial/\partial \tilde{r}_1) c(\tilde{r}_1 - \tilde{r}'_1), \quad (14)$$

$$\Sigma^{(c)}(1, 1'; z) n\phi(p'_1) = ([1/(z+Q^{(1)}L)] Q^{(1)} L f(1), Q^{(1)} L f(1')), \quad (15)$$

where  $Q_N^{(1)} = 1 - P_N^{(1)}$ .

Our method of analysis begins by reducing the field  $Q^{(1)} L f(1)$  which appears in  $\Sigma^{(c)}(z)$ . First, in the  $N$ -particle system one can show that

$$L(1 \cdots N) f(1', 1 \cdots N) = -L(1') f(1', 1 \cdots N) - \int d2' L_1(1'2') f(1'2', 1 \cdots N), \quad (16)$$

thus transferring attention from the internal (here unprimed) coordinates to the field coordinates. From the definition of the first projection operator we can now verify that

$$Q_N^{(1)}L(1 \cdots N)f(1', 1 \cdots N) \\ = - \int d2' L_1(1'2')\delta g(1'2', 1 \cdots N), \quad (17)$$

in terms of a new two-particle field defined by

$$g(1'2', 1 \cdots N) = f(1'2', 1 \cdots N) - \int d3' d4' F(1'2', 3') \\ \times F^{-1}(3', 4')f(4', 1 \cdots N). \quad (18)$$

Clearly  $\delta g(1'2')$  is the part of  $\delta f(1'2')$  which is orthogonal to  $\delta f(1')$ .

The collisional part of the first memory function therefore becomes

$$\Sigma^{(c)}(1, 1'; z) n\phi(p_1') \\ = - \int d2 d2' L_1(12)L_1(1'2')G(12, 1'2'; z), \quad (19)$$

where  $G(12, 1'2'; z)$  is the correlation function in which  $\delta g$  evolves according to the modified propagator

$$G(12, 1'2'; z) = ([1/(z + Q^{(1)}L)] \delta g(12), \delta g(1'2')). \quad (20)$$

The initial value (or the coefficient of  $z^{-1}$  in the large- $z$  expansion) reduces to

$$G(12, 1'2') = F(12, 1'2') - \int d1'' d2'' F(12, 1'') \\ \times F^{-1}(1'', 2'')F(2'', 1'2') \quad (21)$$

and will occur frequently below. We call combinations like  $G(12, 1'2')$  contracted correlation functions.

The net effect of these steps is to extract the interaction operators from the fields which appear in  $\Sigma^{(c)}(z)$ , at the price of introducing the four-point contracted correlation function  $G(z)$ . However, this turns out to be a very convenient representation of the memory function, and all of the following development depends on this step. Note that to second order in the potential,  $\Sigma^{(c)}(z)$  is determined by the free-particle  $G(z)$ . We note in passing that  $G(z)$  can also be expressed in terms of correlation functions which evolve according to  $e^{iLz}$  as opposed to the modified propagator, provided that one works with a  $z$ -dependent inverse. The desired relationship is

$$G(12, 1'2'; z) = F(12, 1'2'; z) - \int d3 d3' F(12, 3; z) \\ \times F^{-1}(3, 3'; z)F(3', 1'2'; z), \quad (22)$$

in which the inverse on the right-hand side satisfies a condition like Eq. (11). We can verify this relationship by comparing the large- $z$  expansions of either side. One is led to this result by formulating the kinetic equation in terms of the BBGKY

hierarchy<sup>8,29</sup>; in that case the memory function is given by Eq. (19), with  $G(z)$  defined by Eq. (22). Thus  $\Sigma^{(c)}(z)$  can be expressed symmetrically in terms of conventional correlation functions. Recently Akcasu<sup>17</sup> has advanced a similar theme by expressing the memory function as the solution of integral equations involving only such correlation functions. His equations can also be derived from (19) and (22).

### III. HIGHER-ORDER PROJECTION OPERATORS: RENORMALIZED EXPANSION

In order to work with the dynamics of  $G(12, 1'2'; z)$ , we introduce a second projection operation  $P^{(2)}$ . In the  $N$ -body system this operator projects onto the  $\delta g(12)$  axis according to

$$P_N^{(2)}a(1 \cdots N) = \int d1' d2' d3' d4' (a, \delta g(1'2')) \\ \times G^{-1}(1'2', 3'4')\delta g(3'4', 1 \cdots N). \quad (23)$$

The definition of the inverse needed above is determined by the extension of Eq. (11) to a two-particle space, namely

$$\int d3 d4 G(12, 34)G^{-1}(34, 1'2') = 1(12, 1'2'), \quad (24)$$

with

$$1(12, 1'2') = \frac{1}{2}[\delta(1-1')\delta(2-2') + \delta(1-2')\delta(2-1')]. \quad (25)$$

The unit matrix above has been symmetrized because  $G(12, 1'2')$  is symmetrical under the interchanges  $1 \leftrightarrow 2$  or  $1' \leftrightarrow 2'$ . We note that  $P_N^{(2)}$  is indeed a projection operator, since  $P_N^{(2)}P_N^{(2)} = P_N^{(2)}$ . Furthermore, it is orthogonal to the  $\delta f(1)$  axis, and we have

$$P_N^{(1)}P_N^{(2)} = P_N^{(2)}P_N^{(1)} = 0. \quad (26)$$

The quantity  $G^{-1}(12, 1'2')$  was introduced by Mazenko.<sup>8</sup> For a free gas it reduces to the very simple expression

$$G^{-1}(12, 1'2') = [1/2n^2\phi(p_1)\phi(p_2)]1(12, 1'2'),$$

and more generally we can show that it has the form

$$G^{-1}(12, 1'2') = [1/2n^2\phi(p_1)\phi(p_2)g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2)]1(12, 1'2') \\ - \{[\delta(1-1')/4n\phi(p_1)]B(\tilde{\mathbf{r}}_1, \tilde{\mathbf{r}}_2\tilde{\mathbf{r}}_2') \\ + \text{cyclic perm. of } 11'22'\} \\ + C(\tilde{\mathbf{r}}_1\tilde{\mathbf{r}}_2, \tilde{\mathbf{r}}_1'\tilde{\mathbf{r}}_2'). \quad (27)$$

Although closed expressions are not yet available

for  $B$  and  $C$ , their density expansions are well-behaved and can be shown to begin as

$$B(\vec{r}_1, \vec{r}_2, \vec{r}'_2) = f(r_2 r'_2) \left[ 1 + n \int d^3 r_3 [f(r_1 r_3) + 1] \right. \\ \left. \times f(r_2 r_3) f(r'_2 r_3) + O(n^2) \right],$$

$$C(\vec{r}_1, \vec{r}_2, \vec{r}'_1, \vec{r}'_2) = \frac{1}{4} [f(r_1 r'_1) f(r_2 r'_2) + f(r_1 r'_2) f(r_2 r'_1) \\ - f(r_1 r'_1) f(r_1 r'_2) f(r_2 r'_1) f(r_2 r'_2)] + O(n),$$

where  $f(r r') = e^{-\beta u(\vec{r} - \vec{r}')} - 1$ . If the potential has a hard core, say of diameter  $r_0$ , then  $G(12, 1'2')$  vanishes when the primed or unprimed coordinates are within a distance  $r_0$  of one another, and the domain of the inverse must be trivially restricted. Thus we define  $G^{-1}(12, 1'2')$  only when both  $|\vec{r}_1 - \vec{r}_2| > r_0$  and  $|\vec{r}'_1 - \vec{r}'_2| > r_0$ , and we consider the condition which it is to satisfy, Eq. (24), only in this domain. Integrations such as those in the definition of the projection operator  $P^{(2)}$  are similarly restricted. One finds that these considerations are completely automatic, since  $G(12, 1'2')$  is never needed within the hard-core diameter.

We now take advantage of the new projection operator to obtain a kinetic equation for  $G(12, 1'2'; z)$ . We describe the details in Appendix A and give here the final result, namely

$$[z - L(12)] G(12, 1'2'; z) \\ = G(12, 1'2') + \int d^3 d^4 [\Sigma^{(s)}(12, 34) + \Sigma^{(c)}(12, 34; z)] \\ \times G(34, 1'2'; z). \quad (28)$$

The left-hand side contains the full two-body streaming operator since  $G(12, 1'2'; t)$  describes two particles at time  $t$ . The right-hand side contains a second memory function, whose static part is

$$\Sigma^{(s)}(12, 1'2') = - \int d^3 d^4 (Lg(12), g(34)) \\ \times G^{-1}(34, 1'2') - L(12)1(12, 1'2'), \quad (29)$$

which is to be compared with the corresponding expression for  $\Sigma^{(s)}(1, 1')$ , Eq. (14). It can be reduced to

$$\int d^3 d^4 \Sigma^{(s)}(12, 34) G(34, 1'2') \\ = \int d^3 [L_1(13) + L_1(23)] G(123, 1'2') \\ - \int d^3 d^4 d^5 F(12, 3) F^{-1}(3, 4) L_1(45) G(45, 1'2'), \quad (30)$$

where  $G(123, 1'2')$  is another static contracted correlation function like  $G(12, 1'2')$ :

$$G(123, 1'2') = F(123, 1'2') - \int d^1 d^2 F(123, 1'') \\ \times F^{-1}(1'', 2'') F(2'', 1'2'). \quad (31)$$

The collisional part of the new memory function is, according to the derivation in Appendix A,

$$\Sigma^{(c)}(12, 1'2'; z) = \int d^3 d^4 ([1/(z + Q^{(2)} Q^{(1)} L)] Q^{(2)} Q^{(1)} \\ \times Lg(12), Q^{(2)} Q^{(1)} Lg(34)) G^{-1}(34, 1'2'), \quad (32)$$

with  $Q_N^{(2)} = 1 - P_N^{(2)}$ . This is the analog of the expression for the first memory function, Eq. (15). Note that  $Q^{(2)}$  and  $Q^{(1)}$  commute.

In direct analogy with the first memory function, the second memory function describes the effect of the medium on two propagating particles. The static part gives a mean-field effect, and the collisional part gives the dynamics. We discuss this in more detail below, after indicating how the expansion proceeds to higher order.

We apply to  $\Sigma^{(c)}(12, 1'2'; z)$  the same program which was developed for  $\Sigma^{(c)}(1, 1'; z)$  beginning in Sec. II. Thus it is possible to extract interaction operators and to identify a new three-body contracted correlation function  $H(123, 1'2'3'; z)$  via

$$\int d^3 d^4 \Sigma^{(c)}(12, 34; z) G(34, 1'2') \\ = - \int d^3 d^3' [L_1(13) + L_1(23)] \\ \times [L_1(1'3') + L_1(2'3')] H(123, 1'2'3'; z), \quad (33)$$

where

$$H(123, 1'2'3'; z) \\ = ([1/(z + Q^{(2)} Q^{(1)} L)] \delta h(123), \delta h(1'2'3')), \quad (34)$$

and  $h(123)$  is the following three-body field:

$$h(123) = f(123) - \int d^4 d^5 F(123, 4) F^{-1}(4, 5) f(5) \\ - \int d^4 d^5 d^6 d^7 G(123, 45) G^{-1}(45, 67) g(67). \quad (35)$$

Physically,  $\delta h(123)$  is the portion of  $\delta f(123)$  which is orthogonal to both  $\delta f(1)$  and  $\delta h(12)$ . Thus  $H(z)$  is related to  $G(z)$  in the same way that  $G(z)$  is related to  $F(z)$ .

We can now construct a natural projection operator  $P^{(3)}$  for  $H(z)$  which projects onto the  $\delta h(123)$  axis via

$$P_N^{(3)} a(1 \cdots N) = \int d1'd2'd3'd4'd5'd6'(a, \delta h(1'2'3')) \\ \times H^{-1}(1'2'3', 4'5'6') \delta h(4'5'6', 1 \cdots N). \quad (36)$$

In this case the projection operator requires the static inverse of  $H$ , which satisfies

$$\int d4d5d6 H(123, 456) H^{-1}(456, 1'2'3') \\ = (1/3!) [\delta(1-1') \delta(2-2') \delta(3-3') + \text{perm. of } 1'2'3'] \quad (37)$$

This inverse is as well-founded as the earlier  $G^{-1}$ . Using the projection operator in the standard way, we find that  $H(z)$  satisfies a three-body kinetic equation of the form

$$[z - L(123)] H(123, 1'2'3'; z) \\ = H(123, 1'2'3') \\ + \int d4d5d6 \Sigma(123, 456; z) H(456, 1'2'3'; z). \quad (38)$$

The static part of the memory function turns out to be

$$\int d4d5d6 \Sigma^{(s)}(123, 456) H(456, 1'2'3') \\ = -(Lh(123), h(1'2'3')) - L(123) H(123, 1'2'3'), \quad (39)$$

in analogy with the two-body result, Eq. (29), and

$$F_{11}(z) = \frac{1}{z - L_{11} - \Sigma_{11}^{(s)} - L_{12} \frac{1}{z - L_{22} - \Sigma_{22}^{(s)} - L_{23} \frac{1}{z - L_{33} - \Sigma_{33}^{(s)} - H_{33} L_{32} G_{22}^{-1}}} G_{22} L_{21} F_{11}^{-1}} F_{11} \quad (44)$$

The kinetic equation for  $F(1, 1'; z)$  follows when each side is multiplied by the principal denominator on the right-hand side. Therefore each memory function also has a continued-fraction expansion given by a subset of the structure in Eq. (44), e.g.,

$$\Sigma_{11}^{(c)}(z) = L_{12} \frac{1}{z - L_{22} - \Sigma_{22}^{(s)} - L_{23} \frac{1}{z - L_{33} - \Sigma_{33}^{(s)} - H_{33} L_{32} G_{22}^{-1}}} G_{22} L_{21} F_{11}^{-1} \quad (45)$$

there is a corresponding expression for the dynamical part.

Thus we have a well-defined prescription for generating the expansion to arbitrary order. Since each level of description adds one more particle to the dynamics, the three-body level probably reaches the limit of practical applications. To summarize the results, it is useful to put the information together as a single kinetic equation for  $F(1, 1'; z)$ . We do this most conveniently by employing an operator notation which was defined earlier.<sup>7</sup> Very briefly, we write

$$F(1, 1'; z) = \langle 1 | F_{11}(z) | 1' \rangle, \\ G(12, 1'2'; z) = \langle 12 | G_{22}(z) | 1'2' \rangle, \text{ etc.} \quad (40)$$

so that the indices on the operators refer to the number of arguments. The Liouville operators are transcribed according to

$$L(1) \delta(1-1') = \langle 1 | L_{11} | 1' \rangle, \\ L(12) 1(12, 1'2') = \langle 12 | L_{22} | 1'2' \rangle, \quad (41) \\ \frac{1}{2} [L_1(11') \delta(1-2') + L_1(12') \delta(1-1')] = \langle 1 | L_{12} | 1'2' \rangle \\ = -\langle 1'2' | L_{21} | 1' \rangle.$$

Then the collisional part of the first memory function becomes, transcribing Eq. (19),

$$\Sigma_{11}^{(c)}(z) F_{11} = L_{12} G_{22}(z) L_{21}, \quad (42)$$

and the two-body kinetic equation becomes

$$[z - L_{22} - \Sigma_{22}^{(s)} - \Sigma_{22}^{(c)}(z)] G_{22}(z) = G_{22}. \quad (43)$$

Thus we arrive at a continued-fraction representation of  $F(1, 1'; z)$  of the form

With the representation in Eq. (44) we can immediately make contact with the Gross theory, in the form developed by the author.<sup>7</sup> We recover the first approximation (the modified Vlasov description) by neglecting all terms beyond  $\Sigma_{11}^{(6)}$ , the second approximation by neglecting all terms beyond  $\Sigma_{22}^{(6)}$ , and so forth. Equivalently, in the first approximation we take  $\Sigma^{(c)}(1, 1'; z) = 0$ , in the second approximation  $\Sigma^{(c)}(12, 1'2'; z) = 0$ , etc., thus ignor-

ing the dynamical effects associated with successive projection operators.

The theory can now be cast into potential-independent form via the steps noted earlier.<sup>6,7</sup> To illustrate, we give the reduced expressions for the kinetic equation in the second and third approximations. The equation of the second approximation has the form of (2) with an approximate collisional memory function given by

$$\begin{aligned} \Sigma^{(c)}(1, 1'; z) n \phi(p'_1) &\simeq \langle 1 | L_{12} (z - L_{22} - \Sigma_{22}^{(6)})^{-1} G_{22} L_{21} | 1' \rangle \\ &= \int d2d3d2'd3' \langle 1 | L_{12} G_{22} | 23 \rangle \langle 23 | [z G_{22} - (L_{22} + \Sigma_{22}^{(6)}) G_{22}]^{-1} | 2'3' \rangle \langle 2'3' | G_{22} L_{21} | 1' \rangle. \end{aligned} \quad (46)$$

The three matrix elements in the last expression have the following potential-independent forms:

$$\begin{aligned} \langle 1 | L_{12} G_{22} | 1'2' \rangle &= -in^2 \beta^{-1} \phi(p'_1) \phi(p'_2) \left( \frac{\partial g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_2)}{\partial \tilde{\mathbf{r}}_1} \cdot \frac{\partial \delta(1-1')}{\partial \tilde{\mathbf{p}}_1} + \frac{\partial g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_1)}{\partial \tilde{\mathbf{r}}_1} \cdot \frac{\partial \delta(1-2')}{\partial \tilde{\mathbf{p}}_1} \right) - in^3 \phi(p_1) \phi(p'_1) \phi(p'_2) \frac{\tilde{\mathbf{p}}_1}{m} \cdot \frac{\partial}{\partial \tilde{\mathbf{r}}_1} \\ &\times \left\{ [c(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_1) + c(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_2)] g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_2) - g(\tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}'_1 \tilde{\mathbf{r}}'_2) + n \int d^3 r_2 c(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2) g(\tilde{\mathbf{r}}_2 \tilde{\mathbf{r}}'_1 \tilde{\mathbf{r}}'_2) \right\}, \end{aligned} \quad (47)$$

$$\begin{aligned} \langle 12 | z G_{22} - (L_{22} + \Sigma_{22}^{(6)}) G_{22} | 1'2' \rangle &= 2n^2 \phi(p_1) \phi(p_2) g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2) [z - \bar{L}(12)] 1(12, 1'2') + (1 + P_{12})(1 + P_{1'2'}) in^3 \phi(p_1) \phi(p_2) \phi(p'_2) \\ &\times \left( -iz [g(\tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 \tilde{\mathbf{r}}'_2) - g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2) g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_2)] \delta(1-1') + \frac{\partial [g(\tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 \tilde{\mathbf{r}}'_2) - g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2) g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_2)]}{\beta \partial \tilde{\mathbf{r}}_1} \cdot \frac{\partial \delta(1-1')}{\partial \tilde{\mathbf{p}}_1} \right. \\ &\left. + [g(\tilde{\mathbf{r}}_1 \tilde{\mathbf{r}}_2 \tilde{\mathbf{r}}'_2) - g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}_2) g(\tilde{\mathbf{r}}_1 - \tilde{\mathbf{r}}'_2)] \frac{\tilde{\mathbf{p}}_1}{m} \cdot \frac{\partial \delta(1-1')}{\partial \tilde{\mathbf{r}}_1} \right) + z g(12, 1'2'), \end{aligned} \quad (48)$$

$$\langle 12 | G_{22} L_{21} | 1' \rangle = -\langle 1' | L_{12} G_{22} | 12 \rangle, \quad (49)$$

where  $\bar{L}(12)$  is the two-body Liouville operator with  $v(r)$  replaced by the potential of mean force  $\bar{v}(r) = -\beta^{-1} \ln g(r)$ ,  $P_{12}$  is the operator which interchanges variables 1 and 2, and  $g(12, 1'2')$  is the part of  $G(12, 1'2')$  which contains no  $\delta$  functions of the arguments.

Although this result looks somewhat complicated, it is still at the level of binary dynamics in an external field. If we make a diagonal approximation to the matrix elements by keeping only the first set of terms (those containing an over-all factor of  $n^2$ ), the memory function reduces to a simple and familiar form, namely the exact low-density memory function<sup>1-3</sup> with  $v(r)$  replaced by  $\bar{v}(r)$ . A result identical to the second approximation was originally obtained by Mazenko.<sup>8</sup> Beyond this point, however, his approach differs from the continued-fraction expansion, as he considers the connected and disconnected parts of the remaining terms taken as a whole.

In the third approximation, the renormalized form of the memory function is similar to that of the second approximation, Eq. (46), with a term added to the denominator; thus we obtain

$$\begin{aligned} \Sigma^{(c)}(1, 1'; z) n \phi(p'_1) &\simeq \int d2d3d2'd3' \langle 1 | L_{12} G_{22} | 23 \rangle \\ &\times \langle 23 | [z G_{22} - (L_{22} + \Sigma_{22}^{(6)}) G_{22} - \Omega_{22}(z)]^{-1} | 2'3' \rangle \\ &\times \langle 2'3' | G_{22} L_{21} | 1' \rangle, \end{aligned} \quad (50)$$

in which  $\Omega_{22}(z)$  serves as a correction to the two-particle motion due to dynamical correlations with a third particle. It is given by

$$\begin{aligned} \langle 12 | \Omega_{22}(z) | 1'2' \rangle &= \int d3d4d5d3'd4'd5' A(12, 345) \\ &\times M^{-1}(345, 3'4'5'; z) A(3'4'5', 1'2'), \end{aligned} \quad (51)$$

where

$$\begin{aligned} A(12, 1'2'3') &= \langle 12 | D_{23} - D_{21} F_{11}^{-1} F_{13} \\ &- (D_{22} - D_{21} F_{11}^{-1} F_{12}) G_{22}^{-1} G_{23} | 1'2'3' \rangle \\ &= -A(1'2'3', 12), \end{aligned} \quad (52)$$

$$\begin{aligned}
M(123, 1'2'3'; z) = & \langle 123 | z H_{33} - D_{33} + D_{32} G_{22}^{-1} G_{23} + G_{32} G_{22}^{-1} D_{23} - G_{32} G_{22}^{-1} D_{22} G_{22}^{-1} G_{23} + (G_{32} G_{22}^{-1} F_{21} - F_{31}) \\
& \times F_{11}^{-1} D_{11} F_{11}^{-1} (F_{12} G_{22}^{-1} G_{23} - F_{13}) | 1'2'3' \rangle, \tag{53}
\end{aligned}$$

and  $D_{j_r}$  is the initial value of the derivative of  $iF_{j_r}(t)$ , as worked out in Ref. 7. Since the  $D_{j_r}$ 's are given entirely in terms of the radial distribution functions, one sees that  $\Omega_{22}(z)$  and, therefore, the memory function of the third approximation are explicitly potential-independent. We have not attempted to reduce these quantities beyond the somewhat formal expressions given above (the radial distribution functions for two through six particles are involved). However, one can make the important checks that  $\Sigma^{(6)}$  has the correct symmetries, that it agrees to order  $n$  with the second approximation (and therefore with the low-density memory function), and that it agrees to order  $n^2$  with the triple-collision memory function.<sup>4</sup>

#### IV. DISCUSSION

In this paper we have shown how the Zwanzig-Mori projection operator formalism<sup>10,11</sup> can be used to deduce a renormalized kinetic theory.<sup>30</sup> In the case of full correlations this theory coincides with the predictions of the theory developed by Gross.<sup>6,31</sup> At a first glance the two approaches seem to have little in common. In the formulation given by Gross, one begins with the time-dependent  $N$ -body distribution function, which can always be written in the form

$$\rho_N(1 \cdots N, t) = \rho_{\text{eq}}(1 \cdots N) [1 + \Psi(1 \cdots N, t) - \langle \Psi(t) \rangle_{\text{eq}}]. \tag{54}$$

The approximation scheme consists in constraining  $\Psi$  first to be one-body additive, then two-body additive, etc. Since  $\rho_N(1 \cdots N, t)$  is symmetric in its arguments, this scheme exhausts all the possibilities, although it is difficult to make quantitative statements about the convergence properties. Combining the scheme with the BBGKY hierarchy and specializing to small departures from equilibrium, one arrives at successively larger systems of linear first-order equations for the family of two-time correlation functions  $\{F(1, 1'; t), F(12, 1'; t), F(123, 1'; t), \dots\}$ . The potential appears in both the streaming terms and the coupling terms. However, it enters in precisely those combinations which give the gradients of the radial distribution functions  $\{g(\vec{r}_1 \vec{r}_2), g(\vec{r}_1 \vec{r}_2 \vec{r}_3), \dots\}$ , and so it can be eliminated. This is a rather delicate process, since the potential cannot be eliminated separately from the streaming terms or the coupling terms. Having thus arrived at renormalized equations, one still has a long distance to go in order to obtain the appropriate kinetic equation,

i.e., an equation of the right form for  $F(1, 1'; t)$ . Eventually the memory function is found to have a symmetrized continued-fraction structure.<sup>7</sup>

Only at this point does one make contact with the approach developed in the present paper. As has long been appreciated, the projection-operator method gives an immediate expression for the memory function, albeit at the price of introducing a modified propagator. The Mori continued-fraction expansion<sup>28</sup> provides a natural continuation of this process, whereby the modified propagator is treated on the same level as the original propagator via the introduction of a second projection operator. One thus obtains a "memory function for the memory function," and so forth. In essence, the theme of the present paper is to extend this program to the correlation functions of interest in kinetic theory. We are led to projection operators which involve successively larger numbers of particles, and this establishes the essential similarity with the Gross theory. We recover the memory functions of that theory by ignoring dynamical effects associated with consecutive projection operators. Although the projection-operator method might appear more direct since it deals directly with the memory functions, it obviously depends upon a proper selection of projection operators. This is often a difficult task in the absence of *a posteriori* considerations.

If one grants that the projection operators are to involve successively more particles, there is an easy way to visualize the sequence derived in this paper. Since the first projection operator<sup>13</sup> projects onto the  $\delta f(1)$  axis, one might expect the second to project onto the  $\delta f(12)$  axis, the third onto the  $\delta f(123)$  axis, etc. [the  $f$ 's are defined in Eqs. (6) and (7)]. This is almost true, except that the axes should be orthogonal; hence one must apply the Gram-Schmidt procedure to the quantities  $\{\delta f(1), \delta f(12), \delta f(123), \dots\}$ . The result is the sequence of fields considered here,  $\{\delta f(1), \delta g(12), \delta h(123), \dots\}$ , and the operators project onto just these axes.

Once the general expansion is worked out, it can also be applied to the self-correlation function. To arrive at self correlations systematically from the full-correlation problem, we could consider a binary mixture and calculate the correlations of one species as its fugacity approaches zero, while using the same masses and potentials. In Appendix B we carry out the expansion within the context of a single tagged particle. The result is less complicated than in the case of full correlations since,

for example, the Vlasov-like kernel vanishes; the over-all structure of the expansions, however, is similar.

#### ACKNOWLEDGMENTS

The author would like to thank Professor N. R. Corngold for discussions concerning this general problem and for support, and J. B. Smith for useful criticism.

#### APPENDIX A: DERIVATION OF THE KINETIC EQUATION FOR $G(12, 1'2'; z)$

We start by considering the evolution of  $\exp(itQ_N^{(1)}L_N)\delta g(12)$ , working in the  $N$ -body system.

$$\begin{aligned} \frac{\partial}{\partial t} G(12, 34; t)G^{-1}(34, 56)\delta g(56) &= G(12, 34; t)G^{-1}(34, 56)(iQ^{(1)}L\delta g(56), \delta g(78))G^{-1}(78, 7'8')\delta g(7'8') \\ &+ (iQ^{(1)}LQ^{(2)}e^{itQ^{(1)}L}\delta g(12), \delta g(34))G^{-1}(34, 56)\delta g(56), \end{aligned} \quad (\text{A2})$$

with integrations implied over repeated variables. Now we multiply by  $\delta g(1'2')$  (again in the restricted domain) and take the ensemble average to obtain

$$\begin{aligned} \frac{\partial}{\partial t} G(12, 1'2'; t) &= -iG(12, 34; t) \\ &\times G^{-1}(34, 56)\bar{\Sigma}^{(s)}(56, 78)G(78, 1'2') \\ &+ (iQ^{(1)}LQ^{(2)}e^{itQ^{(1)}L}\delta g(12), \delta g(1'2')), \end{aligned} \quad (\text{A3})$$

with

$$\bar{\Sigma}^{(s)}(12, 34)G(34, 1'2') = -(L\delta g(12), \delta g(1'2')). \quad (\text{A4})$$

The first term on the right-hand side of Eq. (A3) contains the appropriate frequency matrix  $\bar{\Sigma}^{(s)}$  (to be reduced below), and the second term will give rise to the new collision operator.

In order to isolate the collision operator, i.e., the collisional part of the new memory function, we consider the complement of Eq. (A1), obtained by replacing the leftmost  $P_N^{(2)}$  by  $Q_N^{(2)}$ . Integrating this equation, we have

$$\begin{aligned} Q_N^{(2)}e^{itQ_N^{(1)}L_N}\delta g(12) \\ = i \int_0^t dt' G(12, 34; t')G^{-1}(34, 56) \\ \times e^{i(t-t')Q_N^{(2)}Q_N^{(1)}L_N}Q_N^{(2)}Q_N^{(1)}L_N\delta g(56), \end{aligned} \quad (\text{A5})$$

since the initial value is zero. We can now construct the last quantity in Eq. (A3), which becomes

We have

$$\begin{aligned} \frac{\partial}{\partial t} P_N^{(2)}e^{itQ_N^{(1)}L_N}\delta g(12) \\ = iP_N^{(2)}Q_N^{(1)}L_Ne^{itQ_N^{(1)}L_N}\delta g(12) \\ = iP_N^{(2)}Q_N^{(1)}L_N(P_N^{(2)}+Q_N^{(2)})e^{itQ_N^{(1)}L_N}\delta g(12), \end{aligned} \quad (\text{A1})$$

omitting the internal arguments (if there is a hard core, we consider this equation only in the domain  $|\bar{\mathbf{r}}_1 - \bar{\mathbf{r}}_2| > r_0$ ). Breaking up the right-hand side as indicated, we find that Eq. (A1) reads

$$\begin{aligned} (iQ^{(1)}LQ^{(2)}e^{itQ^{(1)}L}\delta g(12), \delta g(1'2')) \\ = - \int_0^t dt' G(12, 34; t')G^{-1}(34, 56) \\ \times (Q^{(1)}Le^{i(t-t')Q^{(2)}Q^{(1)}L}Q^{(2)}Q^{(1)}L\delta g(56), \delta g(1'2')). \end{aligned} \quad (\text{A6})$$

It is not difficult to see that the projection operators are Hermitian with respect to the inner product. Therefore in the last factor above we bring  $Q^{(1)}$  over to the right, where it can be dropped since  $Q^{(1)}\delta g(1'2') = \delta g(1'2')$ . We then bring  $L$  over to the right and insert  $1 = Q^{(2)}Q^{(1)} + P^{(2)} + P^{(1)}$  before the exponential. The  $P$ 's drop out and the right-hand side of Eq. (A6) becomes

$$\begin{aligned} - \int_0^t dt' G(12, 34; t')G^{-1}(34, 56)\Sigma^{(c)}(56, 78; t-t') \\ \times G(78, 1'2'), \end{aligned}$$

where  $\Sigma^{(c)}$  is as given by Eq. (32). It will be identified as the desired collisional term in the memory function.

Thus far the kinetic equation is given by

$$\begin{aligned} \frac{\partial}{\partial t} G(12, 1'2'; t) &= -iG(12, 34; t)G^{-1}(34, 56) \\ &\times \bar{\Sigma}^{(s)}(56, 78)G(78, 1'2') \\ &- \int_0^t dt' G(12, 34; t')G^{-1}(34, 56) \\ &\times \Sigma^{(c)}(56, 78; t-t')G(78, 1'2'), \end{aligned} \quad (\text{A7})$$

which is nearly in final form, except for the convention that the memory function is to matrix-multiply  $G(12, 1'2'; t)$  from the left. In order to bring this about, we note the following transpose properties:

$$G^{-1}(12, 34)\bar{\Sigma}^{(s)}(34, 56)G(56, 1'2') = -\bar{\Sigma}^{(s)}(1'2', 12), \quad (\text{A8})$$

$$G^{-1}(12, 34)\Sigma^{(c)}(34, 56; t)G(56, 1'2') = \Sigma^{(c)}(1'2', 12; -t), \quad (\text{A9})$$

which, upon substitution into Eq. (A7), give

$$\begin{aligned} & \frac{\partial}{\partial t} G(12, 1'2'; t) \\ &= i\bar{\Sigma}^{(s)}(1'2', 34)G(12, 34; t) \\ & \quad - \int_0^t dt' \Sigma^{(c)}(1'2', 34; -t+t')G(12, 34; t'). \end{aligned} \quad (\text{A10})$$

Next we interchange  $(12) \leftrightarrow (1'2')$  and take  $t \rightarrow -t$ , using the property

$$G(12, 1'2'; t) = G(1'2', 12; -t), \quad (\text{A11})$$

and obtain

$$\begin{aligned} & \frac{\partial}{\partial t} G(12, 1'2'; t) \\ &= -i\bar{\Sigma}^{(s)}(12, 34)G(34, 1'2'; t) \\ & \quad - \int_0^t dt' \Sigma^{(c)}(12, 34; t-t')G(34, 1'2'; t'). \end{aligned} \quad (\text{A12})$$

It is now quite straightforward to show that  $\bar{\Sigma}^{(s)}$  consists of the sum of two kinds of terms, one describing two-particle streaming and the other vanishing when the potential or density vanishes. They are, respectively,

$$\begin{aligned} \bar{\Sigma}^{(s)}(12, 1'2') &= L(12)l(12, 1'2') \\ & \quad + \Sigma^{(s)}(12, 1'2') \text{ (no integration),} \end{aligned} \quad (\text{A13})$$

with  $\Sigma^{(s)}$  as given in Eq. (30). After Laplace transforms are applied, the kinetic equation (A12) finally assumes the form quoted in Eq. (28).

#### APPENDIX B: SELF-CORRELATIONS

In this appendix we apply the projection-operator methods to the case of self-correlations. For convenience we use a field which tags the first particle in the  $N$ -body system according to<sup>29</sup>

$$f_s(1', 1 \cdots N) = N^{1/2} \delta(1' - 1) \quad (\text{B1})$$

in analogy with Eq. (6). This quantity gives the

self-correlation function defined in (5):

$$F_s(1, 1'; t) = (e^{iLt} f_s(1), f_s(1')), \quad (\text{B2})$$

the initial value of which is  $n\phi(p_1)\delta(1-1')$ . The inner product in Eq. (B2) is still the grand canonical average, and fluctuations in the field can be dropped for a sufficiently large system.

The basic kinetic equation for  $F_s(1, 1'; t)$  follows when we introduce a projection operator defined in each  $N$ -body system by

$$\begin{aligned} & P_{N_s}^{(1)} a(1 \cdots N) \\ &= \int d1'd2' (a, f_s(1')) F_s^{-1}(1', 2') f_s(2', 1 \cdots N). \end{aligned} \quad (\text{B3})$$

The resulting equation is<sup>14</sup>

$$\begin{aligned} & [z - L(1)] F_s(1, 1'; z) \\ &= F_s(1, 1') + \int d2 \Sigma_s(1, 2; z) F_s(2, 1'; z), \end{aligned} \quad (\text{B4})$$

with a memory function given by

$$\Sigma_s(1, 1'; z) n\phi(p_1') = \left( \frac{1}{z + Q_s^{(1)} L} Q_s^{(1)} L f_s(1), Q_s^{(1)} L f_s(1') \right). \quad (\text{B5})$$

There is no static part since the average force on a given particle vanishes.

When the interaction operators are removed from the inner product, the memory function is seen to involve a four-point correlation function as follows:

$$\begin{aligned} \Sigma_s(1, 1'; z) n\phi(p_1') &= - \int d2 d2' L_1(12) L_1(1'2') \\ & \quad \times \left( \frac{1}{z + Q_s^{(1)} L} g_s(12), g_s(1'2') \right), \end{aligned} \quad (\text{B6})$$

where  $g_s(1'2')$  is the field which has the tagged particle located at point  $1'$  and any other particle located at point  $2'$ , minus the portion parallel to the previously defined field:

$$\begin{aligned} g_s(1'2', 1 \cdots N) &= f_s(1'2', 1 \cdots N) \\ & \quad - \int d3'd4' (f_s(1'2'), f_s(3')) \\ & \quad \times F_s^{-1}(3', 4') f_s(4', 1 \cdots N), \end{aligned} \quad (\text{B7})$$

with

$$f_s(1'2', 1 \cdots N) = N^{1/2} \delta(1' - 1) \sum_{\alpha=2}^N \delta(2' - \alpha). \quad (\text{B8})$$

Thus  $g_s(12)$  serves as the self-correlation analog

of  $g(12)$ . In Eq. (B6),  $g_s(12)$  and  $g_s(1'2')$  can be replaced by, respectively,  $f_s(12)$  and  $f_s(1'2')$  since the interaction operators wipe out the difference. It is more convenient to leave this equation as it stands, however, since we require the combination which has a well-defined static inverse. Specifically, defining a contracted correlation function by

$$G_s(12, 1'2') = (g_s(12), g_s(1'2')), \quad (\text{B9})$$

we can take

$$\int d3d4 G_s(12, 34) G_s^{-1}(34, 1'2') = \delta(1-1')\delta(2-2'), \quad (\text{B10})$$

whereas such an inverse condition can be shown to be impossible for the quantity  $F_s(12, 1'2') = (f_s(12), f_s(1'2'))$ . (Note that the unit matrix is not symmetrized since one particle is singled out.) For free particles we have

$$[z - L(12)] G_s(12, 1'2'; z) = G_s(12, 1'2') + \int d3d4 [\Sigma_s^{(s)}(12, 34) + \Sigma_s^{(c)}(12, 34; z)] G_s(34, 1'2'; z), \quad (\text{B14})$$

in which the static and collisional parts of the new memory function are

$$\Sigma_s^{(s)}(12, 1'2') = \int d3d4d5 [L_1(13) + L_1(23)] G_s(123, 45) G_s^{-1}(45, 1'2') - \int d3d4 F_s(12, 3) F_s^{-1}(3, 4) L_1(42') \delta(4-1'), \quad (\text{B15})$$

$$\begin{aligned} \int d3d4 \Sigma_s^{(c)}(12, 34; z) G_s(34, 1'2') = & - \int d3d3' [L_1(13) + L_1(23)] [L_1(1'3') + L_1(2'3')] \\ & \times \left( \frac{1}{z + Q_s^{(2)} Q_s^{(1)} L} h_s(123), h_s(1'2'3') \right), \end{aligned} \quad (\text{B16})$$

and the field  $h_s(123)$  is defined as in Eq. (35). We note that the static contribution to the above memory function is nonzero, in contrast with the one-particle case.

To arrive at higher approximations, we introduce a three-body projection operator, etc. The result is a continued-fraction representation of  $F_s(1, 1'; z)$  with the same over-all form as Eq. (44); each term can again be put into potential-independent form.

At the second level of approximation we drop the collisional contribution  $\Sigma_s^{(c)}(12, 1'2'; z)$  in Eq. (B14) and obtain a mean-field equation for self-correlations. In this case the mean field governs the propagation of two particles (the tagged particle and one of the others) through the

$$G_s^{-1}(12, 1'2') = \frac{1}{n^2 \phi(p_1) \phi(p_2)} \delta(1-1') \delta(2-2'). \quad (\text{B11})$$

Now we consider the time development of the correlation function which appears in  $\Sigma_s(1, 1'; z)$ , namely

$$G_s(12, 1'2'; z) = \left( \frac{1}{z + Q_s^{(1)} L} \delta g(12), \delta g(1'2') \right). \quad (\text{B12})$$

In order to do so, we define the new projection operator

$$\begin{aligned} P_{N_s}^{(2)} a(1 \cdots N) = & \int d1' d2' d3' d4' (a, g_s(1'2')) \\ & \times G_s^{-1}(1'2', 3'4') g_s(3'4', 1 \cdots N). \end{aligned} \quad (\text{B13})$$

By following lines similar to those of Appendix A, we arrive at a two-body kinetic equation for  $G_s(z)$  of the form

medium. The corresponding kinetic equation for the self-correlation function has the form of Eq. (B4), and we can show that the appropriate memory function is

$$\begin{aligned} \Sigma_s(1, 1'; z) n \phi(p_1') \approx & \int d2d3d2'd3' A_s(1, 23) \\ & \times M_s^{-1}(23, 2'3'; z) A_s(2'3', 1'), \end{aligned} \quad (\text{B17})$$

where

$$\begin{aligned} A_s(1, 1'2') = & -i n^2 \beta^{-1} \phi(p_1') \phi(p_2') \frac{\partial g(\vec{r}_1 - \vec{r}_2')}{\partial \vec{r}_1} \cdot \frac{\partial \delta(1-1')}{\partial \vec{p}_1} \\ = & -A_s(1'2', 1), \end{aligned} \quad (\text{B18})$$

$$\begin{aligned} M_s(12, 1'2'; z) = & n^2 \phi(p_1) \phi(p_2) g(\vec{r}_1 - \vec{r}_2) [z - \bar{L}(12)] \delta(1-1') \delta(2-2') + i n^3 \phi(p_1) \phi(p_2) \phi(p_2') \\ & \times \left( -iz [g(\vec{r}_1 \vec{r}_2 \vec{r}_2') - g(\vec{r}_1 - \vec{r}_2) g(\vec{r}_1 - \vec{r}_2')] \delta(1-1') + \frac{\partial [g(\vec{r}_1 \vec{r}_2 \vec{r}_2') - g(\vec{r}_1 - \vec{r}_2) g(\vec{r}_1 - \vec{r}_2')]}{\beta \partial \vec{r}_1} \cdot \frac{\partial \delta(1-1')}{\partial \vec{p}_1} \right. \\ & \left. + [g(\vec{r}_1 \vec{r}_2 \vec{r}_2') - g(\vec{r}_1 - \vec{r}_2) g(\vec{r}_1 - \vec{r}_2')] \frac{\vec{p}_1}{m} \cdot \frac{\partial \delta(1-1')}{\partial \vec{r}_1} \right), \end{aligned} \quad (\text{B19})$$

which are simplifications of the corresponding expressions for full correlations, Eqs. (47)–(49). This memory function serves as a renormalized generalization of the low-density memory function,<sup>3,17,19</sup> with which it agrees to lowest order in the density. It is also to be noted that if we make a diagonal approximation to the renormalized propagator by omitting the second term of  $M_s(12, 1'2'; z)$ , we recover the low-density memory function but with  $v(r)$  replaced by the potential of mean force.

In a theory of self-correlations developed recently by Mazenko,<sup>29</sup> a two-body kinetic equation is

constructed for  $F_s(12, 1'2'; z)$ , evolving according to the natural propagator, rather than for  $G_s(12, 1'2'; z)$ . It now appears that various ambiguities stemming from the invertibility question can be avoided if we deal with the latter function, as is done here. One of the chief results of Ref. 29 is obtained by truncating the appropriate two-body memory function at the static level, thus giving rise to a kinetic equation for  $F_s(1, 1'; z)$  with a memory function denoted by  $\varphi_s^0(12)$ . It can be shown that this equation is the same as our second level of approximation.

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\*Research supported by the National Science Foundation under Grant No. GP-9626.

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