

A Diagrammatic Formulation of the Kinetic Theory of Fluctuations in Equilibrium Classical Fluids. II. Equations of Motion of the Fluctuation Fields and Their Diagrammatic Solution

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This is the second of a series of papers that presents a kinetic theory of fluctuations in equilibrium classical fluids that (i) makes extensive use of diagrammatic techniques in its development and (ii) will facilitate the use of diagrammatic techniques in the derivation of approximate kinetic theories. We focus on atomic liquids, but the results are easily generalizable to molecular liquids. The fundamental fluctuating quantity in the theory is $f(\mathbf{R}, \mathbf{P})$, which is the density of atoms at points in single particle phase space. The time correlation function for fluctuations of this quantity from its average, $\langle \delta f(\mathbf{R}, \mathbf{P}, t) \delta f(\mathbf{R}', \mathbf{P}', t') \rangle$, is the most basic correlation function of concern in generalized kinetic theories of fluctuations in liquids. In this paper, we derive a diagrammatic expression for this correlation function and for multipoint generalizations of it. The result allows us to make contact with the fully renormalized kinetic theory of Mazenko and show the equivalence of the results of the current approach to those of Mazenko; it is also the starting point for a graphical analysis of the various multipoint functions that appear in the renormalized kinetic theory.

1. Introduction

In the first paper of this series, denoted as I,¹ we reviewed some of the history of the kinetic theory of fluctuations in equilibrium atomic liquids and, in particular, the history of the development of kinetic equations for the time correlation function of the density of atoms in single particle phase space. This density is often called $f(\mathbf{R}, \mathbf{P}; t)$, and the correlation function of interest is $\langle f(\mathbf{R}, \mathbf{P}; t) f(\mathbf{R}', \mathbf{P}'; 0) \rangle$, where the angular brackets denote an appropriate equilibrium ensemble average. The most extensive formal development along this line was that of Mazenko.^{2,3} He derived expressions for the memory function associated with this correlation function in terms of a function G , which is a function of four positions and momenta and one time interval. He also derived exact expressions to describe the time evolution of G . Much of the formal and quantitative kinetic theory of liquids of the last two decades is based on his work. We noted in I that Boley⁴ and Lindendorf,⁵ who were building on the work of Gross,^{6–8} showed that much of the structure of Mazenko's theory can be obtained by introducing a specific set of basis functions (which we call the "fluctuation basis") for the Hilbert space of dynamical variables and constructing projection operators using this basis set.

In I, we discussed the process by which the fluctuation basis is constructed; this is a process that assumes the existence of certain functions related to equilibrium static correlation functions of the density and the existence of their inverse functions. We proved several theorems about the existence of these functions and about their cluster properties, i.e., about their behavior when one or more of the arguments is separated from the others. These theorems are basic to the development of the cluster theory to be presented in this paper and later papers in this series.

In section 2 of this paper, the results of I are used to construct a field theory that describes the dynamics of density fluctuations. The equations of motion of the fundamental fields are derived. The theory has the remarkable feature of being a linear field theory (with, however, rather complicated fields that are nonlinearly related to the density). Some of the properties of the vertices that appear in the field theory are derived, and it is shown that they are fully renormalized, in the sense of Mazenko. In section 3, the equations of motion are solved exactly and the solution is expressed in a simple diagrammatic form. Section 4 applies the results to the calculation of the usual phase space density correlation function and makes contact with Mazenko's theory.

This work lays the basis for another graphical formulation, to be discussed in the third paper of this series, that goes beyond the formulation of Mazenko. In the new formulation, the dynamics of both the correlation functions and the memory functions are expressed in terms of the same types of diagrams in a way that facilitates the derivation of exact and approximate relationships between them. In particular, the assumptions underlying the various versions of mode-coupling theory are specific types of relationships between the two types of functions, and the diagrammatic theory is of a form that will facilitate the derivation of mode-coupling approximations and corrections to mode-coupling theories.

The system of interest in this paper is an equilibrium fluid of point particles with a pairwise additive interparticle potential. The initial state of the system at time zero is specified by the number of particles N and their positions and momenta $\mathbf{r}_1 \mathbf{p}_1 \dots \mathbf{r}_N \mathbf{p}_N$, which will be abbreviated as $\mathbf{r}^N \mathbf{p}^N$. The probability distribution function for the initial state is that of the grand canonical ensemble. (See I for a more complete discussion of the notation.)

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2. Equations of Motion for the Fundamental Fields

The first paper (I) defined three sets of fields that can be used to discuss density fluctuations of an atomic fluid: $f(1)$, $\psi_n(1...n)$ for $n \geq 0$, and $\phi_n(1...n)$ for $n \geq 0$. Here, an integer, such as 1, is an abbreviation for a point in single particle phase space, such as $(\mathbf{R}_1, \mathbf{P}_1)$. The first field, $f(1)$, is the density in single particle phase space and is defined in eq 2 of I. The ψ_n field is a product of n f fields for its various arguments. For example, $\psi_2(12) = f(1)f(2)$; see eqs 3–6 of I for the complete definition of ψ_n . The subscript n on ψ_n and ϕ_n is a fluctuation index. It tells the number of phase point arguments of the function, and it implies that the function describes correlations among fluctuations at n points in phase space. The ϕ_n fields are members of the fluctuation basis, which is discussed in detail in I. Each ϕ_n field is a linear combination of ψ_m fields for $m \leq n$. Here, we use the phrase “field” to describe a dynamical variable (i.e., a function of $N, \mathbf{r}^N, \mathbf{p}^N$) that is dependent on additional arguments, such as a fluctuation index and one or more phase point variables. Although a dynamical variable for a specific system in the ensemble derives its time dependence from the dynamics of the $\mathbf{r}^N, \mathbf{p}^N$ variables, for these particular fields it is possible to obtain closed equations of motion for the fields themselves, with no direct reference to the time dependence of the $\mathbf{r}^N, \mathbf{p}^N$ variables.

In the case of the $f(1)$ fields, the closed equations of motion are nonlinear, as we shall see below. The nonlinearity is, of course, a source of complication; however, an even greater complication arises from the fact that the formal solution for the time-dependent correlation function $\langle f(1;t)f(1';0) \rangle$ contains infinitely many moments of the f variables at time zero (i.e., averages such as $\langle f(1)f(1') \rangle$ and $\langle f(1)f(2)f(1') \rangle$).

When fields ψ_n for all n are used, the closed equations of motion are *linear*. However, the formal solution for the equivalent correlation function $\langle \psi_1(1;t)\psi_1(1';0) \rangle$ contains infinitely many moments of the form $\langle \psi_m(1...m)\psi_1(1') \rangle$.

However, when the fluctuation basis (ϕ_n for all n) is used, the formal solution for the closely related correlation function $\langle \phi_1(1;t)\phi_1(1';0) \rangle$ contains initial moments only of the form $\langle \phi_1(1'')\phi_1(1') \rangle$. The “cost” of this simplification is that the coupling coefficients in the equations of motion for the fields contain rather complicated functions that represent the renormalized interactions of Gross and Mazenko.

In this section, we derive the three sets of equations of motion and examine some of their formal properties.

The time-dependent version of the f fields is given by

$$f(1;t) = \sum_{i=1}^N \delta(1;i(t)) \quad (1)$$

where $\delta(1;i(t)) = \delta(\mathbf{R}_1 - \mathbf{r}_i(t))\delta(\mathbf{P}_1 - \mathbf{p}_i(t))$. Each term $\mathbf{r}_i(t)$ and $\mathbf{p}_i(t)$ is a function of t and of the initial state $N, \mathbf{r}^N, \mathbf{p}^N$.

By elementary methods, using Hamilton’s equations, it is straightforward to show that

$$\dot{f}(1;t) = \int d1' V_{11}(1;1') f(1';t) + \int d1' d2' V_{12}(1;1'2') f(1';t) f(2';t) \quad (2)$$

where

$$V_{11}(1;1') \equiv -\frac{\mathbf{P}_1}{m} \cdot \nabla_{\mathbf{R}_1} \delta(1;1')$$

$$V_{12}(1;1'2') \equiv \nabla V(\mathbf{R}_1 - \mathbf{R}_{2'}) \cdot \nabla_{\mathbf{P}_1} \delta(1;1')$$

(This form of the result is obtained only if it is assumed that $\nabla V(0) = 0$. Most real and model interatomic potentials do not satisfy this condition; however, by modifying the potential at short distances, where the potential is much larger than kT , it is possible to satisfy this condition without changing the physical effect of the model potential.) The important feature of these equations is that they are closed nonlinear equations of motion for the f fields that are local in time, with the coupling coefficients in the equations of motion being independent of time.

The equations of motion for the set of ψ fields is obtained immediately from the definition of ψ_n and the equation of motions for f (see eq 2). The result is

$$\dot{\psi}_n(1...n;t) = \sum_{i=1}^n \int d1' V_{11}(i;1') \psi_n(1...n[1'/i];t) + \sum_{i=1}^n \int d1' d2' V_{12}(i;1'2') \psi_{n+1}(1...n2'[1'/i];t) \quad (3)$$

where $(1...n[1'/i])$ represents the argument list obtained by replacing i by $1'$ in $(1...n)$. These are closed equations of motion for the ψ_n fields; however, in this case, the equations are linear in the fields.

Each of the fluctuation basis functions ϕ is a linear combination of the ψ functions, with ϕ_n being a linear combination of ψ_m for $0 \leq m \leq n$. The coefficients in these linear combinations are fixed quantities, defined by the construction of the fluctuation basis, and are independent of time. Thus, it follows immediately that the equations of motion for the ϕ fields are a closed linear set of equations with coupling coefficients that are independent of time.

$$\dot{\phi}_n(1...n;t) = \sum_{m=0}^{\infty} \frac{1}{m!} \int d1'...dm' \times Q_{nm}(1...n;1'...m') \phi_m(1'...m';t) \quad (4)$$

Because of the symmetry of ϕ_m with regard to permutation of its m phase point arguments, Q_{nm} can, without loss of generality, be chosen to be symmetric under permutation of its right arguments. In principle, the coefficients Q can be expressed in terms of V_{11} and V_{12} , using the linear relationship between the ψ and ϕ functions. This can be a tedious exercise; moreover, it fails to use an important simplifying feature of the fluctuation basis.

An alternative approach relies on the fact that the quantities Q are independent of time. Thus, we can evaluate them by considering $t = 0$ in the previous equation. At $t = 0$, $\dot{f}_n = iL\phi_n$, where L is the Liouville operator. Thus, the previously described equation, at $t = 0$, is equivalent to the following equation for vectors in the Hilbert space:

$$iL|\phi_n(1...n)\rangle = \sum_{m=0}^{\infty} \frac{1}{m!} \int d1'...dm' \times Q_{nm}(1...n;1'...m') |\phi_m(1'...m')\rangle$$

By taking the inner product with $\langle \phi_p(1''...p'')|$, making use of the orthogonality of the fluctuation functions with different values of the subscript, multiplying on the left by $K_p(1'''...p''';1''...p'')$ (which is the inverse function to F_p ; see eq 2.11 of I), integrating over the doubly primed variables, and using

the symmetry of Q mentioned previously, we get

$$Q_{nm}(1...n;1'...m') = \frac{1}{m!} \int d1''...dm'' K_m(1'...m';1''...m'') \times \langle \phi_m(1''...m'') | iL | \phi_n(1...n) \rangle \quad (5)$$

It can be shown (see Appendix A) that

$$\langle \phi_m | iL | \phi_n \rangle = 0 \quad (\text{if } |m - n| > 1, \text{ or } m = 0, \text{ or } n = 0)$$

for any values of the phase point arguments of the functions. This is a consequence of the way in which the fluctuation basis was constructed, as well as the fact the Liouville operator is Hermitian. It relies also on the assumption that the interparticle interactions are pairwise additive. It follows that

$$Q_{nm}(1...n;1'...m') = 0 \quad (\text{if } |m - n| > 1, \text{ or } m = 0, \text{ or } n = 0) \quad (6)$$

The Q_{nm} terms are the coupling coefficients in the time-dependent field theory that uses the fluctuation basis functions as the fundamental fields. These coefficients are expressed in eq 5 in terms of two types of functions. The first are the K_m functions, which, as shown in I, can be expressed in terms of moments and cumulants of the single point density and of functions closely related to them. The second are matrix elements of the Liouville operator between members of the fluctuation basis. In Appendix A, we show that such matrix elements also can be expressed in terms of moments and cumulants of the single point density, with no explicit reference to the interparticle potential. This establishes that the Q_{nm} coupling coefficients are fully renormalized, in the sense used by Mazenko³ and Gross;⁶⁻⁸ specifically, they can be expressed in terms of the static equilibrium correlation functions of the fluid with no explicit reference to the form of the interparticle potential.

3. Diagrammatic Solution of the Equations of Motion for the ϕ Fields

The linear equations of motion for the ϕ_n fields are simple enough that they can be solved directly without the use of diagrammatic techniques. However, because those techniques will be needed later for other developments of the theory, we will introduce them at this point.

Each $\phi_n(1...n)$ field is dependent on its fluctuation index n and on n phase point variables $(1...n)$, each of which is a combination of a position \mathbf{R}_i and a momentum \mathbf{P}_i . Each $\phi_n(1...n)$ field is also a function of $\mathbf{r}^N \mathbf{p}^N$ and, hence, corresponds to a vector in the Hilbert space $|\phi_n(1...n)\rangle$. Each ϕ field is symmetric under an interchange of its phase point arguments. For example, $\phi_2(12)$ and $\phi_2(21)$ are the same function, and, hence, $|\phi_2(12)\rangle$ and $|\phi_2(21)\rangle$ are the same vector. Let us define a single symbol α that is a combination of a fluctuation index n and n unordered phase point variables. $\alpha \leftrightarrow (n; 1...n) (n; \mathbf{R}_1 \mathbf{P}_1... \mathbf{R}_n \mathbf{P}_n)$. The $|\phi(\alpha)\rangle$ term then denotes a member of the fluctuation basis, and distinct values of α correspond to distinct vectors. With this convention, the sum over m and the integration over the primed variables with the factor of $(m!)^{-1}$ in eq 4 can be replaced by a sum over α with no factor of $(m!)^{-1}$. Equation 4 then becomes

$$\dot{\phi}(\alpha, t) = \sum_{\alpha'} Q(\alpha \alpha') \phi(\alpha', t) \quad (7)$$

where the sum over α' denotes a sum and integration over all the values of the variables in α that correspond to distinct vectors.

The initial condition for this differential equation is the value of $\phi(\alpha)$ at the initial time $t = 0$. It will be convenient to replace this initial condition by the condition that $\phi(\alpha, t) = 0$ for $t \rightarrow -\infty$ and put a source term in the differential equation. Thus, we have

$$\dot{\phi}(\alpha, t) = \sum_{\alpha'} Q(\alpha \alpha') \phi(\alpha', t) + \phi(\alpha) \delta(t)$$

where ϕ_α denotes the initial value. The solution of this equation gives the physically relevant $\phi_\alpha(t)$ function for $t > 0$. This is converted to an integral equation by integrating from $-\infty$ to t :

$$\phi(\alpha, t) = \Theta(t) \phi(\alpha) + \int_{-\infty}^t dt' \sum_{\alpha'} Q(\alpha \alpha') \phi(\alpha', t') \quad (8)$$

where $\Theta(t)$ is the Heaviside function.

To make the diagrammatic formulation more compact than it would otherwise be, we define a variable a that is a combination of variable α and variable t : $a \leftrightarrow (\alpha, t)$ ($n, 1...n, t$) $\leftrightarrow (n, \mathbf{R}_1 \mathbf{P}_1... \mathbf{R}_n \mathbf{P}_n, t)$. We define various functions of a variables in terms of previously defined functions.

$$Q(a; a') \equiv Q(\alpha \alpha') \delta(t - t')$$

$$\phi(a) \equiv \phi(\alpha, t)$$

$$\chi^{(0)}(a; a') \equiv \Theta(t - t') \delta(\alpha, \alpha') \quad (9)$$

$$\bar{\phi}(a) \equiv \phi(\alpha) \delta(t) \quad (10)$$

Let Σ_a be an abbreviation for $\sum_{\alpha} \int_{-\infty}^{\infty} dt$. With a change of variable names, the integral given in eq 8 then can be written as

$$\phi(a_1) = \sum_{a_2} \chi^{(0)}(a_1; a_2) \bar{\phi}(a_2) + \sum_{a_2 a_3} \chi^{(0)}(a_1; a_2) Q(a_2; a_3) \phi(a_3)$$

This equation can be formally solved by iteration.

$$\begin{aligned} \phi(a_1) &= \sum_{a_2} \chi^{(0)}(a_1; a_2) \bar{\phi}(a_2) + \\ &\quad \sum_{a_2, a_3, a_4} \chi^{(0)}(a_1; a_2) Q(a_2; a_3) \chi^{(0)}(a_3; a_4) \bar{\phi}(a_4) + \dots \\ &= \sum_{a_2} \chi(a_1; a_2) \bar{\phi}(a_2) \end{aligned} \quad (11)$$

where

$$\chi(a_1; a_2) \equiv \chi^{(0)}(a_1; a_2) + \sum_{a_3, a_4} \chi^{(0)}(a_1; a_3) Q(a_3; a_4) \chi^{(0)}(a_4; a_2) + \dots \quad (12)$$

This equation for $\chi(a_1; a_2)$ can be expressed in terms of diagrams in the following way:

$$\chi(a_1; a_2) = \text{the sum of all topologically different matrix diagrams} \quad (13)$$

with (i) a left root labeled a_1 , (ii) a right root labeled a_2 , (iii) free points, (iv) $\chi^{(0)}$ bonds, and (v) Q vertices; such that (i) each root is attached to a $\chi^{(0)}$ bond and (ii) each free point is attached to a $\chi^{(0)}$ bond and a vertex Q . (See Figure 1 for pictures of

$$\chi(a_1; a_2) = a_1 \circ \leftarrow \circ a_2 + a_1 \circ \leftarrow \bullet \bigcirc Q \bullet \leftarrow \circ a_2 + a_1 \circ \leftarrow \bullet \bigcirc Q \bullet \leftarrow \bullet \bigcirc Q \bullet \leftarrow \circ a_2 + \text{etc.}$$

Figure 1. Graphical series for the response function $\chi(a_1; a_2)$ given in eq 13. In each diagram, the small open circles on the left and right are root points corresponding to the arguments of the function on the left-hand side of the equation. The small filled circles in all but the first diagram are free points, corresponding to dummy integration and summation variables used in evaluating the diagram. The horizontal lines with arrowheads pointing to the left are $\chi^{(0)}$ bonds. The large circles with the letter Q inside are Q vertices. Each diagram has a value that can be calculated from the structure of the diagram. For example, the value of the second diagram is obtained by assigning dummy variables a_3 and a_4 to the two free points and evaluating the following quantity: $\sum_{a_3 a_4} \chi^{(0)}(a_1; a_3) Q(a_3; a_4) \chi^{(0)}(a_4; a_2)$. (See Appendix A of I for a more complete discussion of the diagrams and their evaluation. In the present paper, the symmetry numbers of all the diagrams are unity.)

some of these diagrams. Also see Appendix A of I for a summary of the graphical theoretic formulation that we use. Note that the function $\chi^{(0)}$ is represented as a line or a bond with an arrowhead on it. The arrow points from the right argument to the left argument.)

The function χ is the Green function for the equations of motion of the fields defined by the fluctuation basis. It is a causal response function, in that it can be regarded as describing the response at a later time to an external perturbation of the fields. (The “turning on” of the initial condition for the fields is an example of such an “external” perturbation.) Each diagram in the series for χ (see Figure 1) consists of an alternating series of arrows (the $\chi^{(0)}$ bonds) and vertices Q, starting at the root corresponding to the right argument, moving left, and ending on the root corresponding to the left argument. The $\chi^{(0)}$ bond is an unperturbed version of the response function.

The correlation function of the fluctuation basis fields can be evaluated using eqs 11 and 10. The result is

$$\langle \phi(\alpha_1, t_1) \phi(\alpha_2, 0) \rangle = \sum_{\alpha_3} \chi(a_1; a_3) \delta(t_3) \langle \phi(\alpha_3) \phi(\alpha_2) \rangle$$

It follows from the orthogonality properties of the fluctuation basis that the average on the right side of this equation is zero unless $n_2 = n_3$. It follows that

$$\langle \phi(\alpha_1, t_1) \phi(\alpha_2, 0) \rangle = \sum_{\alpha_3} \chi(a_1; a_3) \delta(t_3) \delta_{n_3, n_2} \langle \phi(\alpha_3) \phi(\alpha_2) \rangle$$

or

$$C_{nm}(1 \dots n, t_1; 1' \dots m', 0) \equiv \langle \phi_n(1 \dots n, t_1) \phi_m(1' \dots m', 0) \rangle$$

$$= \frac{1}{m!} \int d1'' \dots dm'' \chi_{nm}(1 \dots n, t_1; 1'' \dots m'', 0) \times F_m(1'' \dots m''; 1' \dots m') \quad (15)$$

Here, we are using a notational convention that allows a function of two fluctuation indices to be written with the fluctuation indices as subscripts. In converting from a sum over α_3 (which is a sum over distinct vectors) to a sum over n_3 and an integral over $1'' \dots m''$, a factor of $1/m!$ must be introduced to avoid overcounting.

A remarkable feature of this result, which is one of the important consequences of use of the fluctuation basis, is that

the vertices that represent the *initial conditions* in the solution for $\langle \phi_n(1 \dots n, t) \phi_m(1' \dots m', 0) \rangle$ include only the $F_m = \langle \phi_m \phi_m \rangle$ term for the same index m as the second index on the correlation function. Thus, for example, when calculating $\langle \phi_1(1, t) \phi_1(2, 0) \rangle$, which describes the correlation function of single point fluctuations, no static correlation functions for ϕ_p fields for $p > 1$ appear in the final result, as a result of the initial conditions.

This is very different from the results that are obtained using the ψ functions as the basic fields. The same sort of analyses could be conducted, and a similar graphical expression for the correlation function would appear. However, the graphical expression for $\langle \psi_1(1, t) \psi_1(2, 0) \rangle$ would contain infinitely many functions of the form $\langle \psi_m \psi_1 \rangle$ for all values of m .

The calculation of the time-dependent correlation functions of the fluctuation fields has been reduced to the calculation of the static correlation functions and the calculation of the response function χ , and we have a formally exact diagrammatic series for this function.

4. Density Autocorrelation Function and the Relationship to Mazenko's Theory

Using the latest result, it is straightforward to derive memory function equations for the correlation functions. Let us focus on the correlation function of single point fluctuations: $C_{11}(1, t_1; 2, 0) = \langle \phi_1(1, t_1) \phi_1(2, 0) \rangle = \langle \delta f(1, t_1) \delta f(2, 0) \rangle$, where $\delta f(1) = f(1) - \langle f(1) \rangle$. According to eq 15, the response function to calculate is $\chi_{11}(1, t_1; 2, 0)$.

A straightforward graphical derivation of a memory function equation can be obtained if we decompose the unperturbed response function $\chi^{(0)}$ into three parts:

$$\chi^{(0)}(a; a') = \chi^{(0,0)}(a; a') + \chi^{(0,1)}(a; a') + \chi^{(0,>1)}(a; a') \quad (16)$$

where

$$\chi^{(0,0)}(a; a') = \delta_{n(a),0} \chi^{(0)}(a; a')$$

$$\chi^{(0,1)}(a; a') = \delta_{n(a),1} \chi^{(0)}(a; a')$$

$$\chi^{(0,>1)}(a; a') = (1 - \delta_{n(a),0} - \delta_{n(a),1}) \chi^{(0)}(a; a')$$

In these equations, $n(a)$ refers to the fluctuation index contained in a . The graphical series then becomes the following:

$\chi(a_1; a_2)$ = the sum of all topologically different matrix diagrams (17)

with (i) a left root labeled a_1 ; (ii) a right root labeled a_2 ; (iii) free points; (iv) $\chi^{(0,0)}$, $\chi^{(0,1)}$, and $\chi^{(0,>1)}$ bonds; and (v) Q vertices; such that (i) each root is attached to a $\chi^{(0,0)}$, $\chi^{(0,1)}$, or $\chi^{(0,>1)}$ bond and (ii) each free point is attached to a $\chi^{(0,0)}$, $\chi^{(0,1)}$, or $\chi^{(0,>1)}$ bond and a vertex Q. (See Figure 2 for some examples of these diagrams.) It can easily be shown that $\chi^{(0,0)}$ bonds have a role only in the graphical series for the trivial response function $\chi_{00}(t_1; t_2)$. Therefore, with the understanding that the formulas will be applied only to the nontrivial functions, we shall omit the mention of $\chi^{(0,0)}$ from subsequent expressions.

To derive a memory function equation for this response function, we use a procedure that is familiar from the derivation of the Dyson equation in many-body theory or the graphical derivation of the Ornstein–Zernike equation in the theory of equilibrium liquids. Consider the general diagram in the series for the case of $a_1 = (1, 1, t_1)$ and $a_2 = (1, 2, t_2)$ (see Figure 2). The bonds attached to the two roots must be $\chi^{(0,1)}$ bonds. One possibility is that these two bonds are the same bond; this is

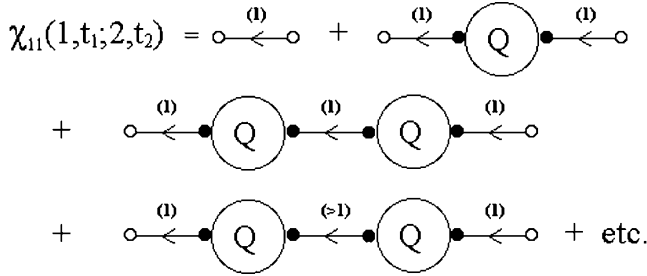


Figure 2. Graphical series for the response function in eq 17 for the specific case of $\chi_{11}(1, t_1; 2, t_2)$. In each diagram, the root point (small open circle) on the left should have the arguments $(1, t_1)$ attached, and the root circle on the right should have $(2, t_2)$ attached; however, these labels have been omitted for simplicity. A horizontal line with an arrowhead and “(1)” above it represents a $\chi^{(0,1)}$ bond. A horizontal line with an arrowhead and “(>1)” above it represents a $\chi^{(0,>1)}$ bond. (See the caption of Figure 1 for additional information.) Note that when the second diagram on the right is evaluated, the only nonzero contribution contains Q_{11} , because there is a $\chi^{(0,1)}$ on each side of the Q vertex. The same is true for the two Q vertices in the third diagram. In the fourth diagram, the same reasoning demands that the first Q vertex can only be Q_{1m} for some $m > 1$ and the second Q vertex can only be Q_{m1} for some $m > 1$. Because of eq 6, the only value of m that gives a nonzero contribution is $m = 2$.

the case in the diagram that has no Q vertices (see the first diagram in Figure 2). The other possibility is that there are at least two $\chi^{(0,1)}$ bonds in the diagram. If we move along the bonds and vertices going from the left root to the right root, we can locate the second $\chi^{(0,1)}$ bond that is encountered, the first being the bond that is attached to the a_1 root. The part of the diagram between those two bonds might be a single Q_{11} vertex (as in the second and third diagrams in Figure 2) or an alternating sequence of Q vertices and $\chi^{(0,>1)}$ lines, ending with a Q vertex (as in the fourth diagram). The second $\chi^{(0,1)}$ bond and everything between it and the a_2 root is a diagram in the series for the same response function that is being calculated, but with a different first argument. It follows that

$$\begin{aligned} \chi_{11}(1, t_1; 2, t_2) &= \chi^{(0,1)}(1, t_1; 2, t_2) + \int_{-\infty}^{\infty} dt_3 \int_0^{\infty} dt_4 \int d^3d^4 \\ &\times \chi^{(0,1)}(1, t_1; 3, t_3) \times (Q_{11}(3, t_3; 4, t_4) \delta(t_3 - t_4) + M(3, t_3; 4, t_4)) \\ &\times \chi_{11}(4, t_4; 2, t_2) \\ &= \chi^{(0,1)}(1, t_1; 2, t_2) + \int_{-\infty}^{t_1} dt_3 \int d^4 Q_{11}(1; 4) \chi_{11}(4, t_3; 2, t_2) + \\ &\int_{-\infty}^{t_1} dt_3 \int_0^{\infty} dt_4 \int d^4 M(1, t_3; 4, t_4) \chi_{11}(4, t_4; 2, t_2) \quad (18) \end{aligned}$$

The first term on the right-hand side is the value of the diagram with no vertex Q . The term containing Q is the value of the diagram with only a Q_{11} vertex separating the first two $\chi^{(0,1)}$ bonds. $M(3, t_3; 4, t_4)$ is the sum of the contributions of all the graphical objects (other than a single Q_{11} vertex) that can appear between the first and second $\chi^{(0,1)}$ bonds in a diagram of the series that we are analyzing. A graphical expression for it can be obtained by starting with the graphical expression for $\chi_{11}(1, t_1; 2, t_2)$, removing the $\chi^{(0,1)}$ bonds on the far left-hand and far right-hand side of each diagram, and discarding any diagrams that still have $\chi^{(0,1)}$ bonds. We get

$$M(1, t_1; 2, t_2) = \text{the sum of all topologically different matrix diagrams} \quad (19)$$

with (i) a left root labeled $(1, t_1)$, (ii) a right root labeled $(2, t_2)$, (iii) free points, (iv) $\chi^{(0,>1)}$ bonds, and (v) Q vertices; such that (i) each root is attached to a vertex Q and (ii) each free point is

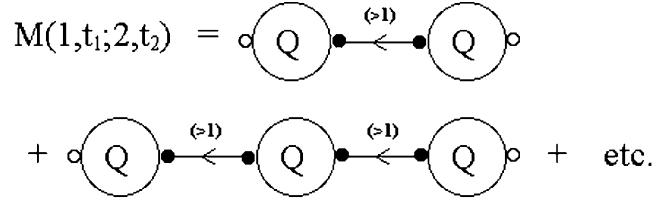


Figure 3. Graphical series for the memory function $M(1, t_1; 2, t_2)$ given in eq 19. In each diagram, the root point on the left should have the arguments $(1, t_1)$ attached, and the root on the right should have $(2, t_2)$; however, these labels have been omitted for simplicity. (See the captions of Figures 1 and 2 for additional information.) Note that, because of the arguments on the left root and other considerations discussed in Figure 2, the Q vertex on the far left of each diagram must be Q_{12} and the Q vertex on the far right must be Q_{21} .

attached to a $\chi^{(0,>1)}$ bond and a vertex Q . (See Figure 3 for some examples of these diagrams. Diagrams in this series have a chain of alternating Q vertices and $\chi^{(0,>1)}$ lines connecting the roots, with the roots being on Q vertices.)

Note that M is nonzero only if its left time argument is later than its right time argument. This follows from the structure of the diagrams and the time dependence of $\chi^{(0,>1)}$. Using this fact in eq 18 and then differentiating with respect to t_1 , we get

$$\begin{aligned} \frac{\partial}{\partial t_1} \chi_{11}(1, t_1; 2, t_2) &= \delta(1, 2) \delta(t_1 - t_2) + \int d^4 Q_{11}(1; 4) \\ &\times \chi_{11}(4, t_1; 2, t_2) + \int_{t_2}^{t_1} dt_4 \int d^4 M(1, t_1; 4, t_4) \chi_{11}(4, t_4; 2, t_2) \end{aligned}$$

To get the result for the corresponding correlation function, we use eq 15 for appropriate values of the arguments.

$$C_{11}(1, t_1; 2, 0) = \int d^3 \chi_{11}(1, t_1; 3, 0) F_1(3; 2)$$

Combining these latter two results, we get the following result for $t_1 > 0$:

$$\begin{aligned} \frac{\partial}{\partial t_1} C_{11}(1, t_1; 2, 0) &= \int d^3 Q_{11}(1; 3) C_{11}(3, t_1; 2, 0) + \\ &\int_0^{t_1} dt_3 \int d^3 M(1, t_1; 3, t_3) C_{11}(3, t_3; 2, 0) \quad (20) \end{aligned}$$

This is the usual kinetic equation for the correlation function of the single point density fluctuations. (See Appendix B for a detailed analysis.) The Q_{11} term contains the flow term and the Vlasov term. M is the “collisional” portion of the memory function. Moreover, we have a graphical series for M .

In each nonzero diagram in the series for M , the Q vertex that is attached to the left root must be a Q_{12} vertex, and the vertex attached to the right root must be a Q_{21} vertex. (See the captions of Figures 2 and 3 for a discussion of the relevant considerations.) Let the integration variables for the free point on the vertex Q attached to the left root be $(2; 34; t_3)$, and use $(2; 56; t_4)$ for the free point attached to the right root. We can then factor out the values of the left and right Q vertices, and obtain, after performing the trivial integrations over t_3 and t_4 ,

$$\begin{aligned} M(1, t_1; 2, t_2) &= \frac{1}{(2!)^2} \int d^3d^4d^5d^6 Q_{12}(1; 34) \\ &\times (\text{a function of } 34, t_1, 56, t_2) \times Q_{21}(56; 2) \quad (21) \end{aligned}$$

The factors of $1/(2!)$ arise because, in evaluating the diagram, we should be integrating over those values of $(34) \leftrightarrow (\mathbf{R}_3 \mathbf{P}_3, \mathbf{R}_4 \mathbf{P}_4)$ that correspond to distinct values of α . However, if we release the restriction and integrate over all (34) , we can correct for

the overcounting by inclusion of one factor of $1/(2!)$. The other factor arises in a similar way from the (56) variables.

The unspecified function in this equation represents the sum of the values of the diagrams in the series for M , except for the factors associated with the two Q vertices that are explicitly contained in this equation. The graphical expression for M leads to the following diagrammatic formulation of that function: the sum of all topologically different matrix diagrams with (i) a left root labeled $(2,34,t_1)$, (ii) a right root labeled $(2,56,t_2)$, (iii) free points, (iv) $\chi^{(0,>1)}$ bonds, and (v) Q vertices; such that (i) each root is attached to a $\chi^{(0,>1)}$ bond and (ii) each free point is attached to a $\chi^{(0,>1)}$ bond and a Q vertex. Compare this relation with that given in eq 17 for χ itself. The two have basically the same structure. The only difference is that eq 17 has three types of $\chi^{(0)}$ bonds, whereas this expression has only one type of χ bond.

This leads us to define the following quantity:

$$\begin{aligned} \chi^{(>1)}(a_1;a_2) &= \text{the sum of all the graphs in eq 17 for} \\ &\chi(a_1;a_2) \text{ that have no } \chi^{(0,0)} \text{ or } \chi^{(0,1)} \text{ bonds} \quad (22) \\ &= \text{the sum of all graphs in eq 13 for} \\ &\chi(a_1;a_2) \text{ with each } \chi^{(0)} \text{ bond replaced by a } \chi^{(0,>1)} \text{ bond} \end{aligned}$$

$\chi^{(>1)}$ is the response function χ with all terms deleted that make reference to the parts of the Hilbert space spanned by ϕ_0 and the set of $\phi_1(1)$. In effect, it contains projection operators that project out contributions from that portion of the Hilbert space. The function in the integral in eq 21 is equal to $\chi_{22}^{(>1)}(34,t_1;56,t_2)$. Hence, we have

$$M(1,t_1;2,t_2) = \frac{1}{(2!)^2} \int d3d4d5d6 Q_{12}(1;34) \times \chi_{22}^{(>1)}(34,t_1;56,t_2) Q_{21}(56;2) \quad (23)$$

This result is equivalent to that of Mazenko for the collisional portion of the memory function. In particular, the response function $\chi_{22}^{(>1)}$ is closely related to Mazenko's four-point G function. (See Appendix B for a discussion of the relationship of this expression to that of Mazenko.)

5. Discussion

In this paper, we have presented a formally exact theory of the time correlation functions of phase space density fluctuations in an atomic fluid at equilibrium. The organizing principles for the construction of the theory are as follows: (i) the use of the fluctuation basis for the Hilbert space of dynamical variables to define the fundamental fields of a field theory; (ii) the solution of the linear equations of motion for these fields by perturbation theory; and (iii) the use of diagrammatic series to represent the various functions that appear in the theory. We have established that the theory has the same structure as that of Mazenko and have obtained diagrammatic expressions for some of the functions that appear in Mazenko's theory.

In the third paper of this series, we will start at this point and derive a second graphical representation that will be more useful in developing approximations for the numerical calculation of correlation functions. It will be used to obtain the fundamental cluster properties of the correlation functions and response functions that are central to the theory, to obtain a new form of graphical series for the memory function of the phase space density correlation function and to indicate how

mode-coupling approximations can be obtained in a straightforward manner.

The methodology in the present paper is a special case of a more general diagrammatic theory for classical systems that we have developed^{9,10} using the ideas of Martin, Siggia, and Rose.¹¹ The more general theory is not needed for the calculation of two-time correlation functions when the fluctuation basis is employed; however, it would be required to investigate correlation functions that involve three or more times. A characteristic of the original Martin–Siggia–Rose method, as well as of our development of it and the special case discussed in this paper, is that response functions have a central role in the theory, on a level that is equally as important as the correlation functions themselves. The response functions have a simple diagrammatic structure, and other functions of interest are obtained directly from them. (Correlation functions are obtained by post-multiplication of a response function by static correlation functions. Memory functions are obtained by sandwiching a response function between two interactions.)

The use of the fluctuation basis for the construction of a kinetic theory is not limited to classical systems that obey Hamiltonian mechanics. We have recently shown^{12,13} how this type of basis can be applied to the derivation of kinetic theories of spin systems that obey stochastic dynamics. We suspect that similar methods would also be useful for colloidal systems and Brownian dynamics.

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Appendix A. Matrix Elements of the Liouville Operator

A.1. Selection Rule for Matrix Elements of the Liouville Operator in the Fluctuation Basis. A.1.1. Theorem. $\langle \phi_m | iL | \phi_n \rangle = 0$ if $|m - n| > 1$ or $m = 0$ or $n = 0$ for any values of the phase point arguments of the functions.

A.1.2. Proof. If $n = 0$, then $L\phi_n = 0$ and the matrix element is clearly zero. If $m = 0$, we use the Hermitian nature of L to conclude that the matrix element is zero.

In I, we defined \mathcal{J}_n for each n as the subspace spanned by the ϕ_n functions. It will be helpful to define \mathcal{T}_n as the subspace of the Hilbert space spanned by all the $|\phi_m\rangle$ for $0 \leq m \leq n$. As a result of the procedure for constructing the fluctuation basis, every vector in \mathcal{J}_n is orthogonal to every vector in \mathcal{T}_m for $n > m$. Each $|\psi_n\rangle$ is in \mathcal{T}_n . Moreover, \mathcal{T}_n is in \mathcal{T}_m if $n < m$.

Equation 3 leads to the conclusion that $|\psi_n\rangle$ is in \mathcal{T}_{n+1} . Using the general relationship $\dot{A} = iLA$ for any dynamical variable, we conclude that $iL|\psi_n\rangle$ is in \mathcal{T}_{n+1} . Because ϕ_n is a linear combination of ψ_m for $m \leq n$, it follows that $iL\phi_n$ is in \mathcal{T}_{n+1} . It follows that $\langle \phi_m | iL | \phi_n \rangle$ is zero if $m > n + 1$. Using the Hermitian character of L , it follows that the matrix element is zero if $n > m + 1$. Q.E.D.

We note that the vanishing of the matrix element for $|m - n| > 1$ is a consequence of the pairwise additivity of the interparticle potential. If there were three-particle terms in the potential energy, the corresponding condition for the vanishing of the matrix element would be $|m - n| > 2$.

A.2. Poisson Bracket Relationships for Matrix Elements of the Liouville Operator and Renormalizability of the Interactions. In the current theory, matrix elements of the Liouville operator, such as $\langle B | iL | A \rangle$, can be calculated directly

by calculating the action of the Liouville operator on A and then calculating the inner product. An alternative method is to use the following general relationship:

$$\langle B|iL|A\rangle = -kT\langle\{B,A\}\rangle$$

where the Poisson bracket of two dynamical variables is defined as

$$\{B,A\} \equiv \sum_{i=1}^N ([\nabla_{\mathbf{r}_i} B][\nabla_{\mathbf{p}_i} A] - [\nabla_{\mathbf{p}_i} B][\nabla_{\mathbf{r}_i} A])$$

(We use the convention that derivative operators do not act beyond the bounds defined by square brackets. Thus, for example, the $\nabla_{\mathbf{r}_i}$ operator in the first term on the right acts only on B .) This relationship, which can be derived in a straightforward manner, has been used by Gross⁸ in the discussion of the renormalizability of kinetic theory.

The derivatives that appear here involve the particle positions and momenta. When the variables A and B are the fundamental fields, such as $\psi_n(1\dots n)$ and $\phi_n(1\dots n)$, it is possible, by straightforward means, to obtain corresponding relationships that involve derivatives with regard to the field point arguments. The basis for this is the simple identity

$$\{\delta(1;i), \delta(2;j)\} = \delta_{ij} \int d3 D(123) \delta(3;i)$$

where $D(123) \equiv [(\nabla_{\mathbf{r}_1} \cdot \nabla_{\mathbf{p}_2} - \nabla_{\mathbf{p}_1} \cdot \nabla_{\mathbf{r}_2}) \delta(1;3) \delta(3;2)]$.

Each of the ψ_n fields is a linear combination of products of δ functions. Using the simple relationships for the Poisson brackets of products of functions, e.g.,

$$\{B_1 B_2, A\} = B_2 \{B_1, A\} + B_1 \{B_2, A\}$$

and its generalizations, it is possible to show that

$$\langle\{\psi_n(1\dots n), \psi_m(1\dots m)\}\rangle = \text{the sum of all topologically different diagrams} \quad (24)$$

with (i) n left roots labeled $1\dots n$; (ii) m right roots labeled $1'\dots m'$; (iii) one free point; and (iv) one D hypervertex and one m_{n+m-1} vertex; such that (i) the first point of the vertex D is a left root, (ii) the second point of the vertex D is a right root, (iii) each other root is on the vertex m , and (iv) the free point is the third point of the vertex D and is attached to the vertex m . In these diagrams, the D vertex has three nonequivalent points.

Thus, $\langle\psi_n|iL|\psi_m\rangle$ can be related to derivatives of m_{n+m-1} with regard to its phase point arguments. Because the fluctuation basis functions are linear combinations of ψ_n , the matrix elements of the Liouville operator in the fluctuation basis can be related to gradients of the fundamental moments of the density, with no reference to the interparticle potential. Ultimately, this implies that the coupling coefficients in the field theory can be expressed in the same way, which implies that the theory is “fully renormalized”, in the sense of Gross and Mazenko.

A.3. Calculation of Matrix Elements of the Liouville Operator. There are several ways of calculating specific matrix elements of the Liouville operator. We will illustrate them here to obtain the matrix elements that are needed in this paper.

To calculate $\langle\phi_1(1)|iL|\phi_1(1')\rangle$, we use the result that $|\phi_1(1)\rangle = |\psi_1(1)\rangle - \langle\psi_1(1)|\phi_0\rangle$, the fact that the Liouville operator is Hermitian, and the fact that $L|\phi_0\rangle = 0$ to obtain the relationship

$$\langle\phi_1(1)|iL|\phi_1(1')\rangle = \langle\psi_1(1)|iL|\psi_1(1')\rangle$$

Using the previously described Poisson bracket relationship and the graphical series in eq 24, we get

$$\begin{aligned} \langle\phi_1(1)|iL|\phi_1(1')\rangle &= -kT\langle\{\psi_1(1), \psi_1(1')\}\rangle \\ &= -kT \int d2 D(11'2) m_1^{(c)}(2) \\ &= \frac{\mathbf{P}_1}{m} \cdot \nabla \delta(\mathbf{R}_1 - \mathbf{R}_{1'}) \delta(\mathbf{P}_1 - \mathbf{P}_{1'}) \rho M(\mathbf{P}_1) \end{aligned}$$

where $\rho = N/V$ and $M(\mathbf{P}_1)$ is a normalized Maxwell–Boltzmann distribution function.

To calculate $\langle\phi_2|iL|\phi_1\rangle$, the same approach could be used, but we get a simple answer more directly using a different procedure. Note that it follows, from eq 3, evaluated for $t = 0$, that

$$\begin{aligned} iL|\psi_n(1\dots n)\rangle &= \sum_{i=1}^n \int d1'' V_{11}(i;1'') |\psi_n(1\dots n[1''/i])\rangle + \\ &\quad \sum_{i=1}^n \int d1'' d2'' V_{12}(i;1''2'') |\psi_{n+1}(1\dots n2''[1''/i])\rangle \quad (25) \end{aligned}$$

It follows, using the orthogonality properties of the ϕ and ψ functions, that

$$\begin{aligned} \langle\phi_{n+1}(1'\dots (n+1'))|iL|\phi_n(1\dots n)\rangle &= \langle\phi_{n+1}(1'\dots (n+1'))|iL|\psi_n(1\dots n)\rangle \\ &= \sum_{i=1}^n \int d1'' d2'' V_{12}(i;1''2'') \\ &\quad \times F_{n+1}(1'\dots (n+1)'; 1\dots n2''[1''/i]) \quad (26) \end{aligned}$$

Applying this relation to $n = 1$, we get

$$\langle\phi_2(1'2')|iL|\phi_1(1)\rangle = \int d1'' d2'' V_{12}(1;1''2'') F_2(1'2'; 1''2'')$$

To calculate $\langle\phi_1|iL|\phi_2\rangle$, the simplest method is to take the complex conjugate of the previous result and use the Hermitian property of L :

$$\langle\phi_1(1)|iL|\phi_2(1'2')\rangle = - \int d1'' d2'' V_{12}(1;1''2'') F_2(1'2'; 1''2'')$$

We note that different methods for calculating the same matrix elements often give results that look quite different but are equivalent.

A.4. Evaluation of Coupling Coefficients Q . Here, we summarize some results of the evaluation of the coupling coefficients Q . These results are obtained using eq 5 of this paper, eq B18 of I, and the results just above for matrix elements of the Liouville operator.

$$Q_{11}(1;1') = \frac{\mathbf{P}_1}{m} \cdot \nabla_{\mathbf{R}_1} (\delta(1';1) - c(\mathbf{R}'_1 \mathbf{R}_1) \rho M(\mathbf{P}_1)) \quad (27)$$

$$Q_{12}(1;1'2') = V_{12}(1;1'2') + V_{12}(1;2'1') \quad (28)$$

$$\begin{aligned} Q_{21}(12;1') &= - \int d1'' d1''' d2''' V_{12}(1'';1'''2''') \\ &\quad \times F_2(12;1'''2''') K_1(1'';1') \quad (29) \end{aligned}$$

Appendix B. Kinetic Equation for the Density Fluctuation Correlation Function

Equation 20 is the kinetic equation for the density fluctuation correlation function. In this appendix, we show that it is

equivalent to the usual memory function result and we establish the association to the theory of Mazenko.

Using eq 27, the kinetic equation can be expressed as

$$\frac{\partial}{\partial t_1} C_{11}(1, t_1; 2, 0) = -\frac{\mathbf{P}_1}{m} \cdot \nabla_{\mathbf{R}_1} C_{11}(1, t_1; 2, 0) + \rho M(\mathbf{P}_1) \frac{\mathbf{P}_1}{m} \cdot \int d\mathbf{3} \nabla c(\mathbf{R}_1, \mathbf{R}_3) C_{11}(3, t_1; 2, 0) + \int_0^{t_1} dt_3 \int d\mathbf{3} M(1, t_1; 3, t_3) C_{11}(3, t_3; 2, 0) \quad (30)$$

The first term on the right-hand side is the usual flow term. The second term is equivalent to the contribution of what is variously called the “static” (or “mean-field” or “self-consistent-field”) portion of the memory function. The third term on the right-hand side is contribution of the “collisional” portion of the memory function.

The function $M(1, t_1; 3, t_3)$ that appears here corresponds to the negative of the quantity that Mazenko calls $\phi^{(c)}$. (See eqs 3.12 and 3.14 of Mazenko² or eqs 35 and 42 of Mazenko and Yip³.) The precise correspondence is that the Laplace transform (using the specific form of Laplace transform that Mazenko uses) of $M(1, t_1; 2, t_2)$, with regard to the time interval $t_1 - t_2$, is equal to $-\phi_c(12)$, with the z dependence of the latter function being understood.

Using eq 23 and eqs 28 and 29, M can be expressed as

$$M(1, t_1; 2, t_2) = -\frac{1}{2!} \int d\mathbf{3} d\mathbf{4} d\mathbf{5} d\mathbf{6} d\mathbf{1}''' d\mathbf{2}''' d\mathbf{1}'' V_{12}(1; 34) \times V_{12}(1''; 1''' 2''') \chi_{12}^{(>1)}(34, t_1; 56, t_2) F_2(56; 1''' 2''') K_1(1''; 2)$$

If we define

$$G(12, t_1; 34, t_2) \equiv \frac{1}{2!} \int d\mathbf{5} d\mathbf{6} \chi_{22}^{(>1)}(12, t_1; 56, t_2) F_2(56; 34) \quad (31)$$

we then have

$$M(1, t_1; 2, t_2) = -\int d\mathbf{3} d\mathbf{4} d\mathbf{5} d\mathbf{6} d\mathbf{7} \times V_{12}(1; 34) V_{12}(7; 56) G(34, t_1; 56, t_2) K_1(7; 2)$$

This expression for the collisional portion of the memory

function, in terms of a four-point function G , is equivalent to that of Mazenko. (For example, see eq 3.16 of Mazenko² or eq 46 of Mazenko and Yip.³) The G function defined in eq 31 has precisely the same relationship to the memory function in the current theory as Mazenko's G function. Moreover, by an explicit calculation, it can be shown that the two functions are equal when the two time arguments are equal. In fact, the two functions are equal at all times, but we shall not demonstrate this here. Such a demonstration would require an analysis of Mazenko's theory that goes beyond the scope of this paper. See Lindenfeld⁵ for a discussion of the basic method of demonstration.

A comparison of eq 31 with eq 15 shows that the $G(12, t_1; 34, t_2)$ function can be given the following interpretation. It is the correlation function $C_{22}(12, t_1; 34, t_2)$ evaluated by keeping only those contributions to χ_{22} that contain no $\chi^{(0,0)}$ or $\chi^{(0,1)}$ bonds. It represents $C_{22}(12, t_1; 34, t_2)$ with the dynamics restricted to the portion of the Hilbert space that is orthogonal to S_0 and S_1 . In effect, this dynamics is a propagation that has been calculated with a modified propagator of the type introduced by Mori. Mazenko specified the dynamics of his G function without reference to projection operators; however, Boley⁴ and Lindenfeld⁵ established the connection between Mazenko's dynamics and projection operators.

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