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Tagged Particle Fluctuations in Uniform Shear Flow[1]

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The nonlinear Boltzmann and Boltzmann–Lorentz equations are used to describe the dynamics of a tagged particle in a nonequilibrium gas. For the special case of Maxwell molecules with uniform shear flow, an exact set of equations for the average position and velocity, and their fluctuations, is obtained. The results apply for arbitrary magnitude of the shear rate and include the effects of viscous heating. A generalization of Onsager's assumption of the regression of fluctuations is found to apply for the relationship between the equations for the average dynamics and those for the time correlation functions. The connection between fluctuations and dissipation is described by the equations for the equal-time correlation function. The source term in these equations indicates that the "noise" in this nonequilibrium state is qualitatively different from that in equilibrium, or even local equilibrium. These equations are solved to determine the velocity autocorrelation function as a function of the shear rate.

KEY WORDS: Nonequilibrium fluctuations; Boltzmann equation; shear flow; velocity autocorrelation function; kinetic theory.

1. INTRODUCTION

Time-dependent fluctuations in systems far from equilibrium can provide a much richer description of the dynamics of a many body system than the corresponding equilibrium fluctuations. The description of such fluctua-

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tions has been developed in recent years at the kinetic[1-4] and hydrodynamic[5-8] levels, from both phenomenological and more fundamental formulations. A complete theory comparable to that for equilibrium fluctuations is still evolving, and applications are limited by the difficulty of solving the associated nonlinear equations. The objectives of this and the following paper are to illustrate some of the similarities and differences between fluctuations in nonequilibrium states and those in equilibrium, for a case where the theory is well-established and exact calculations are possible. The system considered is a tagged particle in a low density gas of Maxwell molecules[9] (r^{-5} force law). The fluid is considered in a state of uniform shear flow with possibly large shear rate and the tagged particle is assumed to be mechanically equivalent to the fluid particles. In the following paper the case of a tagged particle with large mass is considered.

Two general questions regarding fluctuations far from equilibrium are addressed here: (1) What is the relationship (if any) of the dynamics of the average variables to that of their fluctuations? (2) How is the "noise" in the system characterized for these variables? In equilibrium, the answer to the first question is given by Onsager's assumption on the regression of fluctuations[10], i.e., that after an initial aging period the time correlation functions decay according to the same (linear) equations as those for the associated macroscopic variables. Also, the "noise" in equilibrium is simply determined by the thermodynamic parameters of the equilibrium ensemble. To describe the corresponding results obtained here for the nonequilibrium state of uniform shear flow, let z denote a matrix whose elements are the position and velocity of a tagged particle,

$$z_\alpha \leftrightarrow (\mathbf{q}_T, \mathbf{v}_T) \tag{1.1}$$

The average values of z and their fluctuations are defined by

$$Z_\alpha(t) \equiv \langle z_\alpha(t) \rangle \tag{1.2}$$

$$G^{\alpha\beta}(t,\tau) \equiv \big\langle z_\alpha(t+\tau)\big[z_\beta(\tau) - \langle z_\beta(\tau)\rangle\big]\big\rangle \tag{1.3}$$

where the brackets denote an average over the initial state of the system, assumed given at $t=0$. The equations obtained below for Z_α and $G^{\alpha\beta}$ have the form

$$\frac{\partial}{\partial t} Z_\alpha + \mathscr{L}_{\alpha\beta} Z_\beta = 0 \tag{1.4}$$

$$\frac{\partial}{\partial t} G^{\alpha\beta}(t,\tau) + \mathscr{L}_{\alpha\sigma} G^{\sigma\beta}(t,\tau) = 0 \tag{1.5}$$

$$\frac{\partial}{\partial \tau} G^{\alpha\beta}(0,\tau) + \mathscr{L}_{\alpha\sigma} G^{\sigma\beta}(0,\tau) + \mathscr{L}_{\beta\sigma} G^{\alpha\sigma}(0,\tau) = \mathscr{D}_{\alpha\beta}(\tau) \tag{1.6}$$

where $\mathscr{L}_{\alpha\beta}$ is a constant matrix whose elements depend linearly on the shear rate. The source term $\mathscr{D}_{\alpha\beta}$ in Eq. (1.6) depends on time, owing to the viscous heating, and is a nonlinear function of the shear rate. Equations (1.4)–(1.6) have the same general form as those recently shown to apply for nonequilibrium fluctuations in a simple fluid, at both the kinetic and hydrodynamic levels.[4,8] Equations (1.4) and (1.5) may be viewed as a generalization of Onsager's assumption on the regression of fluctuations where the regression matrix, $\mathscr{L}$, depends on the parameters of the nonequilibrium state. Equation (1.6) is a generalization of the fluctuation–dissipation theorem relating the dissipation matrix, $\mathscr{L}$, to the equal time fluctuations. The source term, $\mathscr{D}$, is related to the "noise" in the system (for a Langevin or Fokker–Planck model, $\mathscr{D}$ is simply the amplitude for the correlation of the Langevin force, as is shown in the following paper). In the equilibrium state $\mathscr{D} \propto 2\nu_1 k_B T$, where ν_1 is the friction constant and T is the temperature. Here it is found that $\mathscr{D}$ depends on the irreversible part of the fluid stress tensor as well so that there is a qualitative difference between equilibrium (or even local equilibrium) and nonequilibrium noise.

The solution to Eqs. (1.4)–(1.6) is straightforward but lengthy to obtain. Only the velocity autocorrelation function is considered in some detail. Several new features appear in contrast to the equilibrium case. First, the average is not stationary, owing to viscous heating in the fluid, so the correlation function depends on both times, t and τ, in addition to the initial time. Furthermore, it does not decay to zero for large t. Instead it approaches a value characterized by the tagged particle velocity coming into equilibrium with the local fluid velocity. As expected, there is an anisotropy due to the shear flow. The latter produces an effective force on the particle in the direction of the flow. This force is proportional to the velocity in the direction of the shear, which competes with the collisional damping of the correlation function. Finally, the effects of viscous heating and anisotropy are reflected in the equal time correlation function $\langle v_i(\tau) v_j(\tau) \rangle$ through the source term, $\mathscr{D}$, in Eq. (1.6).

There has been a related discussion of Brownian motion in uniform shear flow based on a modified Langevin equation or Fokker–Planck equation.[11] In the paper following this one,[12] the Boltzmann–Lorentz operator is expanded for the case of small mass ratio between fluid and tagged particles. The result is a Fokker–Planck equation for tagged particle motion in a nonequilibrium fluid, with an associated Langevin description. Its relationship to Ref. 11 and other related work is discussed there.

2. KINETIC THEORY

The kinetic equations for fluctuations and transport in a low density nonequilibrium gas have been derived in Ref. 1 (the derivation there is carried out explicitly only for hard spheres, but applies for continuous potentials as well). The variables of interest are the phase space densities for the fluid and tagged particle, $f(x,t)$ and $h(x,t)$, respectively, and the phase space fluctuations for the tagged particle,

$$C(x_1, t+\tau; x_2, \tau) \equiv \langle \delta(x_1 - \hat{x}_T(t+\tau))[\delta(x_2 - \hat{x}_T(\tau)) - \langle \delta(x_2 - \hat{x}_T(\tau))\rangle]\rangle \quad (2.1)$$

Here, x denotes the position and velocity for the tagged particle. The caret (ˆ) above the variable denotes the degrees of freedom being averaged, in contrast to the associated field point. The equations governing the time dependence of f, h, and C are[1]

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) f = J[f,f] \quad (2.2)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) h = J[f,h] \quad (2.3)$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_1\cdot\nabla_1\right) C(1,2) = J[f,C] \quad (2.4)$$

The function $C(1,2)$ is the same as that defined by Eq. (2.1), in an abbreviated notation. The bilinear Boltzmann operator, J, is[9]

$$J[A,B] \equiv \int d\mathbf{v}_2 \int_0^\infty db\, b \int_0^{2\pi} d\phi |\mathbf{v}_1 - \mathbf{v}_2| \{A(\mathbf{q}_1, \tilde{\mathbf{v}}_2) B(\mathbf{q}_1, \tilde{\mathbf{v}}_1) - A(\mathbf{q}_1, \mathbf{v}_2) B(\mathbf{q}_1, \mathbf{v}_1)\} \quad (2.5)$$

where b is the impact parameter and a tilde on the velocity indicates its value after a binary collision. [It is understood in Eq. (2.4) that the domain for operation of J is the variable labeled 1).] The conditions for the validity of Eqs. (2.2)–(2.4) are discussed in Ref. 1. Equation (2.2) is the usual nonlinear Boltzmann equation. If f is replaced by a Maxwell–Boltzmann distribution in Eqs. (2.3) and (2.4), these degenerate to the linear Boltzmann–Lorentz equations for fluctuations and transport of a tagged particle in an equilibrium fluid.

Fluctuations in any property associated with the tagged particle can be determined from the function $C(1,2)$. For example, let z be given by Eq. (1.1). Then the fluctuations in z are given by

$$G^{\alpha\beta}(t,\tau) = \int dx_1\, dx_2\, z_\alpha(x_1) z_\beta(x_2) C(x_1, t+\tau; x_2, \tau) \quad (2.6)$$

In particular, the velocity autocorrelation function is

$$G_{ij}^{vv}(t,\tau) = \int dx_1\, dx_2\, v_{1i} v_{2j} C(x_1, t+\tau; x_2, \tau) \quad (2.7)$$

Steady shear flow corresponds to a fluid between two parallel plates in relative motion. If the flow velocity is taken to be zero at $\mathbf{q} = 0$, then it has the form

$$u_i(\mathbf{q}, t) = a_{ij} q_j \tag{2.8}$$

where a_{ij} is a constant tensor with zero diagonal elements and

$$a_{ij} a_{jk} = 0 \tag{2.9}$$

To obtain a unique solution to Eqs. (2.2)–(2.4) it is necessary to specify initial conditions (at $t = 0$). For simplicity, the initial fluid state is taken to depend on the position only through the flow velocity,

$$f(x, 0) = f_0(\mathbf{v} - \mathbf{u}(\mathbf{q})) \tag{2.10}$$

Similarly, the tagged particle is taken to be located initially at the origin with the same velocity distribution,

$$h(x, 0) = \delta(\mathbf{q}) \frac{1}{n} f_0(\mathbf{v} - \mathbf{u}(\mathbf{q})) \tag{2.11}$$

where n is the initial (uniform) fluid density (the factor $1/n$ is required by the different normalizations of f and h). The initial condition for $C(1, 2)$ is determined from the definition, (2.1),

$$C(x_1, \tau; x_2, \tau) = h(x_1, \tau)\left[\delta(x_1 - x_2) - h(x_2, \tau)\right] \tag{2.12}$$

The special form of the initial condition, (2.10), suggests a transformation to a local rest frame in which the initial distribution, f_0, is strictly uniform in space. By analogy with the Galilean transformation, a new set of variables $(\mathbf{q}', \mathbf{v}')$ are defined by

$$\mathbf{v}' = \mathbf{v} - \mathbf{u}(\mathbf{q}), \qquad \mathbf{q}' = \mathbf{q} - \mathbf{u}(\mathbf{q})t \tag{2.13}$$

or, with Eq. (2.8),

$$v_i' = v_i - a_{ij} q_j, \qquad q_i' = \Lambda_{ij}(t) q_j \tag{2.14}$$

The tensor $\Lambda_{ij}(t)$ is given by

$$\Lambda_{ij}(t) = \delta_{ij} - a_{ij} t \tag{2.15}$$

Because of the property (2.9) for shear fields, $\Lambda_{ij}(t)$ defines a one-parameter group of transformations, i.e.,

$$\Lambda_{ik}(t)\Lambda_{kj}(\tau) = \Lambda_{ij}(t + \tau), \qquad \Lambda_{ij}^{-1}(t) = \Lambda_{ij}(-t) \tag{2.16}$$

Use of Eqs. (2.16) allows the inversion of Eqs. (2.14) to give

$$v_i = v_i' + a_{ij} q_j', \qquad q_i = \Lambda_{ij}(-t) q_j' \tag{2.17}$$

It is now straightforward to transform the kinetic equations (2.2)–(2.4), and the associated initial conditions, with the results

$$\left(\frac{\partial}{\partial t}+L\right)f' = J[f', f'] \tag{2.18}$$

$$\left(\frac{\partial}{\partial t}+L\right)h' = J[f', h'] \tag{2.19}$$

$$\left(\frac{\partial}{\partial t}+L\right)C' = J[f', C'] \tag{2.20}$$

with

$$f'(x,0) = f_0(v)$$

$$h'(x,0) = \delta(\mathbf{q})\frac{1}{n}f_0(v)$$

$$C'(x_1,\tau;x_2,\tau) = h'(x_1,\tau)\left[\delta(x_1 - x_2) - h'(x_2,\tau)\right] \tag{2.21}$$

and the operator, L, is

$$L = \Lambda_{ij}(t)v_j\frac{\partial}{\partial q_i} - a_{ij}v_j\frac{\partial}{\partial v_i} \tag{2.22}$$

The prime on a function denotes the transformed function of the new variables (the prime on the variables themselves has been deleted for notational simplicity). To obtain Eqs. (2.21) use has been made of the relation

$$\delta(x - x_0) = \frac{1}{\mathrm{Det}J}\delta(x' - x_0')$$

where $\mathrm{Det}J$ is the determinant of the Jacobian for the transformation. The latter is equal to 1. It has also been observed that the collision operators are invariant under the transformation, (2.14).

A similar change of variables has been used by Yamada and Kawasaki.[13] Their velocity transformation is the same, but they transform the coordinate according to $\mathbf{q}' = \mathbf{q}$. The coordinate transformation used here is that for a change from Eulerian to Lagrangian coordinates. An advantage of this representation is that the fluid distribution, $f'(x,t)$, is independent of the position variable. This follows from the fact that the initial condition is spatially homogeneous and Eq. (2.18) itself is translationally invariant. Furthermore, the reduced distribution for the velocity of the tagged particle,

$$\bar{h}'(v,t) \equiv \int d\mathbf{q}\, h'(x,t) \tag{2.23}$$

is proportional to $f'(v,t)$ for all t, i.e.,

$$\bar{h}'(v,t) = \frac{1}{n}f'(v,t) \tag{2.24}$$

This may be proved by noting that the $\phi' \equiv nh' - f'$, obeys a linear first-order differential equation with homogeneous initial condition,

$$\left(\frac{\partial}{\partial t} - a_{ij} v_j \frac{\partial}{\partial v_i}\right)\phi' = J[f', \phi'] \tag{2.25}$$

In particular, the equivalence of these two distributions implies that the velocity moments of the tagged particle in the rest frame may be determined from the corresponding velocity moments of the fluid distribution.

3. MACROSCOPIC DYNAMICS

In this section, the kinetic equations are used to obtain a contracted, or "macroscopic," description in terms of the hydrodynamic variables for the nonequilibrium fluid state, and the average position and velocity for the tagged particle. Consider first the gas as described by Eq. (2.18) in the rest frame. Since $f'(x, t)$ is independent of position for all times, Eq. (2.18) simplifies to

$$\left(\frac{\partial}{\partial t} - a_{ij} v_j \frac{\partial}{\partial v_i}\right) f' = J[f', f'] \tag{3.1}$$

The hydrodynamic equations may now be obtained in the usual way[9] by multiplying Eq. (3.1) with the summational invariants $(1, \mathbf{v}, v^2)$ and integrating over the velocity. The contributions from J vanish, leading to the hydrodynamic equations for uniform shear flow:

$$\frac{\partial n(t)}{\partial t} = 0 = \frac{\partial}{\partial t} \mathbf{u}(\mathbf{q}, t) \tag{3.2}$$

$$\frac{\partial p(t)}{\partial t} = -\frac{2}{3} a_{ij} P_{ij}(t) \tag{3.3}$$

Here n is the density, p is the pressure, and the pressure tensor is defined by

$$P_{ij}(t) = \int d\mathbf{v}\, m v_i v_j f' \tag{3.4}$$

where m is the mass. The temperature is defined by $p = n k_B T$. The independence on n, p, and P_{ij} on $\mathbf{q}$ is a consequence of the homogeneity of f'. Equation (3.2) indicates that the constancy of the initial flow field and density is preserved in time. Consequently, the only dynamical variable is the temperature, which increases at a rate determined by the irreversible stress tensor. To calculate the latter, an equation for P_{ij} is obtained by multiplying Eq. (3.1) with $m v_i v_j$ and integrating over the velocity:

$$\frac{\partial}{\partial t} P_{ij} + a_{ik} P_{kj} + a_{jk} P_{ik} = \int d\mathbf{v}\, m v_i v_j J[f', f'] \tag{3.5}$$

Up to this point, the results apply for a wide class of interatomic forces. In general the evaluation of the term on the right side of Eq. (3.5) would entail the introduction of some approximation scheme. However, for the special case of Maxwell molecules this term can be evaluated exactly in terms of P_{ij} and the pressure. The details are carried out in the Appendix, with the result that Eq. (3.5) becomes[14,15]

$$\left(\frac{\partial}{\partial t} + \nu_3\right)P_{ij} + a_{ik}P_{kj} + a_{jk}P_{ik} = \nu_3 p\delta_{ij} \tag{3.6}$$

where ν_3 is an eigenvalue of the Boltzmann operator. Equations (3.3) and (3.6) may be solved to determine the time dependence of the pressure. (A similar analysis has been given by Zwanzig using a model Boltzmann equation.[16] For the case of Maxwell molecules the results of the model equation agree with the exact results here.) The explicit calculation of $P_{ij}(t)$ is briefly described in the Appendix. It is found that there are two short time transients after which the temperature increases exponentially in time.

Next, consider the average dynamics for the tagged particle. Multiplication of Eq. (2.19) successively by **q** and **v**, and integration over these variables gives

$$\begin{aligned} \frac{\partial R_i'}{\partial t} &= \Lambda_{ij}(t)V_j' \\ \frac{\partial V_i'}{\partial t} + a_{ij}V_j' &= \int dx\, v_i J[f', g'] \end{aligned} \tag{3.7}$$

Here $\mathbf{R}'$ and $\mathbf{V}'$ denote the average position and velocity of the tagged particle in the rest frame. Again, for Maxwell molecules the right side of the velocity equation can be calculated, with the result [see Appendix, Eqs. (A1) and (A7)],

$$\int dx\, v_i J[f', g'] = -\nu_1 V_i' \tag{3.8}$$

Here ν_1 is an eigenvalue of the Boltzmann–Lorentz operator. Substitution of (3.8) in (3.7), and transformation back to the laboratory frame then gives the equations of motion for the tagged particle:

$$\frac{\partial \mathbf{R}}{\partial t} = \mathbf{V}, \qquad \frac{\partial \mathbf{V}}{\partial t} = -\nu_1(\mathbf{V} - \mathbf{u}(\mathbf{R})) \tag{3.9}$$

4. FLUCTUATIONS

The calculation of $G^{\alpha\beta}(t,\tau)$ is simplified by representing it in terms of the local rest frame variables using (2.17),

$$R^{\alpha\beta}(t,\tau) = \int dx_1\, dx_2\, z_\alpha(x_1) z_\beta(x_2) C'(x_1, t+\tau; x_2, \tau) \tag{4.1}$$

where $R^{\alpha\beta}$ (for α or $\beta = \mathbf{q}, \mathbf{v}$) are the position and velocity correlations in the rest frame. A set of equations for $R^{\alpha\beta}(t,\tau)$ with $t \neq 0$ is immediately obtained by multiplying Eq. (2.20) with v_i and q_i and integrating. For

Maxwell molecules the moments of the Boltzmann–Lorentz operator can be calculated exactly (see Appendix), and the resulting equations are

$$\left(\frac{\partial}{\partial t}+\nu_1\right)R_{ij}^{v\alpha}(t,\tau)+a_{ik}R_{kj}^{v\alpha}(t,\tau)=0 \tag{4.2}$$

$$\frac{\partial}{\partial t}R_{ij}^{q\alpha}(t,\tau)-\Lambda_{ik}(t)R_{kj}^{v\alpha}(t,\tau)=0 \tag{4.3}$$

for $\alpha=\mathbf{q},\mathbf{v}$. Transforming back to the laboratory frame then gives

$$\frac{\partial}{\partial t}G_{ij}^{q\alpha}(t,\tau)-G_{ij}^{v\alpha}(t,\tau)=0 \tag{4.4}$$

$$\left(\frac{\partial}{\partial t}+\nu_1\right)G_{ij}^{v\alpha}(t,\tau)-\nu_1 a_{ik}G_{kj}^{q\alpha}(t,\tau)=0 \tag{4.5}$$

Equations for the equal time correlation functions, $R^{\alpha\beta}(0,\tau)$, are obtained in a similar way by integrating Eq. (2.19) for h' with the components of $\mathbf{v}$ and $\mathbf{q}$. Again, the collision integrals can be evaluated (see Appendix), and the resulting equations are

$$\frac{\partial}{\partial \tau}R_{ij}^{qq}(0,\tau)-\Lambda_{ik}(\tau)R_{kj}^{vq}(0,\tau)-\Lambda_{jk}(\tau)R_{ki}^{vq}(0,\tau)=0 \tag{4.6}$$

$$\left(\frac{\partial}{\partial \tau}+\nu_1\right)R_{ij}^{vq}(0,\tau)-\Lambda_{jk}(\tau)R_{ki}^{vv}(0,\tau)+a_{ik}R_{kj}^{vq}(0,\tau)=0 \tag{4.7}$$

$$\left(\frac{\partial}{\partial \tau}+\nu_1+\nu_2\right)R_{ij}^{vv}(0,\tau)+a_{ik}R_{kj}^{vv}(0,\tau)+a_{jk}R_{kj}^{vv}(0,\tau)-\frac{1}{3}\nu_2\delta_{ij}R_{kk}^{vv}(0,\tau)$$
$$=I_{ij}(\tau) \tag{4.8}$$

where R_{kk}^{vv} is the trace of the tensor R_{ij}^{vv}, and

$$I_{ij}(\tau)=\frac{\nu_1-\nu_2}{\rho}t_{ij}^*(\tau)+\delta_{ij}\frac{\nu_1}{\rho}p(\tau) \tag{4.9}$$

Here the pressure tensor has been divided into its diagonal and traceless parts,

$$P_{ij}(\tau)=p(\tau)\delta_{ij}+t_{ij}^*(\tau) \tag{4.10}$$

where the traceless tensor, $t_{ij}^*(\tau)$, represents the irreversible part of the momentum flux in the fluid. Also in Eq. (4.9), $\rho=Mn$, where M is the mass. Transformation of Eqs. (4.6)–(4.8) to the laboratory frame gives the desired results:

$$\frac{\partial}{\partial \tau}G_{ij}^{qq}(0,\tau)-G_{ij}^{vq}(0,\tau)-G_{ij}^{qv}(0,\tau)=0 \tag{4.11}$$

$$\left(\frac{\partial}{\partial \tau}+\nu_1\right)G_{ij}^{vq}(0,\tau)-\nu_1 a_{ik}G_{kj}^{qq}(0,\tau)-G_{ij}^{vv}(0,\tau)=0 \tag{4.12}$$

$$\left(\frac{\partial}{\partial \tau}+2\nu_1\right)G_{ij}^{vv}(0,\tau)-\nu_1\left(a_{ik}G_{kj}^{qv}(0,\tau)+a_{jk}G_{ik}^{vq}(0,\tau)\right)=D_{ij}(\tau) \tag{4.13}$$

with

$$D_{ij}(\tau) = \nu_1\left[\frac{k_B}{M}T(\tau) + \frac{1}{3}R_{kk}^{vv}(0,\tau)\right]\delta_{ij} + (\nu_1 - \nu_2)\left[\frac{t_{ij}^*(\tau)}{\rho} + \left(R_{ij}^{vv}(0,\tau) - \frac{1}{3}\delta_{ij}R_{kk}^{vv}(0,\tau)\right)\right]$$

The expression for $D_{ij}(\tau)$ may be simplified further using the equivalence (2.24), which implies

$$R_{ij}^{vv}(0,\tau) = P_{ij}(\tau)/\rho \tag{4.14}$$

and

$$D_{ij}(\tau) = \frac{2\nu_1 k_B T(\tau)}{M}\delta_{ij} + 2(\nu_1 - \nu_2)t_{ij}^*(\tau)/\rho \tag{4.15}$$

The sets of equations (3.3) and (3.6) for the fluid, (3.9) for the average tagged particle motion, (4.4) and (4.5) for the two-time fluctuations, and (4.11)–(4.13) for the equal time fluctuations give a closed description of the dynamics of the tagged particle and its fluctuations. Inspection of these equations shows they may be expressed in the general form of Eqs. (1.4)–(1.6), with $\mathscr{L}$ and $\mathscr{D}$ defined by

$$\mathscr{L}_{\alpha\beta} \leftrightarrow \left(\begin{array}{c|c} 0 & -1 \\ \hline -\nu_1\overleftrightarrow{a} & \nu_1 \end{array}\right) \tag{4.16}$$

$$\mathscr{D}_{\alpha\beta} \leftrightarrow \left(\begin{array}{c|c} 0 & 0 \\ \hline 0 & \overleftrightarrow{D} \end{array}\right) \tag{4.17}$$

where $\overleftrightarrow{a}$ and $\overleftrightarrow{D}$ are the tensors whose elements are a_{ij} and D_{ij}, respectively. [This abbreviated notation implies a contraction of the tensors $\overleftrightarrow{a}$ and $\overleftrightarrow{D}$ with associated vector elements in the matrix multiplication. For example, $\mathscr{L}_{\alpha\beta}Z_\beta = (-V_i, -\nu_1 a_{ij}R_j + \nu_1 V_i)$.] In the equilibrium state the noise term, D_{ij}, reduces to $(2k_BT/M)\delta_{ij}$ as expected from the usual Langevin theory of equilibrium fluctuations. More generally D_{ij} depends on the nonequilibrium state both through the time dependence of T and the irreversible stress tensor t_{ij}^*. Further comment on this is given in the last section.

5. VELOCITY AUTOCORRELATION FUNCTION

The solution of Eqs. (3.9) determining the average position and velocity of the tagged particle is straightforward to obtain, with the results

$$R_i(t) = \Lambda_{ij}(-t)\left\{R_j(0) + \frac{1}{\nu_1}\left[\Lambda_{jk}\left(\frac{2}{\nu_1}\right)(1 - e^{-\nu_1 t}) + 2a_{jk}te^{-\nu_1 t}\right]V_k'(0)\right\}$$

$$V_i(t) = U_i(0) + T_{ij}(t)V_j'(0) \tag{5.1}$$

Here $V_i'(0) = V_i(0) - U_i(0)$, $U_i(0) = a_{ij}R_j(0)$ and

$$T_{ij}(t) = e^{-\nu_1 t}\delta_{ij} + \frac{a_{ij}}{\nu_1}\left[1 - (1 + \nu_1 t)e^{-\nu_1 t}\right] \tag{5.2}$$

For the special initial condition, (2.11), the average position and velocity vanish at $t = 0$ and therefore are zero at all times.

The two-time correlation functions for the fluctuations in the velocity and position of the tagged particle may be determined by solving Eqs. (4.4) and (4.5). These equations are formally identical to the equations for the average quantities, R_i and V_i; the only difference appears in the initial conditions. The two-time correlation functions are then given by

$$G_{ij}^{q\alpha}(t,\tau) = \Lambda_{ik}(-t)\Bigg\{G_{kj}^{q\alpha}(0,\tau) + \frac{1}{\nu_1}\left[\Lambda_{kl}\left(\frac{2}{\nu_1}\right)(1 - e^{-\nu_1 t}) + 2a_{kl}te^{-\nu_1 t}\right] \times\left[G_{lj}^{v\alpha}(0,\tau) - a_{lm}G_{mj}^{q\alpha}(0,\tau)\right]\Bigg\} \tag{5.3}$$

and

$$G_{ij}^{v\alpha}(t,\tau) = a_{ik}G_{kj}^{q\alpha}(0,\tau) + T_{ik}(t)\left[G_{kj}^{v\alpha}(0,\tau) - a_{kl}G_{lj}^{q\alpha}(0,\tau)\right] \tag{5.4}$$

It is interesting to observe that the velocity autocorrelation function $G_{ij}^{vv}(t,\tau)$ does not decay to zero for long times as in equilibrium. In fact, letting $t \to \infty$ in Eq. (5.4) for $\alpha = v$,

$$\lim_{t\to\infty} G_{ij}^{vv}(t,\tau) = a_{ik}G_{kj}^{qv}(0,\tau) + \frac{a_{ik}}{\nu_1}G_{kj}^{vv}(0,\tau) \tag{5.5}$$

This result may be interpreted in the following way. Since the average velocity is $\mathbf{V} = \mathbf{u}(\mathbf{R})$, it may be expected that $G_{ij}^{vv}(t,\tau)$ has as its long time limit

$$\begin{aligned}\lim_{t\to\infty} G_{ij}^{vv}(t,\tau) &= \lim_{t\to\infty}\langle u_i(\mathbf{q}(t+\tau))v_j(\tau)\rangle \\ &= a_{ik}\lim_{t\to\infty}\langle q_k(t+\tau)v_j(\tau)\rangle\end{aligned} \tag{5.6}$$

or,

$$G_{ij}^{vv}(\infty,\tau) = a_{ik}\langle q_k(\tau)v_j(\tau)\rangle + \int_0^\infty dt'\, a_{ik}G_{kj}^{vv}(t',\tau) \tag{5.7}$$

It is seen from Eq. (5.4) that the right-hand sides of Eqs. (5.5) and (5.7) are indeed identical. Thus, the velocity of the tagged particle equilibrates with the local flow field, but since the latter depends on the position of the particle, correlation with its initial velocity persists indefinitely.

The set of Eqs. (4.11)–(4.13) determining the equal time correlation functions in the laboratory frame, $G_{ij}^{\alpha\beta}(0,\tau)$, is quite complicated. It is convenient to solve instead the set of Eqs. (4.6)–(4.9) for the rest frame correlation functions, and then transform the result back to the laboratory frame. In particular, the velocity autocorrelation function is immediately expressed in terms of the equal time correlations in the rest frame by rewriting Eq. (5.4) for $\alpha = v$ as

$$G_{ij}^{vv}(t,\tau) = T_{ik}(t)\left[R_{kj}^{vv}(0,\tau) + a_{jl}R_{kl}^{vq}(0,\tau)\right] + a_{ik}R_{jk}^{vq}(0,\tau) + a_{ik}a_{jl}R_{kl}^{qq}(0,\tau) \tag{5.8}$$

All four equal time correlation functions $R_{ij}^{\alpha\beta}(0,\tau)$ for $\alpha = q, v$ and $\beta = q, v$ appear in Eq. (5.8). However, the property (2.9) and Eqs. (4.6) and (4.7) can then be used to express $G_{ij}^{vv}(t,\tau)$ entirely in terms of the velocity autocorrelation function $R_{ij}^{vv}(0,\tau)$, with the result

$$\begin{aligned} G_{ij}^{vv}(t,\tau) = {} & T_{ik}(t)R_{kj}^{vv}(0,\tau) + \int_0^\tau ds\left[a_{ik}T_{jl}(\tau-s) + a_{jl}T_{ik}(\tau-s)\right]R_{kl}^{vv}(0,s) \\ & + a_{jl}\left[T_{ik}(t) - \delta_{ik}\right]\int_0^\tau ds\, e^{-\nu_1(\tau-s)}\Lambda_{kn}(\tau-s)R_{nl}^{vv}(0,s) \end{aligned} \tag{5.9}$$

The problem is now reduced to solving the single Eq. (4.8). However, as indicated in Eq. (4.14) the equal time velocity correlations in the rest frame are simply proportional to the pressure tensor components. Consequently, Eq. (5.9) may be expressed as

$$\begin{aligned} \rho G_{ij}^{vv}(t,\tau) = {} & T_{ik}(t)P_{kj}(\tau) \\ & + \int_0^\tau ds\left\{\left[a_{ik}T_{jl}(\tau-s) + a_{jl}T_{ik}(\tau-s)\right]\right. \\ & \left. + a_{jl}\left[T_{in}(t) - \delta_{in}\right]e^{-\nu_1(\tau-s)}\Lambda_{nk}(\tau-s)\right\}P_{kl}(s) \end{aligned} \tag{5.10}$$

The pressure tensor components are calculated in the second part of the Appendix. It is found that $P_{ij}(t)$ is the sum of three exponentials in time, two of which decay and one which grows, for all values of the shear rate. The dominant part for $\nu_3 t \gg 1$ is given by Eq. (A.36),

$$P_{ij}(t)/p(0) = B_{ij}e^{z_1 t} \tag{5.11}$$

where B_{ij} and z_1 are functions of the shear rate defined in the Appendix. Equation (5.10) may be expressed finally as

$$G_{ij}^{vv}(t,\tau) = G_{ij}^{vv}(\infty,\tau) + e^{-\nu_1 t}\Lambda_{ik}(t)\left[G_{kj}^{vv}(0,\tau) - G_{kj}^{vv}(\infty,\tau)\right] \tag{5.12}$$

where, for $\nu_1\tau \gg 1$,

$$\begin{aligned} G_{ij}^{vv}(0,\tau) &= \frac{p(\tau)}{\rho}\left[C_1\delta_{ij} + C_2(a_{ij} + a_{ji}) + (C_3 - C_4 e^{-z_1\tau})a_{ik}a_{jk}\right] \\ G_{ij}^{vv}(\infty,\tau) &= \frac{p(\tau)}{\rho}\left[C_5 a_{ij} + (C_6 - C_4 e^{-z_1\tau})a_{ik}a_{jk}\right] \end{aligned} \tag{5.13}$$

The $\{C_i\}$ are independent of τ but are functions of the shear rate, and are given in the last section of the Appendix.

An alternative form for Eq. (5.12) that expresses the tensorial form of G_{ij}^{vv} more explicitly is

$$G_{ij}^{vv}(t,\tau) = G_1(t,\tau)\delta_{ij} + G_2(t,\tau)a_{ij} + G_3(t,\tau)a_{ji} + G_4(t,\tau)a_{ik}a_{jk} \quad (5.14)$$

The scalar functions $\{G_i(t,\tau)\}$ may be identified in terms of the constants, $\{C_i\}$,

$$\begin{aligned} G_1(t,\tau) &= \frac{p(\tau)}{\rho} C_1 e^{-\nu_1 t} \\ G_2(t,\tau) &= \frac{p(\tau)}{\rho} \left[C_5 + e^{-\nu_1 t}(C_2 - C_1 t - C_5) \right] \\ G_3(t,\tau) &= \frac{p(\tau)}{\rho} e^{-\nu_1 t} C_2 \\ G_4(t,\tau) &= \frac{p(\tau)}{\rho} \left[C_6 - C_4 e^{-z_1 \tau} + e^{-\nu_1 t}(C_3 - C_2 t - C_6) \right] \end{aligned} \quad (5.15)$$

The fact that $G_2 \neq G_3$ for $t > 0$ means that $G_{ij}^{vv}(t,\tau)$ is not a symmetric tensor, owing to the presence of the shear in the fluid. To illustrate this, consider the antisymmetric part of $G_{ij}^{vv}(t,\tau)$:

$$\Delta_{ij}(t,\tau) \equiv G_{ij}^{vv}(t,\tau) - G_{ji}^{vv}(t,\tau) = \left[G_2(t,\tau) - G_3(t,\tau) \right](a_{ij} - a_{ji}) \quad (5.16)$$

To be specific, let the flow velocity be in the x direction and the gradient in the y direction, $a_{ij} = a\delta_{ix}\delta_{jy}$. Then Figure 1 shows $\rho\Delta_{xy}(t,\tau)/p(\tau)$ for several values of the shear rate. These results may be interpreted qualitatively as

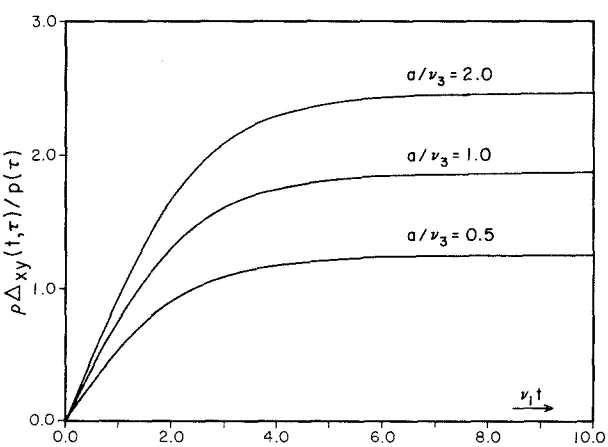

Fig. 1. $\rho\Delta_{xy}(t,\tau)/p(\tau)$, Eq. (5.16), as a function of t for several values of a/ν_3.

follows. At $t = 0$, $\Delta_{xy} = 0$ since $G_{ij}^{vv}(0,\tau)$ is symmetric. For $t > 0$ particles with an initial velocity component along the positive y axis will have an increase in the x component of the velocity due to the flow field. This arises from the second term of Eq. (2.22) which is an inertial force, $F_x = av_y$. In contrast particles with an initial velocity component in the x direction will have no corresponding increase in the y component of the velocity. Consequently, $\Delta_{xy}(t,\tau)$ increases for $t > 0$. However, this increase saturates after a time $1/\nu_1$, owing to collisional damping of the initial velocity. On the average a particle will move to the position $q_i(t+\tau) \sim q_i(\tau) + v_i(\tau)\nu_1^{-1}$. Accordingly, the large t limit should be given by Eq. (5.6) with this value of $q_i(t+\tau)$,

$$\Delta_{xy}(t,\tau) \xrightarrow[\nu_1 t \gg 1]{} \left\langle a\left[y(\tau) + \nu_1^{-1} v_y(\tau)\right] v_y(\tau) \right\rangle$$

which is indeed the correct result, (5.5).

Much of the dependence of $G_{ij}^{vv}(t,\tau)$ on the shear rate is simply due to convective transport of the particle by the fluid. Much of this can be eliminated by the transformation to the local rest frame. The rest frame velocity autocorrelation function is then simply given by

$$R_{ij}^{vv}(t,\tau) = e^{-\nu_1 t} \Lambda_{ik}(t) R_{kj}(0,\tau) \tag{5.18}$$

In contrast to $G_{ij}^{vv}(t,\tau)$, this function clearly decays rapidly to zero. It is shown in the following paper that the diffusion coefficient for this system is related to the time integral of the rest frame velocity autocorrelation function in a way similar to the Green–Kubo expression for linear transport.

6. DISCUSSION

The model considered here is idealized in many respects (e.g., low density, Maxwell molecules, uniform shear flow). However, it serves as a nontrivial example of a highly nonequilibrium system for which the equations for fluctuations and transport can be determined unambiguously and without phenomenological considerations. Of particular interest is the verification of the relationship between the equations for transport and the dynamics of fluctuations as indicated in Eqs. (1.4)–(1.6). The structure of these equations is similar to that for equilibrium fluctuations and in fact may be interpreted as a generalization of Onsager's assumption on the regression of fluctuations. Its validity here is perhaps not too surprising, since the macroscopic equations, (1.4), remain linear even for large shear rates due to the uniformity of the flow field considered. However, these results are in agreement with a more general statement of Onsager's regression hypothesis for nonequilibrium states whose macroscopic dynamics is possibly nonlinear.[4,8] The equation for the equal time fluctuations, (1.6), relates the regression matrix, $\mathscr{L}$, to the microscopic degrees of freedom as expressed by the "noise" term, $\mathscr{D}$. In this sense it may be considered as a type of fluctuation–dissipation relation. Most discussions of such relationships for nonequilibrium systems are restricted to stationary states. The viscous heating here, however, leads to a nonstationary state and the resulting time derivative in Eq. (1.6) introduces a qualitative change in the relationship of $\mathscr{L}$ to $\mathscr{D}$ from that in stationary states.

The interpretation of $\mathscr{D}$ as a noise amplitude is confirmed in the following paper where a Langevin description for tagged particle motion in uniform shear flow is derived. The tensor, $D_{ij}(t)$, that characterizes $\mathscr{D}$, (Eq. 4.17), may be written in the form

$$D_{ij} = \frac{2\nu_1 k_B T(t)}{M} d_{ij} \tag{6.1}$$

In equilibrium d_{ij} reduces to the identity tensor, δ_{ij}. More generally, d_{ij} is not diagonal and its elements are functions of the shear rate. The difference between d_{ij} and δ_{ij} reflects the extent of nonthermal noise in the system. If each small element of the fluid could be considered in a local equilibrium state, the noise in the global nonequilibrium state would be the same as that in equilibrium, except with the macroscopic variables replaced by their nonequilibrium values. Such an approximation would correspond to Eq. (6.1) with $d_{ij} = \delta_{ij}$. Here d_{ij} is given by Eq. (4.15) with additional contributions from the irreversible stress tensor. These contributions indicate the relative importance of differences between the true ensemble and the local equilibrium ensemble. The elements of d_{ij} are readily calculated from the results in the Appendix. For the case of shear flow in the x direction with gradient in the y direction, d_{xx} and d_{xy} are shown in Fig. 2 for the range $0 < a/\nu_3 < 2$. The dashed line (---) denotes the value of d_{xy} for a Newtonian fluid (constant shear viscosity). Consequently, at $a/\nu_3 = 2$ the fluid is highly non-Newtonian but the maximum nonthermal component of the noise is only about a 20% contribution. For very large shear rate d_{xx} has a maximum of 1.44. Similar deviations from local equilibrium noise have been found in other contexts.[17]

In the following paper this problem is reconsidered for the case of a massive tagged particle in the low-density gas. A nonequilibrium Fokker–Planck equation is obtained from the Boltzmann–Lorentz equation, to leading order in the mass ratio. The associated Langevin equations are identified and lead to the same set of equations, (1.4)–(1.6), for the dynamics of fluctuations (although with different values for ν_1 and ν_2). The possibility of diffusion in the Lagrangian frame of the fluid is investigated as a function of shear rate.

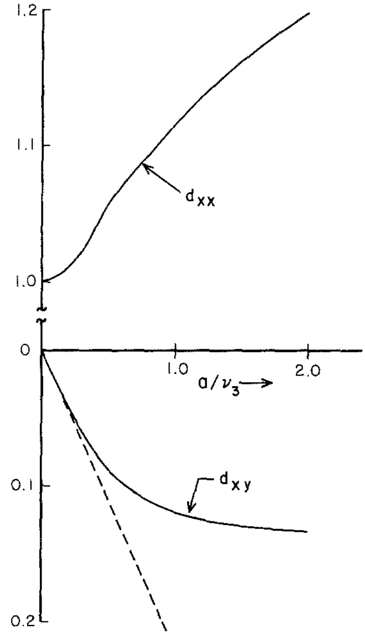

Fig. 2. d_{xx} and d_{xy}, Eq. (6.1), as a function of a/ν_3. The dashed line denotes d_{xy} for a Newtonian fluid.

APPENDIX A

1. Equations for the Rest Frame Correlation Functions

The velocity moments of the nonlinear Boltzmann operator and of the bilinear Boltzmann–Lorentz operator can be calculated exactly for a gas of Maxwell molecules. In particular the first two moments, which are needed in the equations for the position and velocity correlation functions in the rest frame, are evaluated here, with the results

$$\int d\mathbf{v}\, v_i J[f', A] = -\nu_1 \int d\mathbf{v}\, v_i A(x) \tag{A1}$$

and

$$\int d\mathbf{v}\, v_i v_j J[f', A] = -(\nu_1 + \nu_2)\int d\mathbf{v}\, v_i v_j A(x) + \frac{1}{3}\delta_{ij}\nu_2 \int d\mathbf{v}\, v^2 A(x) + \frac{\nu_1 - \nu_2}{\rho} t^*_{ij} + \frac{\nu_1}{\rho}\delta_{ij} p \tag{A2}$$

where A is any function of the phase space variable $x = (\mathbf{q}, \mathbf{v})$ and the irreversible stress tensor t_{ij}^* is defined in Eq. (4.10). The parameters ν_1 and ν_2 are eigenvalues of the Boltzmann–Lorentz operator. Their definition is given in the following.

The proof of Eqs. (A1) and (A2) follows closely the one presented in Appendix C of Ref. 15. The first moment, given in Eq. (A1) is considered first. By making use of the symmetry properties of the collision operator, Eq. (A1) can be rewritten as

$$\int d\mathbf{v}\, v_i J[f', A] = \int d\mathbf{v}\, d\mathbf{v}_1 f'(\mathbf{v}_1, t) A(x) \int_0^\infty db\, b|\mathbf{v} - \mathbf{v}_1| \times \int_0^{2\pi} d\phi\, (\tilde{v}_i - v_i) \tag{A3}$$

Here, $\tilde{v}_i$ denotes the velocity after the collision. Introducing center-of-mass and relative velocities,

$$\mathbf{G} = \tfrac{1}{2}(\mathbf{v} + \mathbf{v}_1), \qquad \mathbf{g} = \mathbf{v} - \mathbf{v}_1 \tag{A4}$$

Eq. (A3) becomes

$$\int d\mathbf{v}\, v_i J[f', A] = \int d\mathbf{v}\, d\mathbf{v}_1\, f'(\mathbf{v}_1, t) A(x) \int_0^\infty db\, bg \int_0^{2\pi} d\phi\, \tfrac{1}{2}(\tilde{g}_i - g_i) \tag{A5}$$

Now let $\tilde{g}_i = g_i \cos\theta + a_i g \sin\theta$, where $\hat{a}$ is a unit vector orthogonal to $\mathbf{g}$. Then, since $\int_0^{2\pi} d\phi\, a_i = 0$,

$$\int d\mathbf{v}\, v_i J[f', A] = \int d\mathbf{v}\, d\mathbf{v}_1\, f'(\mathbf{v}_1, t) A(x) g_i \pi \int_0^\infty db\, bg(\cos\theta - 1) \tag{A6}$$

For Maxwell molecules, $\int_0^\infty db\, bgh(\theta)$ is independent of the velocity, for any function h. Thus

$$\begin{aligned} \int d\mathbf{v}\, v_i J[f', A] &= -\frac{\nu_1}{n} \int d\mathbf{v}\, d\mathbf{v}_1\, f'(\mathbf{v}_1, t) A(x)(v_i - v_{1i}) \\ &= -\nu_1 \int dx\, v_i A(x) \end{aligned} \tag{A7}$$

where the vanishing of the average fluid velocity in the rest frame has been used, and

$$\nu_1 = n\pi \int_0^\infty db\, bg(1 - \cos\theta) \tag{A8}$$

or

$$\nu_1 = \pi n \sigma^2 (V_0/m)^{1/2} 1.19 \tag{A9}$$

Here, V_0 and σ are the parameters characterizing the Maxwell potential,

$$V(r) = V_0(\sigma/r)^4$$

The second moment (A2) can be evaluated in a similar way. Using $\int_0^{2\pi} d\phi\, a_i a_j = \pi(\delta_{ij} - g_i g_j/g^2)$, it becomes

$$\begin{aligned}
&\int d\mathbf{v}\, v_i v_j J[f', A] \\
&\quad = \int d\mathbf{v}\, d\mathbf{v}_1\, f'(\mathbf{v}_1, t) A(x) \Big\{ (g_i G_j + g_j G_i) \int_0^\infty db\, bg\pi(\cos\theta - 1) \\
&\qquad\qquad - \tfrac{3}{4}\big(g_i g_j - \tfrac{1}{3}\delta_{ij} g^2\big) \int_0^\infty db\, bg\pi \sin^2\theta \Big\} \qquad \text{(A10)}
\end{aligned}$$

or

$$\begin{aligned}
&\int d\mathbf{v}\, v_i v_j J[f', A] \\
&\quad = -\frac{\nu_1}{n} \int d\mathbf{v}\, d\mathbf{v}_1\, f'(\mathbf{v}_1, t) A(x)(v_i v_j - v_{1i} v_{1j}) \\
&\qquad - \frac{\nu_2}{n} \int dv\, dv_1\, f'(\mathbf{v}_1, t) A(x) \\
&\qquad \times \Big[v_i v_j + v_{1i} v_{1j} - (v_i v_{1j} + v_j v_{1i}) - \tfrac{1}{3}\delta_{ij}\big(v^2 + v_1^2 - 2\mathbf{v}\cdot\mathbf{v}_1\big)\Big] \qquad \text{(A11)}
\end{aligned}$$

where ν_1 is defined in Eq. (A8) and

$$\nu_2 = \tfrac{3}{4}\pi n \int_0^\infty db\, bg \sin^2\theta \qquad \text{(A12)}$$

or

$$\nu_2 = \tfrac{3}{4}\pi n\sigma^2 (V_0/m)^{1/2} 1.23 \qquad \text{(A13)}$$

The cross term in Eq. (A11) vanishes upon integration over $\mathbf{v}_1$. Making use of the definition (4.10) of the irreversible stress tensor, Eq. (A2) is then obtained.

When $A = f'$ the operator in Eqs. (A1) and (A2) reduces to the nonlinear Boltzmann operator. The right-hand side of Eq. (3.5) describing the time evolution of the pressure tensor is then immediately evaluated by substituting $A = f'$ in Eq. (A2). The result is

$$m \int d\mathbf{v}\, v_i v_j J[f', f'] = -\nu_3 (P_{ij}^* - \delta_{ij} p) \qquad \text{(A14)}$$

where ν_3 is found to equal $2\nu_2$. When Eq. (A14) is substituted on the right-hand side of Eq. (3.5), Eq. (3.6) is obtained.

The set of Eqs. (4.2) and (4.3) for the two-time position and velocity correlation functions in the rest frame, $R_{ij}^{\alpha\beta}(t,\tau)$, are obtained my multiplying Eq. (2.20) with v_i and q_i and integrating. The right-hand side of Eq. (2.20) gives no contribution for $\alpha = q_i$ because the velocity integral of the Boltzmann–Lorentz operator vanishes (i.e., 1 is a left eigenfunction with zero eigenvalue). Equation (4.3) is then immediately obtained. For $\alpha = v_i$ the equation becomes

$$\begin{aligned}\frac{\partial}{\partial t} R_{ij}^{v\beta}(t,\tau) + a_{ik} R_{kj}^{v\beta}(t,\tau) &= \int dx_1\, dx_2\, v_{1i} \beta_{2j} J[f', C'] \\ &= -\nu_1 \int dx_1\, dx_2\, v_{1i} \beta_{2j} C'(x_1, t+\tau; x_2, \tau)\end{aligned} \tag{A15}$$

or

$$\left(\frac{\partial}{\partial t} + \nu_1\right) R_{ij}^{v\beta}(t,\tau) + a_{ik} R_{kj}^{v\beta}(t,\tau) = 0 \tag{A16}$$

Similarly, the equations for the equal time position and velocity correlation functions in the rest frame,

$$R_{ij}^{\alpha\beta}(0,\tau) = \int dx\, \alpha_i \beta_j h'(x,\tau) \tag{A17}$$

are obtained by multiplying Eq. (2.19) with v_i and q_i and integrating. Again, for $\alpha = \beta = q$ the right-hand side of Eq. (2.19) gives no contribution and Eq. (4.6) is obtained. Choosing $\alpha_i = v_i$ and $\beta_j = q_j$ gives

$$\begin{aligned}&\frac{\partial}{\partial t} R_{ij}^{vq}(0,\tau) - \Lambda_{jk}(\tau) R_{kj}^{vv}(0,\tau) + a_{ik} R_{kj}^{vq}(0,\tau) \\ &\quad = \int dx\, v_i q_j J[f', h'] \\ &\quad = -\nu_1 R_{ij}^{vq}(0,\tau)\end{aligned} \tag{A18}$$

where use has been made of Eq. (A1) in writing the second identity. The equation for $R_{ij}^{qv}(0,\tau)$ is immediately obtained by observing that

$$R_{ij}^{\alpha\beta}(0,\tau) = R_{ji}^{\beta\alpha}(0,\tau) \tag{A19}$$

Finally, in the case $\alpha = \beta = v$ the resulting equation is

$$\frac{\partial}{\partial t} R_{ij}^{vv}(0,\tau) + a_{ik} R_{kj}^{vv}(0,\tau) + a_{jk} R_{ki}^{vv}(0,\tau) = \int dx\, v_i v_j J[f', h'] \tag{A20}$$

Making use of Eq. (A2) for $A = h'$, Eq. (4.8) is immediately obtained.

2. Evaluation of $P_{ij}(t)$ and $p(t)$

The coupled equations for the pressure tensor and the pressure are given by Eqs. (3.3) and (3.6):

$$\frac{\partial p}{\partial t} = -\tfrac{2}{3}a_{ij}P_{ij} \tag{A21}$$

$$\left(\frac{\partial}{\partial t} + \nu_3\right)P_{ij} + a_{ik}P_{kj} + a_{jk}P_{ik} = \nu_3\delta_{ij}p \tag{A22}$$

These equations are not independent since $P_{kk} = 3p$. Consider first Eq. (A22) and make the substitution

$$P_{ij}(t) = \Lambda_{ik}(t)\Lambda_{jl}(t)\bar{P}_{kl}(t) \tag{A23}$$

where Λ_{ij} is defined by Eq. (2.15). Then the equation for $\bar{P}_{ij}$ is

$$\left(\frac{\partial}{\partial t} + \nu_3\right)\bar{P}_{ij} = \nu_3\Lambda_{ik}(-t)\Lambda_{jk}(-t)p(t) \tag{A24}$$

Integration of this equation then gives $P_{ij}(t)$ in terms of the pressure

$$P_{ij}(t) = K_{ij}(t)p(0) + \int_0^t d\tau\, K_{ij}(t-\tau)\nu_3 p(\tau) \tag{A25}$$

with

$$K_{ij}(t) \equiv e^{-\nu_3 t}\Lambda_{ik}(t)\Lambda_{jk}(t) \tag{A26}$$

Here, the initial condition $P_{ij}(0) = p(0)\delta_{ij}$ has been chosen for simplicity. To proceed it is convenient to take the Laplace transform of Eqs. (A21) and (A25) to get

$$z\tilde{p}(z) - p(0) = -\tfrac{2}{3}a_{ij}\tilde{P}_{ij}(z) \tag{A27}$$

$$\tilde{P}_{ij}(z) = \tilde{K}_{ij}(z)\left[p(0) + \nu_2\tilde{p}(z)\right] \tag{A28}$$

where the tilde denotes the transform of the corresponding time-dependent function. This set of linear algebraic equations is easily solved to give

$$\tilde{p}(z) = p(0)\frac{(z+\nu_3)^2 + 2a^2/3}{D(z)} \tag{A29}$$

$$\tilde{P}_{ij}(z) = \frac{p(0)}{D(z)}\left[(z+\nu_3)^2\delta_{ij} - (z+\nu_3)(a_{ij}+a_{ji}) + 2a_{ik}a_{jk}\right] \tag{A30}$$

with

$$D(z) \equiv z(z+\nu_3)^2 - \tfrac{2}{3}a^2\nu_3 \tag{A31}$$

The cubic form, $D(z)$, is expressed in terms of its roots by

$$D(z) = (z - z_1)(z - z_2)(z - z_3) \tag{A32}$$

where

$$\begin{aligned} z_1 &= \nu_3 \lambda(a/\nu_3) \\ z_2 &= -\nu_3 \left\{ \left[\frac{1}{2} \lambda\left(\frac{a}{\nu_3} \right) + 1 \right] + i \frac{2}{\sqrt{3}} \sinh \frac{1}{3} \alpha\left(\frac{a}{\nu_3} \right) \right\} \\ z_3 &= z_2^\dagger \end{aligned} \tag{A33}$$

The dagger in the last equation denotes complex conjugation, and

$$\begin{aligned} \lambda(x) &= \tfrac{4}{3} \sinh^2\left[\tfrac{1}{6} \alpha(x) \right] \\ \alpha(x) &= \cosh^{-1}\left[1 + 9x^2 \right] \end{aligned} \tag{A34}$$

The constants, z_1, z_2, and z_3 are the locations of the poles of both $\tilde{p}(z)$ and $\tilde{P}_{ij}(z)$, and represent the only singularities of these functions in the complex plane. The real part of z_2 and z_3 is negative for all values of the shear rate, a, and leads to exponentially decaying components in time. The characteristic time for such decay is of the order of ν_3^{-1}. In contrast, the real part of z_1 is always positive, and leads to an exponential growth in time.

While it is straightforward to invert the Laplace transform in Eqs. (A29) and (A30) for the complete time dependence of $p(t)$ and $\tilde{P}_{ij}(t)$, only the results for $\nu_3 t \gg 1$ will be given here. For such times the exponentially decaying components may be neglected, and the dominant behavior is found to be

$$p(t)/p(0) \to A e^{z_1 t} \tag{A35}$$

$$P_{ij}(t)/p(0) \to B_{ij} e^{z_1 t} \tag{A36}$$

with

$$A = \frac{(z_1 + \nu_3)^2 + 2a^2/3}{(z_1 - z_2)(z_1 - z_3)} \tag{A37}$$

$$B_{ij} = \frac{1}{(z_1 - z_2)(z_1 - z_3)} \left[(z_1 + \nu_3)^2 \delta_{ij} - (z_1 + \nu_3)(a_{ij} + a_{ji}) + 2a_{ik}a_{jk} \right] \tag{A38}$$

The temperature is determined from the ideal gas equation of state, $p(t) = nk_B T(t)$.

3. VELOCITY AUTOCORRELATION FUNCTION

The time-independent functions of the shear rate, C_i, in Eq. (5.13) for the velocity autocorrelation function are given by

$$C_1 = \frac{(z_1+\nu_3)^2}{(z_1+\nu_3)^2+2a^2/3}$$

$$C_2 = \frac{(z_1+\nu_3)(\nu_3-\nu_1)}{(z_1+\nu_1)\left[(z_1+\nu_3)^2+2a^2/3\right]}$$

$$C_3 = 2\,\frac{\nu_1(z_1+\nu_3)^2+z_1(z_1+\nu_1)^2-z_1(z_1+\nu_1)(z_1+\nu_3)}{z_1(z_1+\nu_1)^2\left[(z_1+\nu_3)^2+2a^2/3\right]}$$

$$\begin{aligned} C_4 = {} & 2\left\{z_2z_3(z_2-z_3)(z_1+\nu_3)^2 - z_1z_3(z_1-z_3)(z_2+\nu_3)^2\right. \\ & \left. + z_1z_2(z_1-z_2)(z_3+\nu_3)^2\right\}\left\{\nu_1z_1z_2z_3(z_1-z_3)\left[(z_1+\nu_3)^2+2a^2/3\right]\right\}^{-1} \end{aligned} \tag{A39}$$

$$C_5 = \frac{z_1+2\nu_1}{\nu_1(z_1+\nu_1)}\,C_1$$

$$C_6 = \frac{(z_1+\nu_3)\left[z_1^2(\nu_3-\nu_1)+2\nu_1\nu_3(z_1+\nu_3)\right]}{z_1\nu_1(z_1+\nu_1)^2\left[(z_1+\nu_3)^2+2a^2/3\right]}$$

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