Transport far from equilibrium: Uniform shear flow

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(Received 3 October 1996; revised manuscript received 9 May 1997)

The Bhatnager-Gross-Krook model kinetic equation is applied to spatially inhomogeneous states near steady uniform shear flow. The shear rate of the reference steady state can be large, so the states considered include those very far from equilibrium. The single-particle distribution function is calculated exactly to first order in the deviations of the hydrodynamic field gradients from their values in the reference state. Corresponding nonlinear hydrodynamic equations are obtained, and the set of transport coefficients are identified as explicit functions of the shear rate. The spectrum of the linear hydrodynamic equations is studied in detail, and qualitative differences from the spectrum for equilibrium fluctuations are discussed. Conditions for instabilities at long wavelengths are identified and discussed. [S1063-651X(97)11708-1]

PACS number(s): 05.20.Dd, 51.10.+y, 83.50.Ax, 83.20.−d

I. INTRODUCTION

Nonequilibrium phenomena are well understood for states near equilibrium. However, even the qualitative features of transport and fluctuations far from equilibrium are poorly understood, due to the complexity of the physical states and the lack of an adequate controlled theoretical description in general. It is useful in this context to consider more restrictive conditions and specialized states for which greater progress in this difficult area can be made. Here we consider a low-density simple atomic gas for which transport properties are described by the nonlinear Boltzmann equation. For states near equilibrium, the Chapman-Enskog expansion of the distribution function about the local equilibrium distribution in terms of gradients of the hydrodynamic fields provides approximations to a normal solution (one for which all space and time dependence occurs through the hydrodynamic variables) [1]. From this solution the corresponding hydrodynamic equations are obtained, including explicit expressions for the associated transport coefficients. In principle, this method applies to states far from equilibrium as well, although calculation of the Chapman-Enskog expansion to higher orders in the gradients is prohibitively difficult, and questions of convergence remain unresolved. An alternative approach is to expand in small gradients about a more relevant reference state than local equilibrium. For example, consider states near a homogeneous reference steady state. Deviations of the hydrodynamic variables from their values in this state are characterized by small relative spatial gradients. A modified Chapman-Enskog expansion can be implemented to obtain the distribution function and hydrodynamic equations to leading order in these gradients. Since the reference state can be far from equilibrium, the form of the hydrodynamic equations and the dependence of the transport coefficients on parameters of the steady state will be quite different from those for states near equilibrium.

In practice this program has not been carried out since determination of a nontrivial reference steady state far from the equilibrium from the Boltzmann equation is exception-

ally rare [2]. In contrast, exact results have been obtained for a number of physically interesting special steady states [3] using a model kinetic equation designed to preserve the essential features of the Boltzmann equation while admitting more practical analysis [4]. In some cases these results have been compared with those from Monte Carlo simulation far from equilibrium, indicating that the kinetic model provides both qualitative and semiquantitative representations of the underlying Boltzmann equation [5]. The objective here is to use this kinetic model approach for the special class of states at or near uniform shear flow. Uniform shear flow is a particularly well-studied nonequilibrium state using numerical methods (both Monte Carlo simulation at low density [5] and molecular-dynamics simulation at high density [6,7]), illustrating rheological properties normally associated with complex molecular fluids [8]. More importantly, it is one of the special cases for which an exact solution to the model kinetic equation has been obtained [9,10], providing the necessary reference state for the modified Chapman-Enskog expansion developed here. We look for solutions to the kinetic equation as an expansion in small spatial gradients relative to an exact solution for local uniform shear rather than around local equilibrium. The heat and momentum fluxes are calculated from this solution to linear order in these gradients, and a closed set of generalized hydrodynamic equations is obtained. This is analogous to the nonlinear Navier-Stokes equations near equilibrium, except that here the reference state is non-Maxwellian and a complex function of the shear rate. The associated nonlinear transport coefficients are identified, and examples calculated for arbitrary values of the shear rate.

To expose the physical content of these hydrodynamic equations and their differences from those for states near equilibrium, hydrodynamic modes are calculated from the associated linearized equations. In addition to their dependence on the shear rate, these modes have a more complex wave-vector dependence than those from the Navier-Stokes equations due to the broken symmetry of the reference state. More surprisingly, a new long wavelength instability is

found such that the hydrodynamic modes are growing initially for any finite shear rate and sufficiently long wavelength [11]. A more detailed study of this instability and its verification via computer simulation is described elsewhere [12].

II. KINETIC THEORY AND UNIFORM SHEAR FLOW

In this section the kinetic theory is defined, the associated macroscopic conservation laws obtained, and the special solution for steady uniform shear flow is described. In the next section, this solution is generalized to a local reference state for an expansion to describe a class of states near uniform shear flow and to obtain the associated hydrodynamic equations.

Exact or even approximate solutions to the Boltzmann equation far from equilibrium are exceptionally rare, due to the complexity of the nonlinear collision operator. Therefore kinetic models have been introduced to replace the Boltzmann collision operator with a simpler, more tractable operator. The best studied of these is a single relaxation time model due to Bhatnager, Gross, and Krook (the BGK model) [4]. The essential qualities of this model are its preservation of the exact equilibrium solution and all five conservation laws. The BGK Boltzmann kinetic equation is given by

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla_r\right) f + m^{-1} \nabla_v \cdot (\mathbf{F}_{\text{ext}} f) = -\nu(f - f_\ell), \quad (2.1)$$

where $\mathbf{F}_{\text{ext}}$ is an external force. The parameter ν in Eq. (2.1) is a collision frequency which depends on an interaction law. This frequency is a function of the density and temperature. At low density, it can be written as

$$\nu \sim n(\mathbf{r},t) T^b(\mathbf{r},t), \quad (2.2)$$

when the potential has a form $V(r) \sim r^{-l}$, with $b = 1/2 - 2/l$. In the case of Maxwell molecules ($l=4$), b is zero so ν becomes independent of temperature. For the hard sphere case $l \to \infty$, resulting in a value for b of $\frac{1}{2}$. Finally, $f_\ell(\mathbf{r},\mathbf{v},t)$ is the local equilibrium distribution

$$f_\ell(\mathbf{r},\mathbf{v},t) = n(\mathbf{r},t)\left(\frac{\beta(\mathbf{r},t)m}{2\pi}\right)^{3/2}$$

$$\times \exp\left[-\frac{1}{2}\beta(\mathbf{r},t)m(\mathbf{v}-\mathbf{u}(\mathbf{r},t))^2\right], \quad (2.3)$$

where $n(\mathbf{r},t)$, $T(\mathbf{r},t) \equiv [k_B\beta(\mathbf{r},t)]^{-1}$, and $\mathbf{u}(\mathbf{r},t)$ are the density, temperature, and flow velocity of the nonequilibrium state. These hydrodynamic fields are defined such that

$$\int d\mathbf{v} \begin{pmatrix} 1 \\ \mathbf{v} \\ v^2 \end{pmatrix} (f(\mathbf{r},\mathbf{v},t) - f_\ell(\mathbf{r},\mathbf{v},t)) = 0, \quad (2.4)$$

which assures that the BGK equation yields the correct conservation laws and equilibrium stationary state in the absence of driving forces. More explicitly, Eq. (2.4) gives

$$n(\mathbf{r},t) \equiv \int d\mathbf{v}\, f(\mathbf{r},\mathbf{v},t), \quad n(\mathbf{r},t)\mathbf{u}(\mathbf{r},t) \equiv \int d\mathbf{v}\, \mathbf{v} f(\mathbf{r},\mathbf{v},t),$$

$$\tfrac{3}{2} n(\mathbf{r},t) k_B T(\mathbf{r},t) \equiv \int d\mathbf{v} \tfrac{1}{2} m c^2 f(\mathbf{r},\mathbf{v},t), \quad (2.5)$$

where $\mathbf{c} = \mathbf{v} - \mathbf{u}$.

The macroscopic conservation laws are obtained by taking moments of Eq. (2.1) and using the definitions (2.5)

$$D_t n(\mathbf{r},t) + n(\mathbf{r},t)\nabla \cdot \mathbf{u}(\mathbf{r},t) = 0, \quad (2.6)$$

$$D_t T(\mathbf{r},t) + \frac{2}{3k_B n(\mathbf{r},t)}[\nabla \cdot \mathbf{q}(\mathbf{r},t) + t_{ij}(\mathbf{r},t)\partial_i u_j(\mathbf{r},t)],$$

$$= s(\mathbf{r},t), \quad (2.7)$$

$$D_t u_i(\mathbf{r},t) + [mn(\mathbf{r},t)]^{-1}\partial_j t_{ij} = 0, \quad (2.8)$$

where $D_t \equiv \partial_t + \mathbf{u} \cdot \nabla$ is the material derivative. The heat and momentum fluxes $\mathbf{q}(\mathbf{r},t)$ and $t_{ij}(\mathbf{r},t)$ are linear functionals of $f(\mathbf{r},\mathbf{v},t)$ given by

$$\mathbf{q}(\mathbf{r},t) = \int d\mathbf{v} \tfrac{1}{2} m\, c^2 \mathbf{c} f(\mathbf{r},\mathbf{v},t),$$

$$t_{ij}(\mathbf{r},t) = \int d\mathbf{v}\, m\, c_i c_j f(\mathbf{r},\mathbf{v},t). \quad (2.9)$$

The inhomogeneous term on the right side of the temperature equation, $s(\mathbf{r},t)$, is due to the external force $\mathbf{F}_{\text{ext}}$, introduced to serve as a thermostat. Several thermostats that have been used in both theory and computer simulations. Here we choose a force that is proportional to the relative velocity $\mathbf{c} = \mathbf{v} - \mathbf{u}(\mathbf{r},t)$,

$$\mathbf{F}_{\text{ext}}(\mathbf{r},\mathbf{c},t) = -m\lambda(n(\mathbf{r},t),T(\mathbf{r},t))\mathbf{c}. \quad (2.10)$$

The resulting source term $s(\mathbf{r},t)$ in the equation for the temperature becomes

$$s(\mathbf{r},t) = -2T(\mathbf{r},t)\lambda(n(\mathbf{r},t),T(\mathbf{r},t)). \quad (2.11)$$

The proportional ''constant'' $\lambda(n(\mathbf{r},t),T(\mathbf{r},t))$ is determined by requiring stationarity of the system in the uniform shear flow state (see below), and may depend on the local density, temperature, and shear rate. In Appendix A a different thermostat is considered for comparison. The primary changes are the degree to which the external force compensates for viscous heating away from the state of uniform shear flow.

The fact that the fields are functionals of $f(\mathbf{r},\mathbf{v},t)$ makes the BGK Boltzmann equation highly nonlinear and difficult to solve in general. However, in many cases an implicit solution can be given as an explicit function of the velocity and functional of the fields. Then, the fields must be determined self-consistently from the above macroscopic conservation laws. One of the cases for which an exact solution is known is uniform shear flow [3,9,10]. The uniform shear state is a planar flow whose x component of the flow velocity has a gradient along the y axis, $u_{si} = a_{ij} r_j$ and $a_{ij} = a \delta_{ix}\delta_{jy}$, where a is a constant shear rate. In addition, the density n_s, temperature T_s, heat flux, and momentum flux are spatially

constant. This state is generated by a periodic boundary condition in the local Lagrangian frame [13]. The viscous heating induced by these boundary conditions is compensated by the external force. It is easily verified that this macroscopic state is an exact stationary solution to the above conservation laws (2.6)–(2.8) if $\lambda(n(\mathbf{r},t),T(\mathbf{r},t))$ is chosen to be

$$\lambda_s \equiv \lambda(n_s,T_s) = -\frac{a\, t_{xy,s}(a)}{3 n_s k_B T_s}. \tag{2.12}$$

Due to the simplicity of uniform shear flow state at the macroscopic level, it has been studied extensively as a prototype of nonequilibrium states far from equilibrium in theory [10,14–17] and in computer simulations [6,7,18,19]. To obtain the distribution function for this state it is useful to express the kinetic equation (2.1) in terms of the velocity in the local rest frame, defined by $v_i' = v_i - a_{ij}r_j$. In this frame, the flow field vanishes and the macroscopic state becomes spatially homogeneous. Consequently, we look for a stationary solution to Eq. (2.1) of the form $f(\mathbf{r},\mathbf{v},t) = f_s(\mathbf{v}')$,

$$L(v',a)f_s(\mathbf{v}') = -\nu_s f_{s\ell}(\mathbf{v}'),$$

$$L(v',a) \equiv a_{ij}v_j'\frac{\partial}{\partial v_i'} + \lambda_s \mathbf{v}' \cdot \nabla_{v'} + 3\lambda_s - \nu_s. \tag{2.13}$$

The subscript s denotes the stationary state value and $f_{s\ell}$ is the corresponding local equilibrium distribution function with the hydrodynamic fields for uniform shear flow. The solution to Eq. (2.13) is

$$f_s(\mathbf{v}') = \nu_s \int_0^\infty d\tau\, e^{\tau L} f_\ell(\mathbf{v}')$$

$$= \nu_s \int_0^\infty dt\, e^{-t(\nu_s - 3\lambda_s)} f_{s\ell}(e^{\lambda_s t}\Lambda_{ij}(-t)v_j'). \tag{2.14}$$

The second equality follows from the property for an arbitrary function $X(\mathbf{v})$

$$e^{tL}X(\mathbf{v}') = e^{(3\lambda_s - \nu_s)t}X(e^{\lambda_s t}\Lambda_{ij}(-t)v_j'), \quad \Lambda_{ij}(t) = \delta_{ij} - a_{ij}t, \tag{2.15}$$

where use has been made of $\exp(atv_x\partial_{v_x})X(v_x) = X(e^{at}v_x)$ and $\exp(atv_y\partial_{v_x})X(v_x) = X(v_x + atv_y)$. To determine λ_s as an explicit function of a, the component of the momentum flux $t_{xy,s}(a)$ can be calculated from Eqs. (2.9) and (2.14) to obtain the self-consistent equation

$$3\lambda_s(2\lambda_s + \nu_s)^2 = \nu_s a^2. \tag{2.16}$$

This has one real solution and two complex conjugate solutions. The physically relevant real value is

$$\lambda_s(a) = \frac{2}{3}\nu_s \sinh\left[\cosh^{-1}\frac{1}{6}\left(1 + 9\frac{a^2}{\nu_s^2}\right)\right]^2. \tag{2.17}$$

With λ_s known, the velocity distribution given by Eq. (2.14) is completely determined.

Any transport property of interest now can be calculated by integration. A detailed discussion can be found in Ref.

[10], and comparison with Monte Carlo simulations of the Boltzmann equation for shear flow is given in Ref. [19]. Only the transport properties associated with the heat and momentum fluxes are considered further here. These can be calculated directly from Eqs. (2.9) and (2.14), with the results

$$\mathbf{q}(a) = 0,$$

$$t_{ij,s}(a) = (p_s + \tfrac{1}{3}a^2\Psi_1(a))\delta_{ij} - \eta(a)(a_{ij} + a_{ji})$$
$$- \Psi_1(a)a_{ik}a_{jk} \tag{2.18}$$

Thus, the heat flux vanishes but the momentum flux describes nontrivial rheological effects in terms of the hydrostatic pressure $p = nk_B T$, the shear viscosity $\eta(a) \equiv -a^{-1}t_{xy}(a)$, and the viscometric function $\Psi_1(a) \equiv a^{-2}[t_{yy}(a) - t_{xx}(a)]$, where

$$\eta(a) = \frac{\nu_s}{(2\lambda_s(a) + \nu_s)^2}p_s,$$

$$\Psi_1(a) = -\frac{6\lambda_s(a)}{a^2(2\lambda_s(a) + \nu_s)}p_s. \tag{2.19}$$

In general there is a second independent viscometric function $\Psi_2(a) \equiv a^{-2}[t_{zz}(a) - t_{yy}(a)]$ which vanishes for our kinetic model. The magnitudes of these transport coefficients are monotonically decreasing functions of the shear rate, and have been discussed in detail elsewhere [10].

III. HYDRODYNAMICS NEAR UNIFORM SHEAR FLOW

In this section we consider states that deviate from uniform shear flow by small spatial gradients. A solution to the BGK Boltzmann equation (2.1) is obtained by a variant of the Chapman-Enskog method, whereby the distribution function is expanded about a *local* uniform shear flow reference state in terms of the small spatial gradients of the hydrodynamic fields relative to those of uniform shear flow. This is analogous to the usual Chapman-Enskog expansion about a local equilibrium distribution. The solution obtained in this way can be used to calculate the heat and momentum fluxes in terms of the hydrodynamic variables, so that Eqs. (2.6)–(2.8) become a closed set of hydrodynamic equations. The analysis here is carried out to first order in the gradients. For small shear rate the usual Navier-Stokes results are recovered, where the heat flux is given by Fourier's law and the momentum flux is given by Newton's viscosity law. However, for large shear rates these fluxes and the corresponding hydrodynamic equations are more complex.

To construct the Chapman-Enskog expansion we look for solutions of the form

$$f(\mathbf{r},\mathbf{v},t) = f(\mathbf{v}',y_\alpha(\mathbf{r},t)), \tag{3.1}$$

where $y_\alpha(\mathbf{r},t)$ are the hydrodynamic fields, and $v_i' = v_i - a_{ij}r_j$. This representation expresses the fact that the space dependence of the reference shear flow is completely absorbed in the relative velocity variable, $\mathbf{v}'$, and all other space and time dependence occurs entirely through a functional dependence on the hydrodynamic variables, $y_\alpha(\mathbf{r},t)$.

This is an example of a ''normal'' solution, which is expected to result from a wide class of initial conditions at long times and large space scales. It is essential for a hydrodynamic description since the velocity average of any quantity becomes a functional of the hydrodynamic fields. Approximate solutions to the BGK equation are obtained by expanding Eq. (3.1) in a formal uniformity parameter ϵ that measures the spatial gradients of the fields $y_\alpha(\mathbf{r},t)$,

$$f(\mathbf{v}',y_\alpha(\mathbf{r},t))=f^{(0)}(\mathbf{v}',y_\alpha(\mathbf{r},t))+\epsilon f^{(1)}(\mathbf{v}',y_\alpha(\mathbf{r},t))+\cdots. \tag{3.2}$$

This expansion leads to a corresponding expansion for the heat and momentum fluxes when substituted into Eq. (2.9),

$$t_{ij}=t_{ij}^{(0)}+\epsilon\, t_{ij}^{(1)}+\cdots, \quad \mathbf{q}=\mathbf{q}^{(0)}+\epsilon\,\mathbf{q}^{(1)}+\cdots, \tag{3.3}$$

$$t_{ij}^{(r)}=\int d\mathbf{v}mc_ic_jf^{(r)}, \quad \mathbf{q}^{(r)}=\int d\mathbf{v}\tfrac{1}{2}mc^2\mathbf{c}f^{(r)}. \tag{3.4}$$

Finally, use of this expansion for the fluxes in the conservation laws (2.6)–(2.8) identifies an expansion for the time derivatives of the fields in powers of the uniformity parameter

$$\frac{\partial}{\partial t}=\frac{\partial^{(0)}}{\partial t}+\epsilon\frac{\partial^{(1)}}{\partial t}+\cdots. \tag{3.5}$$

These results provide the basis for generating the Chapman-Enskog solution to the BGK Boltzmann equation.

The BGK Boltzmann equation in terms of the variable $\mathbf{v}'$ is obtained directly from Eq. (2.1),

$$\left(\frac{\partial}{\partial t}+(v_i'+a_{ij}r_j)\frac{\partial}{\partial r_i}-L(v',a)+\lambda\,\delta\mathbf{u}\cdot\boldsymbol{\nabla}_{\mathbf{v}'}\right)f(\mathbf{r},\mathbf{v}',t)$$
$$=\nu f_\ell(\mathbf{r},\mathbf{v}',t), \tag{3.6}$$

where $\delta\mathbf{u}=\mathbf{u}-\mathbf{u}_s$. Also, the operator $L(v',a)$ is defined by Eq. (2.13) except with ν_s,λ_s replaced by ν,λ as functions of $n(\mathbf{r},t)$ and $T(\mathbf{r},t)$. The form of λ is still to be determined at this point. The spatial gradient in the second term on the left side is taken at constant $\mathbf{v}'$, and consequently this term is of first order in the uniformity parameter. Substituting the expansions (3.2) and (3.5) into (3.6) and equating coefficients of each degree in the uniformity parameter leads to the equations for $f^{(0)}$ and $f^{(1)}$:

$$\left(\frac{\partial^{(0)}}{\partial t}-L(v',a)+\lambda\,\delta\mathbf{u}\cdot\boldsymbol{\nabla}_{\mathbf{v}'}\right)f^{(0)}=\nu f_\ell, \tag{3.7}$$

$$\left(\frac{\partial^{(0)}}{\partial t}-L(v',a)+\lambda\,\delta\mathbf{u}\cdot\nabla_{\mathbf{v}'}\right)f^{(1)}$$
$$=-\left(\frac{\partial^{(1)}}{\partial t}+(v_i'+a_{ij}r_j)\frac{\partial}{\partial r_i}\right)f^{(0)}. \tag{3.8}$$

To lowest order in the expansion the conservation laws give

$$\frac{\partial^{(0)}n}{\partial t}=0, \quad \frac{\partial^{(0)}\delta u_i}{\partial t}+a_{ij}\delta u_j=0,$$

$$\frac{3}{2}nk_B\frac{\partial^{(0)}T}{\partial t}+a_{ij}t_{ij}^{(0)}+3\lambda nk_BT=0, \tag{3.9}$$

where $t_{ij}^{(0)}$ is defined by Eq. (3.4). The parameter λ of the external force is now chosen to impose $\partial^{(0)}T/\partial t=0$, i.e.,

$$\lambda(n(\mathbf{r},t),T(\mathbf{r},t))=-at_{xy}^{(0)}(\mathbf{r},t)/3n(\mathbf{r},t)k_BT(\mathbf{r},t). \tag{3.10}$$

The solution to Eq. (3.7) is obtained in a way similar to that for Eq. (2.13), with the result

$$f^{(0)}(\mathbf{v}',y_\alpha(\mathbf{r},t))=\nu(\mathbf{r},t)n(\mathbf{r},t)\left(\frac{m}{2\pi k_BT(\mathbf{r},t)}\right)^{3/2}$$
$$\times\int_0^\infty d\tau\ e^{-\nu(\mathbf{r},t)\tau}e^{3\lambda(\mathbf{r},t)\tau}$$
$$\times\exp\left(-\frac{m}{2k_BT(\mathbf{r},t)}e^{2\lambda(\mathbf{r},t)\tau}\right.$$
$$\left.\times[\Lambda_{ij}(-\tau)(v_j'-\delta u_j(\mathbf{r},t))]^2\right), \tag{3.11}$$

where $\Lambda_{ij}(t)$ is defined in Eq. (2.15). The relationship of Eq. (3.11) to Eq. (2.14) is analogous to the relationship of the local equilibrium distribution to the strict equilibrium distribution, where the former is obtained from the latter by replacing the hydrodynamic fields with their actual nonequilibrium values. To determine $\lambda(\mathbf{r},t)\equiv\lambda(n(\mathbf{r},t),T(\mathbf{r},t))$, the momentum flux $t_{xy}^{(0)}(\mathbf{r},t)$ is calculated using Eqs. (3.4) and (3.11) to obtain

$$t_{xy}^{(0)}(\mathbf{r},t)=\frac{-a\nu(\mathbf{r},t)}{(2\lambda(\mathbf{r},t)+\nu(\mathbf{r},t))^2}\,n(\mathbf{r},t)k_BT(\mathbf{r},t), \tag{3.12}$$

where $\nu(\mathbf{r},t)\equiv\nu(n(\mathbf{r},t),T(\mathbf{r},t))$. Use of Eq. (3.10) then gives, finally,

$$3\lambda(\mathbf{r},t)(2\lambda(\mathbf{r},t)+\nu(\mathbf{r},t))^2=\nu(\mathbf{r},t)a^2. \tag{3.13}$$

This shows that $\lambda(n(\mathbf{r},t),T(\mathbf{r},t))$ is the same as Eq. (2.16) for uniform shear flow, except that the density and temperature are replaced by their values for the general nonequilibrium state. With this result for $\lambda(\mathbf{r},t)$, solution (3.11) is completely determined.

Next, consider the solution to Eq. (3.8) for the contributions to first order in the spatial gradients. As shown in Appendix B, the right side is a linear combination of the hydrodynamic gradients. Consequently, $f^{(1)}$ necessarily has the same form,

$$f^{(1)}(\mathbf{v}',y_\alpha(\mathbf{r},t))=X_{n,i}\frac{\partial n}{\partial r_i}+X_{T,i}\frac{\partial T}{\partial r_i}+X_{u_k,i}\frac{\partial\delta u_k}{\partial r_i}, \tag{3.14}$$

where the coefficients $X_{\beta,i}(y_\alpha(\mathbf{r},t),\mathbf{v}')$ are functions of the velocity to be determined from substitution of Eq. (3.14) into Eq. (3.8),

$$\left(\frac{\partial^{(0)}}{\partial t}-L(v',a)+\lambda\ \delta\mathbf{u}\cdot\nabla_{\mathbf{v}'}\right)X_{\beta,k}-aX_{u_x,k}\delta_{\beta,u_y}=-Y_{\beta,k}.$$

$$(3.15)$$

Here β denotes n,T,u_x,u_y, and u_z, and i,k represents Cartesian coordinates. The last term on the left side originates from $(\partial^{(0)}/\partial t)(\partial\delta u_k/\partial r_i)=(\partial/\partial r_i)(\partial^{(0)}/\partial t)\delta u_k$ and Eq. (3.9). The functions $Y_{\beta,k}$ are given explicitly in terms of $f^{(0)}$ and the flux $t_{ij}^{(1)}$, which must be determined self-consistently from $f^{(1)}$. The procedure is to solve Eq. (3.15) to find $f^{(1)}$ in terms of $t_{ij}^{(1)}$ and then to use this result to derived a self-consistent equation for $t_{ij}^{(1)}$. Further details can be found in Appendix B along with the explicit solution to Eq. (3.15).

In this way the complete normal solution near the uniform shear state is constructed to order ϵ. The heat and momentum fluxes then are calculated from Eq. (3.4). The first terms $t_{ij}^{(0)}(a)$ and $q_i^{(0)}(a)$ represent the transport properties of the *local* reference state. They are the same as those of Sec. II, Eq. (2.18), except that the density and temperature are replaced by their values for the general nonequilibrium state. An important consequence of this replacement is that their gradients are no longer zero and thus they now contribute to the hydrodynamic equations. The second terms $t_{ij}^{(1)}(a)$ and $q_i^{(1)}(a)$ provide new transport coefficients describing dissipation due to spatial deviations uniform shear flow,

$$q_i^{(1)}(a)=-\left(\xi_{T,j}^i(a)\frac{\partial T}{\partial r_j}+\xi_{n,j}^i(a)\frac{\partial n}{\partial r_j}\right),$$

$$t_{ij}^{(1)}(a)=-\gamma_{lk}^{ij}(a)\frac{\partial\delta u_l}{\partial r_k}.\qquad(3.16)$$

It is understood that ν, $\lambda(a)$, and p, and the transport coefficients all are functions of the local nonequilibrium temperature and density, as well as the shear rate a. The method for calculating $\gamma_{lk}^{ij}(a)$ and $\xi_{\alpha,j}^i(a)$ and some detailed forms of the coefficients are given in Appendix C; a more complete listing can be obtained on request from the authors. Since the reference state is anisotropic there are new transport coefficients, reflecting the broken fluid symmetry, which do not exist for hydrodynamics near equilibrium. Fourier's law for the heat flux is modified by a thermal conductivity tensor $\xi_{T,j}^i(a)$, which has the form

$$\xi_{T,j}^i(a)=\xi_T^{(1)}(a)\delta_{ij}+\xi_T^{(2)}(a)a_{ij}+\xi_T^{(3)}(a)a_{ji}+\xi_T^{(4)}(a)a_{ik}a_{jk}$$

$$+\xi_T^{(5)}(a)a_{ki}a_{kj}\qquad(3.17)$$

characterized by five scalar ''thermal conductivities'' characterizing this tensor. The anisotropy is in the x,y plane so, for example, a temperature gradient in the x direction leads to a heat flux in both the x and y directions. At zero shear rate only the contribution from $\xi_T^{(1)}(a)$ survives with $\xi_T^{(1)}(0)=\kappa$, where $\kappa=5k_Bp/2m\nu$ is the thermal conductivity for the BGK model. An additional difference from Fourier's law is a contribution to the heat flux from a density gradient characterized by the transport tensor, $\xi_{n,j}^i(a)$. This has a representation like Eq. (3.17) in terms of five additional scalar transport coefficients. The asymptotic behavior for small

shear rates is $\xi_{n,j}^i(a)\rightarrow(a_{ij}+a_{ji})m(\beta/\nu)^2$, which vanishes for zero shear rate as expected. The momentum flux is expressed in terms of a viscosity tensor, $\gamma_{lk}^{ij}(a)$, of degree 4 which is symmetric and traceless in ij. There are 19 independent viscosity coefficients. At zero shear rate $\gamma_{lk}^{ij}(a)$ reduces to Newton's viscosity law, $\gamma_{lm}^{ij}(a=0)=\eta(\delta_{il}\delta_{jm}+\delta_{im}\delta_{jl}-\frac{2}{3}\delta_{ij}\delta_{lm})$, where $\eta=p/\nu$ is the shear viscosity for the BGK model.

The corresponding nonlinear hydrodynamic equations are obtained directly from these results and the conservation laws

$$D_tn+n\boldsymbol{\nabla}\cdot\delta\mathbf{u}=0,\qquad(3.18)$$

$$\frac{3}{2}nk_BD_tT-a_{ij}\gamma_{lm}^{ij}\frac{\partial\delta u_l}{\partial r_m}+\frac{\partial\delta u_i}{\partial r_j}\left[t_{ij}^{(0)}-\gamma_{lm}^{ij}\frac{\partial\delta u_l}{\partial r_m}\right]$$

$$-\frac{\partial}{\partial r_i}\left[\xi_{n,j}^i\frac{\partial n}{\partial r_j}+\xi_{T,j}^i\frac{\partial T}{\partial r_j}\right]=0,\qquad(3.19)$$

$$D_t\delta u_k+\rho^{-1}\frac{\partial}{\partial r_i}\left[t_{ik}^{(0)}-\gamma_{lm}^{ik}\frac{\partial\delta u_l}{\partial r_m}\right]+a_{kj}\delta u_j=0,\quad(3.20)$$

where $D_t=\partial_t+\mathbf{u}\cdot\nabla$. This is a primary result of our analysis. These equations are analogous to the nonlinear Navier-Stokes equations for a fluid near local equilibrium, and reduce to them for zero shear rate. More generally, the reference state is local shear flow, which can be very far from equilibrium. Furthermore, there is no restriction on the deviations from this reference state, δy_a, since the nonlinear dependence of all coefficients on $y_a(\mathbf{r},t)$ has been retained. The spatial gradients relative to shear flow must be small, however, and the equations are accurate to second order in these gradients. The terms proportional to γ_{lm}^{ij} and $t_{ij}^{(0)}$ in Eq. (3.19) represent viscous heating due to the excess gradient of the flow velocity relative to the reference state. There is no viscous heating from the reference state alone, since the local thermostat has been chosen to cancel it, but for states near uniform shear flow the thermostat cannot compensate for effects due to the gradients relative to the reference state. The implications of this new hydrodynamic description far from equilibrium are elaborated in Sec. IV by an analysis of the associated linear hydrodynamic modes.

IV. HYDRODYNAMIC MODES

The above hydrodynamic equations are restricted to small spatial gradients relative to the reference state of uniform shear flow. If in addition the initial perturbations $\delta y_a(0)$ are small then these equations can be linearized with respect to $\delta y_a(t)$. The resulting set of five linear equations defines the hydrodynamic modes, or linear response excitations to small perturbations. If all of these modes decay in time, the state is linearly stable. Otherwise, a growth of these modes signals an onset of instability that is ultimately controlled by the dominance of nonlinear terms. In this section we determine the hydrodynamic modes for states far from equilibrium and contrast them with those for states near equilibrium.

The linearized hydrodynamic equations follow directly from Eqs. (3.18)–(3.20):

$$\left(\frac{\partial}{\partial t}+a_{ij}r_j\frac{\partial}{\partial r_i}\right)\delta n+n_s\mathbf{\nabla}\cdot\delta\mathbf{u}=0, \qquad (4.1)$$

$$\left(\frac{\partial}{\partial t}+a_{ij}r_j\frac{\partial}{\partial r_i}\right)\delta T+\frac{2}{3n_sk_B}(-a\gamma_{ij,s}^{xy}+t_{ij,s}^{(0)})\frac{\partial\delta u_i}{\partial r_j}$$

$$-\frac{2}{3n_sk_B}\left[\xi_{nj,s}^i\frac{\partial^2\delta n}{\partial r_i\partial r_j}+\xi_{Tj,s}^i\frac{\partial^2\delta T}{\partial r_i\partial r_j}\right]=0, \qquad (4.2)$$

$$\left(\frac{\partial}{\partial t}+a_{ij}r_j\frac{\partial}{\partial r_i}\right)\delta u_k+\rho_s^{-1}\left[\left(\frac{\partial t_{ik}^{(0)}}{\partial n}\right)_s\frac{\partial\delta n}{\partial r_i}+\left(\frac{\partial t_{ik}^{(0)}}{\partial T}\right)_s\frac{\partial\delta T}{\partial r_i}\right.$$

$$\left.-\gamma_{lm,s}^{ik}\frac{\partial^2\delta u_l}{\partial r_i\partial r_m}\right]+a_{kj}\delta u_j=0. \qquad (4.3)$$

To analyze these equations it is convenient to transform to the local Lagrangian frame, $r_i'=r_i-u_{si}(r)t=\Lambda_{ij}(t)r_j$. The Lees-Edwards boundary conditions then become simple periodic boundary conditions in the variable $\mathbf{r}'$. A Fourier representation is defined by

$$\delta\widetilde{y}_\alpha(\mathbf{k},t)=\int d\mathbf{r}'\,e^{i\mathbf{k}\cdot\mathbf{r}'}\delta y_\alpha(\mathbf{r},t)=\int d\mathbf{r}\,e^{i\mathbf{k}(t)\cdot\mathbf{r}}\delta y_\alpha(\mathbf{r},t), \qquad (4.4)$$

where the periodicity requires $k_i=2n_i\pi/L_i$, where n_i are integers and L_i are the linear dimensions of the system. In the second equality, $\mathbf{k}(t)$ is given by

$$k_i(t)=k_j\Lambda_{ji}(t). \qquad (4.5)$$

The linearized hydrodynamic equations in this Fourier representation are

$$\frac{\partial}{\partial t}\delta\widetilde{y}_\alpha+[A_{\alpha\nu}-ik_j(t)B_{\alpha\nu,j}+k_j(t)k_l(t)D_{\alpha\nu,jl}]\delta\widetilde{y}_\nu=0, \qquad (4.6)$$

where, in addition, the dependent variables now have been scaled to dimensionless forms,

$$\delta\widetilde{y}_\alpha=\left\{\frac{\delta\widetilde{n}}{n_s},\left(\frac{3}{2}\right)^{1/2}\frac{\delta\widetilde{T}}{T_s},\left(\frac{m}{k_BT_s}\right)^{1/2}\delta\widetilde{\mathbf{u}}\right\}. \qquad (4.7)$$

A summation convention applies and Latin indices denote Cartesian coordinates. The three matrices $A_{\alpha\beta},B_{\alpha\beta}$, and $D_{\alpha\beta}$ are

$$A_{\alpha\beta}=a\delta_{\alpha3}\delta_{\beta4}, \qquad (4.8)$$

$$B_{\alpha\beta j}=\left(\frac{k_BT_s}{m}\right)^{1/2}\begin{pmatrix} 0 & 0 & \delta_{jx} & \delta_{jy} & \delta_{jz} \\ 0 & 0 & B_{2xj} & B_{2yj} & B_{2zj} \\ \frac{n}{p_s}\left(\frac{\partial t_{jx}^{(0)}}{\partial n}\right)_s & \left(\frac{2}{3}\right)^{1/2}\frac{T_s}{p_s}\left(\frac{\partial t_{jx}^{(0)}}{\partial T}\right)_s & 0 & 0 & 0 \\ \frac{n}{p_s}\left(\frac{\partial t_{jy}^{(0)}}{\partial n}\right)_s & \left(\frac{2}{3}\right)^{1/2}\frac{T_s}{p_s}\left(\frac{\partial t_{jy}^{(0)}}{\partial T}\right)_s & 0 & 0 & 0 \\ \frac{n}{p_s}\left(\frac{\partial t_{jz}^{(0)}}{\partial n}\right)_s & \left(\frac{2}{3}\right)^{1/2}\frac{T_s}{p_s}\left(\frac{\partial t_{jz}^{(0)}}{\partial T}\right)_s & 0 & 0 & 0 \end{pmatrix}, \qquad (4.9)$$

where $B_{2ij}=\sqrt{2/3}(1/p_s)(-a\gamma_{ij,s}^{xy}+t_{ij,s}^{(0)})$. The matrix $D_{\alpha\beta}$ is

$$D_{\alpha\beta jl}=\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \left(\frac{2}{3}\right)^{1/2}\frac{n_s}{p_s}\xi_{nl,s}^j & \frac{2}{3}\frac{T_s}{p_s}\xi_{Tl,s}^j & 0 & 0 & 0 \\ 0 & 0 & \rho^{-1}\gamma_{xl,s}^{jx} & \rho^{-1}\gamma_{yl,s}^{jx} & \rho^{-1}\gamma_{zl,s}^{jx} \\ 0 & 0 & \rho^{-1}\gamma_{xl,s}^{jy} & \rho^{-1}\gamma_{yl,s}^{jy} & \rho^{-1}\gamma_{zl,s}^{jy} \\ 0 & 0 & \rho^{-1}\gamma_{xl,s}^{jz} & \rho^{-1}\gamma_{yl,s}^{jz} & \rho^{-1}\gamma_{zl,s}^{jz} \end{pmatrix}. \qquad (4.10)$$

The homogeneous solution to equations (4.6) can be calculated easily by setting $\mathbf{k}=0$,

$$\delta\widetilde{y}_\alpha(t)=[e^{-At}]_{\alpha\beta}\delta\widetilde{y}_\beta(0)=[1-At]_{\alpha\beta}\delta\widetilde{y}_\beta(0). \qquad (4.11)$$

The second equality follows from the property $A^2=0$. Consequently, all fields are constant except δu_x, which behaves as

$$\delta\widetilde{u}_x(t)=\widetilde{u}_x(0)-at\delta\widetilde{u}_y(0). \qquad (4.12)$$

The homogeneous state is unstable to an initial perturbation in $\delta \widetilde{u}_y$, leading to an unbounded linear change in time. Stability is still possible at finite k if this behavior is modulated by exponential hydrodynamic damping factors $\sim e^{-\alpha k^2 t}$, with $\alpha > 0$.

To simplify the analysis at $\mathbf{k} \neq 0$ we allow perturbation only along the velocity gradient direction, i.e., $\mathbf{k} = k\hat{\mathbf{y}}$. In this case the linear hydrodynamic equations have time-independent coefficients (i.e., $\mathbf{k}(t) = \mathbf{k}$),

$$\left(\frac{\partial}{\partial t} + F\right)_{\alpha \nu} \delta \widetilde{y}_\nu = 0, \quad F_{\alpha \beta} = A_{\alpha \beta} - ik\, B_{\alpha \beta} + k^2\, D_{\alpha \beta}, \tag{4.13}$$

and the matrices B and D now take the simpler forms

$$B_{\alpha \beta} = \left(\frac{k_B T_s}{m}\right)^{1/2} \begin{pmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & B_{2xy} & B_{2yy} & 0 \\ \dfrac{n_s}{p_s}\left(\dfrac{\partial t_{yx}^{(0)}}{\partial n}\right)_s & \left(\dfrac{2}{3}\right)^{1/2}\dfrac{T_s}{p_s}\left(\dfrac{\partial t_{yx}^{(0)}}{\partial T}\right)_s & 0 & 0 & 0 \\ \dfrac{n_s}{p_s}\left(\dfrac{\partial t_{yy}^{(0)}}{\partial n}\right)_s & \left(\dfrac{2}{3}\right)^{1/2}\dfrac{T_s}{p_s}\left(\dfrac{\partial t_{yy}^{(0)}}{\partial T}\right)_s & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \tag{4.14}$$

$$D_{\alpha \beta} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \left(\dfrac{2}{3}\right)^{1/2}\dfrac{n_s}{p_s}\xi_{ny,s}^y & \dfrac{2}{3}\dfrac{T_s}{p_s}\xi_{Ty,s}^y & 0 & 0 & 0 \\ 0 & 0 & \rho_s^{-1}\gamma_{xy,s}^{yx} & \rho_s^{-1}\gamma_{yy,s}^{yx} & 0 \\ 0 & 0 & \rho_s^{-1}\gamma_{xy,s}^{yy} & \rho_s^{-1}\gamma_{yy,s}^{yy} & 0 \\ 0 & 0 & 0 & 0 & \rho_s^{-1}\gamma_{zy,s}^{yz} \end{pmatrix}. \tag{4.15}$$

Equation (4.13) can be solved by Laplace transformation,

$$\widehat{\delta y}_\alpha(\mathbf{k},z) = \int_0^\infty dt\, e^{-tz}\, \delta\widetilde{y}_\alpha(\mathbf{k},t) = [zI + F(\mathbf{k},z)]_{\alpha\nu}^{-1}\, \delta\widetilde{y}_\nu(\mathbf{k},t=0). \tag{4.16}$$

The eigenvalues $\omega^{(i)}(\mathbf{k},a)$ of the matrix $F(\mathbf{k},z)$ define the five simple hydrodynamic poles at $z = -\omega^{(i)}(\mathbf{k},a)$, which determine the dominant dynamics of the $\delta\widetilde{y}_\alpha(\mathbf{k},t)$ at large t and small k. At equilibrium ($a=0$), the hydrodynamic modes of the Navier-Stokes equations are recovered (two sound modes, a heat mode and a twofold-degenerate shear mode) for long wavelengths ($k \to 0$),

$$\omega^{(i)}(\mathbf{k},0) \to \omega_{NS}^{(i)}(k) = \begin{pmatrix} ick + \Gamma k^2 \\ -ick + \Gamma k^2 \\ D_T k^2 \\ (\eta/\rho)k^2 \\ (\eta/\rho)k^2 \end{pmatrix}, \tag{4.17}$$

where $c = \sqrt{5/3\beta m}$ is the sound velocity, $\Gamma = D_T/3 + (2\eta/3\rho) = 1/\beta m \nu$ is the sound damping constant, $D_T = \xi_{Ty,s}^y(a=0)/\rho C_p = 1/\beta m \nu$ is the heat diffusion coefficient, C_p is the specific heat per unit mass, and $\eta/\rho = 1/\beta m \nu$ is the kinematic viscosity. The equilvalence of T, D_T, and η/ρ is a peculiarity of the BGK model. These coefficients are positive so that Eqs. (4.17) represent damped excitations. Corrections to these dispersion relations are of order k^3, describing an expansion that is analytic in k about $k=0$.

For finite shear rate, the modes are more complicated and the behavior at long wavelengths is qualitatively different. To be more precise, consider the case of $k \to 0$ at fixed, finite a. It follows directly from Eq. (4.16) that hydrodynamic modes have the asymptotic behavior

$$\omega^{(i)}(\mathbf{k},a) \rightarrow \begin{pmatrix} c_1(a)k^2 \\ -\frac{1}{2}(1+i\sqrt{3})c_2(a)k^{2/3}+\frac{1}{2}(1-i\sqrt{3})c_3(a)k^{4/3}+c_4(a)k^2 \\ -\frac{1}{2}(1-i\sqrt{3})c_2(a)k^{2/3}+\frac{1}{2}(1+i\sqrt{3})c_3(a)k^{4/3}+c_4(a)k^2 \\ c_2(a)k^{2/3}+c_3(a)k^{4/3}+c_4(a)k^2 \\ (\eta(a)/\rho)k^2 \end{pmatrix}, \tag{4.18}$$

with the coefficients $c_i(a)$ given by

$$c_1(a)=\left[\frac{\partial\eta(a)}{\partial T}\frac{\partial t_{yy}^{(0)}(a)}{\partial n}-\frac{\partial\eta(a)}{\partial n}\frac{\partial t_{yy}^{(0)}(a)}{\partial T}\right]\left(m\frac{\partial t_{yy}^{(0)}(a)}{\partial T}\right)^{-1}, \tag{4.19}$$

$$c_2(a)=\left[\frac{2a^2}{3n^2mk_B}(\eta(a)+\gamma_{xy}^{xy}(a))\frac{\partial t_{yy}^{(0)}(a)}{\partial T}\right]^{1/3}, \tag{4.20}$$

$$c_3(a)=\frac{2}{9n^2mk_Bc_2(a)}\left[\frac{\partial t_{yy}^{(0)}(a)}{\partial T}(-a\gamma_{yy}^{xy}(a)+t_{yy}^{(0)}(a))-a(\eta(a)+\gamma_{xy}^{xy}(a))\frac{\partial t_{xy}^{(0)}(a)}{\partial T}\right]+\frac{1}{3nmc_2(a)}\left(n\frac{\partial t_{yy}^{(0)}(a)}{\partial n}-a\gamma_{xy}^{yy}(a)\right), \tag{4.21}$$

$$c_4(a)=-\frac{c_1(a)}{3}+\frac{1}{3}\left[\rho^{-1}(\gamma_{xy}^{xy}(a)+\gamma_{yy}^{yy}(a))+\frac{2}{3nk_B}\xi_{T,y}^y(a)\right]. \tag{4.22}$$

The modes (4.18) represent two oscillating modes and three purely damped modes, just as in the Navier-Stokes case (4.17). However, there are two important qualitative differences. First, the long-wavelength behavior is nonanalytic in k about $k=0$, and is given by a power series in $k^{2/3}$. Thus, for example, the purely damped modes do not represent diffusive behavior as in the Navier-Stokes case. This nonanalytic behavior with respect to k is due to the fact that the reference matrix at $k=0$ is not diagonalizable, and the eigenvalues are not analytic about $k=a=0$. Therefore, recovery of the form of the modes near equilibrium requires that k and a be taken to zero in a related way (see below). The hydrodynamics for an alternative choice of thermostat, discussed in Appendix A, has dispersion relations that are analytic about $k=a=0$. A second critical difference between Eqs. (4.18) and (4.17) is that the two oscillating modes are unstable in the long-wavelength limit because the coefficient $c_2(a)$ is positive for all a. This means the modes include excitations that grow in time. Eventually, the deviations $\delta\tilde{y}_\alpha$ grow beyond the limitations of the linear equations, and full nonlinear hydrodynamic equations are required to determine their ultimate values. These will be different from those of the reference state, representing the fact that the reference state itself is unstable.

It is possible that the hydrodynamic modes are stable at shorter wavelengths. This is in fact the case, as can be seen by solving $\text{Re}[\omega^{(i)}(\mathbf{k}_s,a)]=0$ to determine the stability line $k_s(a)$ in the k-a plane. This is illustrated in Fig. 1, where the calculation was performed using the exact eigenvalues rather than the small k expansion of Eq. (4.18). Dimensionless variables are used, $k^*=k\ell$ and $a^*=a\tau$, where $\tau=\nu^{-1}$ is the mean free time, $\ell=v_0/\nu$ is the mean free path, and $v_0=\sqrt{2k_BT/m}$ is the thermal velocity. Above this line the modes are stable, while below this line they are unstable.

This prediction of a long-wavelength instability has been verified quantitatively by comparison with Monte Carlo simulation of the same kinetic equation from which this hydrodynamics was derived [11]. Further analysis of this instability and comparisons to simulations is reported in detail elsewhere [12]. In the following we focus on the stable domain of Fig. 1. To study the stable dynamics a new dimensionless variable $x=k^*/a^*$ is introduced. The hydrodynamic modes are expressed as functions of k and x, i.e., $\omega^{(i)}(\mathbf{k},a)=\bar{\omega}^{(i)}(\mathbf{k},x)$, and the expansion about $k=0$ is performed at fixed x. Physically, this involves controlling both the shear rate and the wavelength simultaneously to assure that the system is stable (sufficiently large x) while approaching the long-wavelength limit. To simplify the calculation, a system of Maxwell molecules is considered (interatomic potential $\sim r^{-4}$). In this case $\nu(n,T)$ and $\lambda(n,T)$ are independent of the temperature. The hydrodynamic modes for the stable domain are then obtained for $x>2/\sqrt{5}$, which lies above the dashed line shown in Fig. 1,

$$\omega^{(i)}(\mathbf{k},a) \rightarrow \begin{pmatrix} ick+\Gamma k^2-\frac{2}{5\nu}a^2 \\ -ick+\Gamma k^2-\frac{2}{5\nu}a^2 \\ D_Tk^2 \\ D_Tk^2+\frac{4}{5\nu}a^2 \\ (\eta/\rho)k^2 \end{pmatrix}. \tag{4.23}$$

For this expansion at fixed x the eigenvalues are again analytic functions of k and can be interpreted as perturbations of the Navier-Stokes modes due to small but finite shear rate.

The restrictions on x imply $(2/\sqrt{5})a^*<k^*<1$, so the shear rate dependence is small but not necessarily in the Navier-Stokes limit. More generally, the entire stable domain including larger shear rates can be accessed for $x_s = k/k_s(a) > 1$, and evaluating $\omega(\mathbf{k}, x_s)$ as a function of k exactly.

The linearized hydrodynamic variables $\delta \widetilde{y}_\alpha(\mathbf{k}, t)$ can be expressed in terms of the eigenvalues and eigenfunctions,

$$\delta \widetilde{y}_\alpha(\mathbf{k}, t) = \sum_i e^{-\omega^{(i)}(\mathbf{k}, x)t} \zeta_\alpha^{(i)}(\mathbf{k}, x)(\eta_\beta^{(i)})^\dagger(\mathbf{k}, x) \delta \widetilde{y}_\beta(\mathbf{k}, 0),$$
(4.24)

where $\{\zeta^{(i)}\}$ are the eigenvectors and $\{\eta^{(i)}\}$ are the associated biorthogonal set defined by $\sum_\alpha (\eta_\alpha^{(i)})^\dagger \zeta_\alpha^{(j)} = \delta_{ij}$. To illustrate the effects of the shear rate the analytic results for small k, Eq. (4.23), will be used. The corresponding eigenvectors are

$$\zeta^{(i)} = \begin{pmatrix} \left(\left(\frac{3}{5}\right)^{1/2}, \left(\frac{2}{5}\right)^{1/2}, \left(\frac{6}{5}\right)^{1/2} \frac{i}{x}, -1, 0 \right) \\[2mm] \left(\left(\frac{3}{5}\right)^{1/2}, \left(\frac{2}{5}\right)^{1/2}, \left(\frac{6}{5}\right)^{1/2} \frac{i}{x}, 1, 0 \right) \\[2mm] \left(-\left(\frac{2}{3}\right)^{1/2}, 1, 0, 0, 0 \right) \\[2mm] \left(-\left(\frac{2}{3}\right)^{1/2}, 1, -\frac{2i}{\sqrt{3}x}, 0, 0 \right) \\[2mm] (0, 0, 0, 0, 1) \end{pmatrix}, \quad (4.25)$$

$$\eta^{(i)} = \begin{pmatrix} \left(\frac{1}{2}\left(\frac{3}{5}\right)^{1/2}, \frac{1}{\sqrt{10}}, 0, -\frac{1}{2}, 0 \right) \\[2mm] \left(\frac{1}{2}\left(\frac{3}{5}\right)^{1/2}, \frac{1}{\sqrt{10}}, 0, \frac{1}{2}, 0 \right) \\[2mm] \left(-\left(\frac{3}{2}\right)^{1/2}, 0, \frac{i\sqrt{3}x}{2}, 0, 0 \right) \\[2mm] \left(\frac{3}{5}\left(\frac{3}{2}\right)^{1/2}, \frac{3}{5}, -\frac{i\sqrt{3}x}{2}, 0, 0 \right) \\[2mm] (0, 0, 0, 0, 1) \end{pmatrix}, \quad (4.26)$$

where it is understood that $\mathbf{k}$ is restricted to the stable domain. Then the response of the density to an initial density perturbation is found to be

$$\delta n(\mathbf{k}, t) = \left[\frac{3}{5} e^{-(\Gamma k^2 - (2a^2/5\nu))t} \cos(kct) + e^{-D_T k^2 t} \left(1 - \frac{3}{5} e^{-4a^2 t/5\nu} \right) \right] \delta n(\mathbf{k}, 0). \quad (4.27)$$

Thus, for small shear rates there is an enhancement of the amplitudes for both the sound and heat modes. All other hydrodynamic variables can be calculated in a similar way from Eq. (4.24), as well for both the stable and unstable regions, including small and large shear rates.

V. DISCUSSION

The objective here has been to study transport far from equilibrium for the special nonequilibrium states near uniform shear flow. Dynamical properties of states far from equilibrium are not well understood due to their complexity and technical difficulties with the formal theories of nonequilibrium statistical mechanics. However, at low density the Boltzmann kinetic theory provides a controlled formulation of this problem. There are still difficulties for practical applications, so a kinetic model has been used to allow a detailed analysis for a special class of states near uniform shear flow. First, the BGK Boltzmann equation was solved exactly for the steady state distribution at uniform shear flow, and the corresponding transport properties given as a function of the shear rate. Next, a solution to the kinetic equation was obtained for a class of states deviating from uniform shear flow by small spatial gradients in the hydrodynamic fields, using a variant of the Chapman-Enskog approximation method. By ''variant'' we mean that a local form of the stationary solution for shear flow is used as a reference function rather than the local equilibrium distribution function. In general this reference state is very different from a Maxwellian and can be very far from equilibrium if the shear rate is large. The Chapman-Enskog expansion was used to determine the distribution function to first order in the gradients. The result is a ''normal solution'' for which all space and time dependence occurs through the hydrodynamic fields. These fields must be determined from hydrodynamic equations which follow from the exact conservation laws. The irreversible parts of the hydrodynamic fluxes were determined as functions of the hydrodynamic fields and their gradients using the normal solution with results of the form $t_{ij}^* = -\eta(\partial u_{s,i}/\partial r_j) - \gamma_{lk}^{ij}(\partial \delta u_l/\partial r_k)$ for the momentum flux and $q_i^* = -\xi_{T,j}^i(\partial \delta T/\partial r_j) - \xi_{n,j}^i(\partial \delta n/\partial r_j)$ for the heat flux. Since these coefficients are calculated near the stationary state of broken symmetry there are many new transport coefficients ($\gamma_{lk}^{ij}, \xi_{T,j}^i, \xi_{n,j}^i$), in comparison to the case of states near equilibrium, which depend on the shear rate. With these
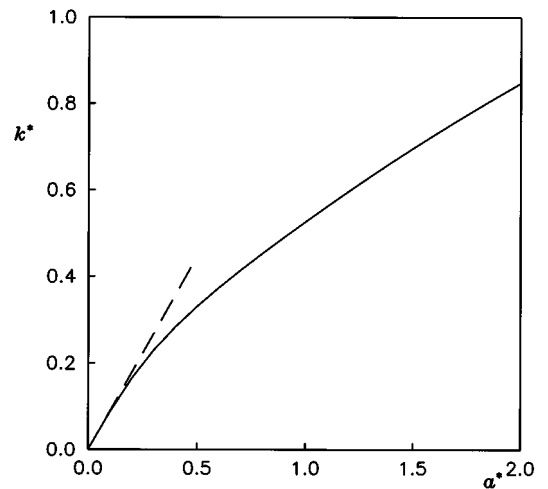
FIG. 1. The solid line separates the stable (above) and unstable (below) domains in the $k^* = k\ell$, $a^* = a/\nu$ parameter space. The dotted line is the asymptotic form obtained from Sec. IV ($x > 2/\sqrt{5}$).

new expressions for the fluxes, a closed set of the generalized hydrodynamic equations was derived near uniform shear flow. In summary, a complete description at both the kinetic and hydrodynamic levels has been given for a wide class of states arbitrarily far from equilibrium. In particular, the analysis provides a rare example of the relevance of a hydrodynamic description far from equilibrium. The corresponding hydrodynamic modes were calculated to order k^2 for arbitrary shear rate from the linearized hydrodynamic equations. An unexpected result is an instability for any finite value of the shear rate at sufficiently long wavelengths. This prediction has been verified quantitatively by comparison with direct Monte Carlo computer simulation of the kinetic equation, confirming the validity of the hydrodynamic description [11,12].

The hydrodynamic analysis was carried out here only for spatial variations along the velocity gradient. More complex dynamics is expected in the general case of arbitrary direction for the spatial perturbation and a description will be given elsewhere. In addition to the stable and unstable exponential time dependence of the hydrodynamic modes, there will be algebraic modulations due to the fact that the hydrodynamic matrix at $k=0$ cannot be diagonalized. This can lead to initial growth of perturbations of uniform shear flow even when the hydrodynamic modes are stable.

The approach taken here can be extended to several other physically interesting reference nonequilibrium states such as a constant temperature gradient, or combined heat and momentum transport. Exact solutions to the BGK kinetic equation are known for these cases [3,20,21], so the reference distribution for the Chapman-Enskog expansion is available. Other directions of extension include applications at higher densities. Recently, a BGK-like kinetic model for the dense fluid Enskog kinetic equation has been described and applied with success to shear flow [22]. This provides theoretical access to densities relevant for molecular-dynamics simulations.

Although attention has been focused on transport, the analysis can be extended in a straightforward way to describe fluctuations in uniform shear flow. The reason for this is the close relationship of the kinetic equations for fluctuations to that for transport [23,24]. For example, the kinetic equation for phase-space fluctuations at two times is governed by the linearization of the kinetic equation for transport. As a consequence, the linear hydrodynamic equations studied in Sec. IV also can be used to compute the hydrodynamic part of time correlation functions such as the dynamic structure factor measured in light scattering. Recently, kinetic models for fluctuations have been developed that are self-consistent with the BGK kinetic model for transport [25]. Their detailed application to fluctuations in uniform shear flow, including anomalous long range spatial correlations [26] will be discussed elsewhere.

ACKNOWLEDGMENTS

APPENDIX A: THERMOSTATS

To establish a steady state for uniform shear flow a nonconservative external force is introduced in Sec. II to compensate for viscous heating generated by the Lees-Edwards boundary conditions. In Sec. III for states *near* uniform shear flow, a local form for this nonconservative force is used,

$$\mathbf{F}_{\text{ext}}(\mathbf{r},t) = -m\lambda(n(\mathbf{r},t),T(\mathbf{r},t))(\mathbf{v}-\mathbf{u}(\mathbf{r},t)). \quad (A1)$$

With this local form it is possible to impose $\partial_t^{(0)}T=0$, which lead to the results that $\lambda(n(\mathbf{r},t),T(\mathbf{r},t))$ is the same as $\lambda_s(n_s,T_s)$ at uniform shear flow given by Eq. (2.17), except that the temperature and density are replaced by those for the general nonequilibrium state. The resulting hydrodynamic equations express viscous heating only due to the gradients relative to uniform shear flow. An alternative choice is to use the simpler case of the constant $\lambda(n_s,T_s)$ in Eq. (A1) even for states near uniform shear flow. The advantage of this choice is a simpler implementation of the Monte Carlo simulation method for the solution to the kinetic model equations. Obviously, this is consistent with the conditions for the steady-state uniform shear flow. However, this choice only partially compensates for the viscous heating at local uniform shear flow, i.e., $\partial_t^{(0)}T\neq0$. In this appendix, the changes from the results of Sec. III in both the Chapman-Enskog solution and the hydrodynamic equations due to this alternative choice are described.

To lowest order in the uniformity parameter, the BGK equation with the new thermostat becomes

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda_s\delta\mathbf{u}\cdot\mathbf{\nabla}_{v'}\right)f^{(0)} = \nu f_{\ell}. \quad (A2)$$

Here and below it is understood that $\lambda_s=\lambda(n_s,T_s)$ is independent of space and time. Since the solution is normal, its time dependence occurs only through the hydrodynamic variables, and the contributions from the time derivative $\partial_t^{(0)}$ can be calculated using the conservation laws to lowest order in the uniformity parameter,

$$\frac{\partial^{(0)}n(\mathbf{r},t)}{\partial t} = 0, \quad \frac{\partial^{(0)}\delta u_i(\mathbf{r},t)}{\partial t} + a_{ij}\delta u_j(\mathbf{r},t) = 0, \quad (A3)$$

$$\tfrac{3}{2}n(\mathbf{r},t)k_B\frac{\partial^{(0)}T(\mathbf{r},t)}{\partial t} + a_{ij}t_{ij}^{(0)}(\mathbf{r},t) + 3\lambda_s n(\mathbf{r},t)k_BT(\mathbf{r},t)$$

$$= 0. \quad (A4)$$

These differ from the results of the Sec. III because it is no longer possible to choose λ_s to compensate for the viscous heating, i.e., $a_{ij}t_{ij}^{(0)}(\mathbf{r},t)\neq-3\lambda_s n(\mathbf{r},t)k_BT(\mathbf{r},t)$. Instead, Eq. (A2) becomes

$$\left[-\frac{2}{3nk_B}(a_{ij}t_{ij}^{(0)}+3\lambda_s nk_BT)\frac{\partial}{\partial T} - L((\mathbf{v}'-\delta\mathbf{u}),a)\right]f^{(0)}$$

$$= \nu f_{\ell}, \quad (A5)$$

where the temperature derivative term is new. To solve Eq. (A5), we need to know the temperature dependence of the zeroth momentum flux, $t_{xy}^{(0)}$. For power-law potentials this

follows from the temperature dependence of ν. The analysis is simplest for Maxwell molecules where ν is independent of the temperature. Then $t_{xy}^{(0)} \sim T$ (as is verified *a posteriori*) and the solution to Eq. (A5) is

$$f^{(0)}(\mathbf{v}', y_\alpha(\mathbf{r},t)) = \nu(\mathbf{r},t)\, n(\mathbf{r},t) \left(\frac{m}{2\pi k_B T(\mathbf{r},t)} \right)^{3/2}$$

$$\times \int_0^\infty d\tau\, e^{-\nu(\mathbf{r},t)\tau} e^{3w(\mathbf{r},t)\tau}$$

$$\times \exp\left(-\frac{m}{2k_B T(\mathbf{r},t)} e^{2w(\mathbf{r},t)\tau} \right.$$

$$\left. \times [\Lambda_{ij}(-\tau)(v_j' - \delta u_j(\mathbf{r},t))]^2 \right), \qquad (A6)$$

$$w(n(\mathbf{r},t), T(\mathbf{r},t)) \equiv -\frac{a\, t_{xy}^{(0)}(\mathbf{r},t)}{3n(\mathbf{r},t)k_B T(\mathbf{r},t)}. \qquad (A7)$$

The solution is still only implicit since $t_{xy}^{(0)}(\mathbf{r},t)$, or equivalently $w(\mathbf{r},t)$, must be determined self-consistently using Eq. (A6). The result is

$$3\, w(\mathbf{r},t)(2w(\mathbf{r},t) + \nu(\mathbf{r},t))^2 = \nu(\mathbf{r},t)a^2. \qquad (A8)$$

This equation is the same as that for $\lambda(n(\mathbf{r},t), T(\mathbf{r},t))$, Eq. (3.13), showing that $w(\mathbf{r},t)$ has the same functional dependence on a, $\nu(\mathbf{r},t)$, and $T(\mathbf{r},t)$. This proves that the zeroth order solutions to the BGK Boltzmann equation, Eqs. (A6) and (3.11), for the two different thermostats are the same. The lowest order equations for the temperature differ, however. Use of Eq. (A7) in Eq. (A4) gives

$$\partial_t^{(0)} T(\mathbf{r},t) = 2\,(w - \lambda_s)\,T(\mathbf{r},t), \qquad (A9)$$

which vanishes only at the steady state.

Now consider the first-order solution in the Chapman-Enskog expansion,

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda_s \delta\mathbf{u}\cdot\boldsymbol{\nabla}_{\mathbf{v}'} \right) f^{(1)}$$

$$= -\left(\frac{\partial^{(1)}}{\partial t} + (v_i' + a_{ij}r_j)\frac{\partial}{\partial r_i} \right) f^{(0)}, \qquad (A10)$$

and look for solutions of the form

$$f^{(1)}(\mathbf{v}', y_\alpha(\mathbf{r},t)) = X_{n,i}(\mathbf{v}', y_\alpha(\mathbf{r},t))\frac{\partial n}{\partial r_i} + X_{T,i}(\mathbf{v}', y_\alpha(\mathbf{r},t))\frac{\partial T}{\partial r_i}$$

$$+ X_{u_k,i}(\mathbf{v}', y_\alpha(\mathbf{r},t))\frac{\partial \delta u_k}{\partial r_i}. \qquad (A11)$$

The equations for the coefficients, $X_{\beta,i}(\mathbf{v}'; y_\alpha(\mathbf{r},t))$, are determined from substitution of into Eq. (A10), and they are

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda_s \delta\mathbf{u}\cdot\boldsymbol{\nabla}_{\mathbf{v}'} \right) \begin{pmatrix} X_{n,k} \\ X_{T,k} \\ X_{u_j,k} \end{pmatrix}$$

$$+ \begin{pmatrix} 2\,T\left(\dfrac{\partial w}{\partial n}\right) X_{T,k} \\ 2\,(\lambda_s - w)\,X_{T,k} \\ a\,\delta_{j,y}\, X_{u_j,k} \end{pmatrix} = - \begin{pmatrix} Y_{n,k} \\ Y_{T,k} \\ Y_{u_j,k} \end{pmatrix}, \qquad (A12)$$

where i, j, and k represent Cartesian coordinates. The functions $Y_{\beta,k}$ are same as those given in Appendix B. Since the equations for $X_{n,k}$ and $X_{T,k}$ are different from Eq. (3.15), the transport coefficients for the heat flux, $\xi_{n,j}^i$ and $\xi_{T,j}^i$, are also different for this new thermostat. However, the equation for $X_{u_i,k}$ is unchanged, so the transport coefficients for the momentum flux, γ_{lm}^{ij}, are unchanged. The corresponding hydrodynamic equations are the same as in Sec. III, except for the temperature equation, which becomes

$$\frac{3}{2}nk_B\, D_t T - a_{ij}\gamma_{lm}^{ij}\frac{\partial \delta u_l}{\partial r_m} + \frac{\partial \delta u_i}{\partial r_j}\left[t_{ij}^{(0)} - \gamma_{lm}^{ij}\frac{\partial \delta u_l}{\partial r_m} \right]$$

$$- \frac{\partial}{\partial r_i}\left[\xi_{n,j}^i \frac{\partial n}{\partial r_j} + \xi_{T,j}^i \frac{\partial T}{\partial r_j} \right] = 3(w - \lambda_s)nk_B T. \quad (A13)$$

The new term $3(w - \lambda_s)nk_B T$ on the right side represents the viscous heating due to spatially uniform deviations from the steady state.

APPENDIX B: CHAPMAN-ENSKOG EXPANSION

In this appendix, Eq. (3.8) for $f^{(1)}$ is solved,

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda\,\delta\mathbf{u}\cdot\boldsymbol{\nabla}_{\mathbf{v}'} \right) f^{(1)} = -(D_t^{(1)} + \mathbf{v}'\cdot\boldsymbol{\nabla})f^{(0)}, \qquad (B1)$$

where $D_t^{(1)} \equiv (\partial^{(1)}/\partial t) + a_{ij}r_j(\partial/\partial r_i)$. The right side of Eq. (B1) can be written in terms of hydrodynamic derivatives,

$$(D_t^{(1)} + \mathbf{v}'\cdot\boldsymbol{\nabla})f^{(0)} = \sum_{\alpha=1}^5 \frac{\partial f^{(0)}}{\partial y_\alpha}(D_t^{(1)} + \mathbf{v}'\cdot\boldsymbol{\nabla})y_\alpha, \quad (B2)$$

where $y_\alpha = \{n(\mathbf{r},t),\, T(\mathbf{r},t),\, \delta\mathbf{u}(\mathbf{r},t)\}$. The time derivatives can be replaced by first-order spatial gradients of hydrodynamic variables using the corresponding hydrodynamic equations obtained from Eqs. (2.6)–(2.8)

$$D_t^{(1)} n + \boldsymbol{\nabla}\cdot(n\,\delta\mathbf{u}) = 0, \qquad (B3)$$

$$\frac{3}{2}nk_B(D_t^{(1)} + \delta\mathbf{u}\cdot\boldsymbol{\nabla})T + a_{ij}t_{ij}^{(1)} + t_{ij}^{(0)}\frac{\partial \delta u_i}{\partial r_j} + \boldsymbol{\nabla}\cdot\mathbf{q}^{(0)} = 0, \qquad (B4)$$

$$D_t^{(1)}\delta u_l + \delta\mathbf{u}\cdot\boldsymbol{\nabla}\,\delta u_l + \rho^{-1}\frac{\partial t_{il}^{(0)}}{\partial r_i} = 0. \qquad (B5)$$

Use of these equations in Eq. (B2) gives

$$(D_t^{(1)} + \mathbf{v}' \cdot \boldsymbol{\nabla})f^{(0)} = Y_{n,i}(\mathbf{v}'; y_\alpha(\mathbf{r},t))\frac{\partial n}{\partial r_i}$$

$$+ Y_{T,i}(\mathbf{v}'; y_\alpha(\mathbf{r},t))\frac{\partial T}{\partial r_i}$$

$$+ Y_{u_k,i}(\mathbf{v}'; y_\alpha(\mathbf{r},t))\frac{\partial \delta u_k}{\partial r_i}. \quad (B6)$$

The coefficients $Y_{\alpha,i}$ are given by

$$Y_{n,i} = \frac{\partial f^{(0)}}{\partial n}(v_i' - \delta u_i) - \rho^{-1}\frac{\partial f^{(0)}}{\partial \delta u_l}\frac{\partial t_{il}^{(0)}}{\partial n}, \quad (B7)$$

$$Y_{T,i} = \frac{\partial f^{(0)}}{\partial T}(v_i' - \delta u_i) - \rho^{-1}\frac{\partial f^{(0)}}{\partial \delta u_l}\frac{\partial t_{il}^{(0)}}{\partial T}, \quad (B8)$$

$$Y_{u_k,i} = -n\frac{\partial f^{(0)}}{\partial n}\delta_{ki} - \frac{2}{3nk_B}\frac{\partial f^{(0)}}{\partial T}\left(t_{ki}^{(0)} + a_{lm}\frac{\partial t_{lm}^{(1)}}{\partial\left(\frac{\partial \delta u_k}{\partial r_i}\right)}\right)$$

$$+ \frac{\partial f^{(0)}}{\partial \delta u_k}(v_i' - \delta u_i), \quad (B9)$$

where i,l,k,m denote x,y,z. The derivatives of $f^{(0)}$ can be obtained simply from Eq. (3.11),

$$\frac{\partial f^{(0)}}{\partial n} = \frac{f^{(0)}}{n} + \left(\frac{\partial \nu}{\partial n}\right)\frac{1}{\nu}[f^{(0)} - \nu^2 h_\nu] + \left(\frac{\partial \lambda}{\partial n}\right)\nu h_\lambda, \quad (B10)$$

$$\frac{\partial f^{(0)}}{\partial T} = -\frac{3}{2T}f^{(0)} + \frac{m}{2k_B T^2}\nu h_T$$

$$+ \left(\frac{\partial \nu}{\partial T}\right)\frac{1}{\nu}[f^{(0)} - \nu^2 h_\nu] + \left(\frac{\partial \lambda}{\partial T}\right)\nu h_\lambda, \quad (B11)$$

$$\frac{\partial f^{(0)}}{\partial \delta u_l} = \frac{m}{k_B T}\nu h_{u_l}. \quad (B12)$$

Here the functions h_α are defined by

$$h_\nu = \int_0^\infty d\tau\, \tau e^{-\nu\tau + 3\lambda\tau}f_\ell(e^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j)), \quad (B13)$$

$$h_\lambda = \int_0^\infty d\tau\, e^{-\nu\tau + 3\lambda\tau}\left\{3\tau - \frac{m}{k_B T}e^{2\lambda\tau}\tau\right.$$

$$\times [\Lambda_{ij}(-\tau)(v_j' - \delta u_j)]^2 \Big\}$$

$$\times f_\ell(e^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j)), \quad (B14)$$

$$h_T = \int_0^\infty d\tau\, e^{-\nu\tau + 3\lambda\tau}e^{2\lambda\tau}[\Lambda_{ij}(-\tau)(v_j' - \delta u_j)]^2$$

$$\times f_\ell(e^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j)), \quad (B15)$$

$$h_{u_k} = \int_0^\infty d\tau\, e^{-\nu\tau + 3\lambda\tau}e^{2\lambda\tau}g_k(\mathbf{v}',\tau)$$

$$\times f_\ell(e^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j)), \quad (B16)$$

where the functions $g_k(\mathbf{v}',t)$ in the expression for h_{u_k} are

$$g_x = (v_x' - \delta u_x) + at(v_y' - \delta u_y),$$

$$g_y = at(v_x' - \delta u_x) + (1 + a^2t^2)(v_y' - \delta u_y),$$

$$g_z = v_z' - \delta u_z. \quad (B17)$$

The right side of Eq. (B1) now can be written in terms of the coefficients, $Y_{\alpha,i}$, and the hydrodynamic gradients. Note that $Y_{\alpha,i}$ are given only implicitly since they depend on the unknown flux $t_{ij}^{(1)}$. The procedure is therefore to determine $f^{(1)}$ in terms of $t_{ij}^{(1)}$, and then use that result to obtain a self-consistent equation for $t_{ij}^{(1)}$.

Clearly, $f^{(1)}$ must have the same form as the right side of Eq. (B6),

$$f^{(1)} = X_{n,i}(\mathbf{v}', y_\alpha(\mathbf{r},t))\frac{\partial n}{\partial r_i} + X_{T,i}(\mathbf{v}', y_\alpha(\mathbf{r},t))\frac{\partial T}{\partial r_i}$$

$$+ X_{u_k,i}(\mathbf{v}', y_\alpha(\mathbf{r},t))\frac{\partial \delta u_k}{\partial r_i}. \quad (B18)$$

Substitution of this form into Eq. (B1) gives the equations

$$\left(\frac{\partial^{(0)}}{\partial t} - L(v',a) + \lambda\,\delta u_i\frac{\partial}{\partial v_i'}\right)X_{\alpha,k} - aX_{u_x,k}\delta_{\alpha,u_y} = -Y_{\alpha,k}, \quad (B19)$$

where $\alpha = n, T, u_x, u_y$, and u_z. These equations have a form similar to Eq.(4.8) and can be solved in a similar way to obtain

$$X_{\alpha,k} = \int_0^\infty d\tau\, e^{-\nu\tau}e^{3\lambda\tau}[a\,\delta_{\alpha,u_y}X_{u_x,k}(e^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j))$$

$$- Y_{\alpha,k}(e^{\lambda\tau}\Lambda_{ij}(-\tau)(v_j' - \delta u_j))]. \quad (B20)$$

This implicit result is sufficient for determination of the transport coefficients, as described in Appendix C.

APPENDIX C: TRANSPORT COEFFICIENTS

In this appendix, the transport coefficients defined in Eqs. (3.16) are calculated using the solution to Eq. (3.15). First, the coefficients from momentum flux are considered,

$$\gamma_{lm}^{ij} = -\int d\mathbf{v}'\, mc_i c_j X_{u_l,m}, \quad (C1)$$

where $\mathbf{c} = \mathbf{v}' - \delta\mathbf{u}$. As an example, γ_{xy}^{xy} is analyzed in detail. Substitution of the solution, $X_{u_x,y}$, Eq. (B20), into the definition of γ_{xy}^{xy}, Eq. (C1), gives

$$\gamma_{xy}^{xy} = \int d\mathbf{v}'\ mc_x c_y \int_0^\infty dt\ e^{-\nu t} e^{3\lambda t} Y_{u_x,y}(e^{\lambda t}\Lambda_{ij}(-t)c_j). \tag{C2}$$

To proceed it is necessary to know the temperature dependence of ν and λ. The simplest case is that of Maxwell molecules for which ν and λ are constants. Then γ_{xy}^{xy} can be calculated with a sequence of change of variables: first $\mathbf{v}' \rightarrow \mathbf{v}' + \delta\mathbf{u}$, then $\mathbf{v}' \rightarrow e^{-\lambda t}\mathbf{v}'$, and finally $v_i' \rightarrow \Lambda_{ij}(t)v_j'$. In this way γ_{xy}^{xy} is found to be

$$\gamma_{xy}^{xy} = \int_0^\infty dt\ e^{-(\nu+2\lambda)t} m \int d\mathbf{v}(v_x - atv_y)v_y$$

$$\times \left[-\frac{2}{3nk_B}\frac{\partial f^{(0)}}{\partial T}(t_{xy}^{(0)} + a_{lm}\gamma_{xy}^{lm}) + \frac{\partial f^{(0)}}{\partial \delta u_x}v_y \right]$$

$$= (t_{xy}^{(0)} + a\gamma_{xy}^{xy})\left(\frac{2\nu a}{(2\lambda+\nu)^3} - \frac{10\nu a}{3(2\lambda+\nu)^3} \right) - \frac{\nu}{(2\lambda+\nu)^2}p. \tag{C3}$$

Use of result (3.12) for $t_{xy}^{(0)}$ and relation (3.13) for λ gives the final value of γ_{xy}^{xy},

$$\gamma_{xy}^{xy} = \frac{\nu(\nu-2\lambda)}{(2\lambda+\nu)^2(6\lambda+\nu)}p. \tag{C4}$$

The same method can be applied for all the transport coefficients, γ_{lm}^{ij}, $\xi_{n,j}^i$, and $\xi_{T,j}^i$. A complete listing of the results can be obtained from the authors on request.

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