

## Heat and momentum transport far from equilibrium

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Explicit expressions for the heat and momentum transport are given for a gas in a stationary state with temperature and velocity gradients. The results are obtained from a formally exact analysis of the normal solution to the Bhatnagar-Gross-Krook model for the nonlinear Boltzmann equation, and are not restricted to small gradients. The irreversible momentum and heat fluxes are found to be nonanalytic functions of the velocity gradients, indicating that the Chapman-Enskog expansion does not converge for this state. However, these fluxes are analytic in the temperature gradients; in particular, the heat flux is simply proportional to the temperature gradient so that Fourier's law applies even for large gradients. The space dependence of the thermodynamic and velocity fields is determined as a function of the interaction potential, and the results for Maxwell molecules and hard spheres are compared.

### I. INTRODUCTION

The transport properties of a simple fluid near equilibrium are well understood in the following sense: The constitutive equations for the heat and momentum fluxes are known (Newton's viscosity law and Fourier's heat law) and the resulting linear hydrodynamic equations can be solved for a wide class of boundary conditions. For states far from equilibrium the constitutive relations must be generalized to nonlinear functions of the hydrodynamic variables and their gradients. Although the Chapman-Enskog<sup>1</sup> method provides a systematic expansion to compute these functions as a power series in the gradients, calculations beyond Navier-Stokes order (Burnett equations) are prohibitively difficult and not applicable for large gradients. Furthermore, even when the fluxes are known as functions of the gradients, there still remains the difficult problem of solving the resulting nonlinear hydrodynamic equations to determine the explicit space dependence of the hydrodynamic variables. Consequently, very little is known about the mechanism of heat and momentum transport far from the Navier-Stokes domain even for the simplest boundary conditions.

The prototype fluid for the study of transport properties is a monatomic low-density gas with short-range interactions. The state of the system is specified by a solution to the nonlinear Boltzmann equation with appropriate initial and boundary conditions. Very few solutions to this equation are known for spatially inhomogeneous states. The first was due to Ikenberry and Truesdell for Maxwell molecules.<sup>2</sup> They showed that the hierarchy of equations for velocity moments of the Boltzmann equation could be solved self-consistently under the assumption of a linear velocity field, and spatially constant temperature and pressure (momentum transport). A second

solution for Maxwell molecules has been obtained recently<sup>3</sup> for a suitably chosen temperature field with constant pressure and zero-flow velocity (heat transport). More detailed information has been obtained for these two cases using the Bhatnagar-Gross-Krook (BGK) model for the nonlinear Boltzmann equation.<sup>4,5</sup> This model preserves the important qualitative features of the transport properties, while allowing for more complete calculations. The objective here is to extend this analysis of the BGK equation to describe transport in a steady state with combined heat and momentum transport.

The physical situation considered is the stationary state of a gas between two parallel plates maintained at different temperatures and in relative motion. Let  $y$  denote the coordinate normal to the plates. Then the stationary BGK equation determines the velocity distribution function at the position  $y$  between the plates,  $f(y, \mathbf{v})$ . A unique solution is obtained by specification of boundary conditions on  $f$  at the upper and lower plates. In general, it is possible to separate the solution into two parts,  $f = f_B + f_N$ . The function  $f_B$  accounts for the prescribed boundary conditions and decays rapidly to zero at distances greater than a mean free path from either plate. The other solution  $f_N$  is a particular solution to the BGK equation that depends on  $y$  only through the hydrodynamic variables. The latter property characterizes the "normal" solutions (e.g., that constructed by the Chapman-Enskog method). This qualitative discussion indicates that a normal solution is expected to apply if attention is limited to the "bulk" domain of the gas, outside the boundary layer. The boundary conditions appear only indirectly in the normal solution through the explicit space dependence of the hydrodynamic variables, which must be determined from the complete solution including  $f_B$  or from an appropriate solution to the

hydrodynamic equations. Here we suppress the detailed kinetic theory boundary-value problem<sup>6</sup> by restricting attention to transport properties associated with the normal solution, and by looking for self-consistent solutions to the corresponding hydrodynamic equations.

In Sec. II a solution to the usual Navier-Stokes hydrodynamic equations for the assumed geometry and boundary conditions is reviewed. It is then shown that this is also a solution to the general macroscopic conservation laws beyond the Navier-Stokes domain, if the heat and momentum fluxes have a suitable form. The consistency of these results with a formal expression for the normal solution to the BGK equation is verified and the relevant transport coefficients are calculated. The primary results are (1) the momentum flux is a nonanalytic function of the shear rate, (2) the heat flux is given by Fourier's law, even for large temperature gradients, with an effective thermal conductivity that depends on the shear rate, and (3) the temperature and velocity profiles depend on the interparticle-force law. Further comment on these results is given in Sec. VI.

## II. STEADY-STATE HYDRODYNAMIC EQUATIONS

The BGK kinetic equation implies the steady-state conservation laws in their usual form

$$\begin{aligned} \nabla \cdot (\rho \mathbf{U}) &= 0, \\ \mathbf{U} \cdot \nabla u + h \nabla \cdot \mathbf{U} + \nabla \cdot \mathbf{q}^* + t_{ij}^* \frac{\partial U_i}{\partial r_j} &= 0, \\ \mathbf{U} \cdot \nabla U_i + \rho^{-1} \left[ \frac{\partial p}{\partial r_i} + \frac{\partial t_{ij}^*}{\partial r_j} \right] &= 0, \end{aligned} \quad (2.1)$$

where  $\rho$  is the density,  $u$  is the internal energy density,  $p$  is the pressure,  $h = u + p$ , and  $\mathbf{U}$  is the flow velocity. The irreversible parts of the heat and momentum fluxes are denoted by  $\mathbf{q}^*$  and  $t_{ij}^*$ , respectively. We choose as independent variables the temperature, pressure, and flow velocity, where the temperature  $T$  is given by  $u = \frac{3}{2} n k_B T$ . For the physical conditions considered it is appropriate to look for solutions of the form

$$\begin{aligned} \mathbf{U} &= \hat{\mathbf{x}} U_x(y), \quad T = T(y), \quad p = \text{const}, \\ \mathbf{q}^* &= \mathbf{q}^*(y), \quad t_{ij}^* = t_{ij}^*(y), \end{aligned} \quad (2.2)$$

where  $\hat{\mathbf{x}}$  is a unit vector in the  $x$  direction. The hydrodynamic equations then take the simpler form

$$\begin{aligned} \frac{\partial}{\partial y} q_y^* &= - \frac{\partial U_x}{\partial y} t_{xy}^*, \\ \frac{\partial}{\partial y} t_{xy}^* &= \frac{\partial}{\partial y} t_{yy}^* = \frac{\partial}{\partial y} t_{zy}^* = 0. \end{aligned} \quad (2.3)$$

For positions sufficiently far from the boundaries, the fluxes are determined entirely by the normal solution and therefore depend on  $y$  only through  $T(y)$  and  $U_x(y)$ . Consider first the Navier-Stokes form for small gradients,

$$\begin{aligned} q_y^* &= -\lambda_0 \frac{\partial T}{\partial y}, \\ t_{xy}^* &= -\eta_0 \frac{\partial U_x}{\partial y}. \end{aligned} \quad (2.4)$$

For the BGK model the thermal conductivity  $\lambda_0(T(y))$  and shear viscosity  $\eta_0(T(y))$  are given by<sup>1,6</sup>

$$\lambda_0 \equiv \frac{5}{2m} k_B p \nu^{-1}(T(y)), \quad \eta_0 \equiv p \nu^{-1}(T(y)), \quad (2.5)$$

where  $\nu(T)$  is an average collision frequency. The dependence of these transport coefficients on  $T(y)$  occurs entirely through this collision frequency, and the hydrodynamic equations are simplified by the change of variables,

$$dl = \nu(T(y)) dy. \quad (2.6)$$

Substitution of (2.4) and (2.6) into (2.3) leads to the steady-state Navier-Stokes equations

$$\begin{aligned} \frac{\partial^2 T}{\partial l^2} &= -(\eta_0/\lambda_0) \left[ \frac{\partial U_x}{\partial l} \right]^2, \\ \frac{\partial^2 U_x}{\partial l^2} &= 0. \end{aligned} \quad (2.7)$$

Now, since the combination  $\eta_0/\lambda_0$  is a constant, these equations are easily solved to give

$$\begin{aligned} U_x &= U_x(0) + al, \\ T &= T(0) + \epsilon l - (\eta_0/2\lambda_0) a^2 l^2, \end{aligned} \quad (2.8)$$

where  $a$  and  $\epsilon$  are constants fixed by the boundary conditions. The relationship of  $l$  to the space variable  $y$  is obtained from the integration of (2.6). Since the dependence of  $\nu$  on  $T$  depends on the interatomic-force law, the velocity and temperature profiles will also have this dependence.

Returning to the exact hydrodynamic equations, the heat and momentum fluxes are written in a form suggestive of the Navier-Stokes expressions,

$$\begin{aligned} q_y^* &= -\lambda[T, \mathbf{U}] \frac{\partial T}{\partial y}, \\ t_{xy}^* &= -\eta[T, \mathbf{U}] \frac{\partial U_x}{\partial y}, \end{aligned} \quad (2.9)$$

where  $\lambda$  and  $\eta$  are a generalized thermal conductivity and shear viscosity, defined by Eq. (2.9). (The square brackets indicate that  $\lambda$  and  $\eta$  are functionals of  $T$  and  $U$ , or, equivalently, functions of these variables and their gradients.) It is now easily verified that the Eqs. (2.8) are also solutions to the exact hydrodynamic equations (with  $\lambda_0$  and  $\eta_0$  replaced by  $\lambda$  and  $\eta$ ) if  $\lambda$  and  $\eta$  have the forms

$$\begin{aligned} \lambda[T, \mathbf{U}] &= \lambda_0(T) F_\lambda(a), \\ \eta[T, \mathbf{U}] &= \eta_0(T) F_\eta(a), \end{aligned} \quad (2.10)$$

where  $F_\lambda(a)$  and  $F_\eta(a)$  are arbitrary functions of the dimensionless shear rate  $a$ , with the limits  $F_\lambda(0) = F_\eta(0) = 1$ . In Sec. III it is verified that (2.9) and (2.10) are formally consistent with a normal solution to the BGK equation, and explicit expressions for  $F_\lambda(a)$  and  $F_\eta(a)$  are obtained. With these results, the fluxes and the hydrodynamic variables are completely determined.

### III. CONSISTENCY WITH THE BGK EQUATION

The exact solution to the hydrodynamic equations obtained in Sec. II applies only if the heat and momentum fluxes have the forms given by (2.9) and (2.10). These fluxes can be expressed as averages over the velocity distribution function  $f$ ,

$$\begin{aligned} q_y^* &= \int d\mathbf{v} v_y \frac{1}{2} m (\mathbf{v} - \mathbf{U})^2 f, \\ t_{xy}^* &= \int d\mathbf{v} v_y m (v_x - U_x) f. \end{aligned} \quad (3.1)$$

As discussed in the introduction, we consider the case where  $f$  is the normal solution to the BGK equation. The steady-state BGK equation for the conditions described in Sec. II takes the form

$$v_y \frac{\partial}{\partial l} f = -(f - f_L), \quad (3.2)$$

where  $l$  is defined as in (2.6) and  $f_L$  is the local equilibrium distribution function

$$\begin{aligned} f_L &= \frac{2p(y)}{m v_0^5(y) \pi^{3/2}} \exp \left[ - \left[ \frac{\mathbf{v} - \mathbf{u}(y)}{v_0(y)} \right]^2 \right], \\ v_0^2(y) &\equiv 2k_B T(y) / m. \end{aligned} \quad (3.3)$$

The pressure  $p(y)$ , temperature  $T(y)$ , and flow velocity  $\mathbf{U}(y)$  are now defined in terms of the first five moments of the distribution function,

$$\int d\mathbf{v} \psi_\alpha(v) (f - f_L) = 0, \quad \psi_\alpha \leftrightarrow (1, \mathbf{v}, v^2). \quad (3.4)$$

This definition of the parameters in the local equilibrium distribution is required for the BGK equation to imply the general macroscopic conservation laws. More specifically, if (3.4) is satisfied for some given  $p$ ,  $T$ , and  $\mathbf{U}$ , then these variables are also exact solutions to the associated hydrodynamic equations. Conversely, given an exact solution to the hydrodynamic equations, the condition (3.4) is satisfied. Consequently, results in Sec. II are consistent with the BGK equation if and only if the assumed form of the hydrodynamic equations is correct. This requires that Eqs. (2.9) and (2.10) agree with (3.1).

To evaluate (3.1) the normal solution must be specified. In spite of its apparent simplicity, the BGK equation is a highly nonlinear equation [due to (3.4)] and we have not been able to construct an explicit solution for the conditions considered. However, a formal solution is sufficient for calculation of the fluxes,

$$f = \lim_{n \rightarrow \infty} f^{(n)}, \quad f^{(n)} \equiv \sum_{j=0}^n \left[ -v_y \frac{\partial}{\partial l} \right]^j f_L. \quad (3.5)$$

Consider first the momentum flux. Substitution of (3.5) into (3.1) gives

$$t_{xy}^* = \lim_{n \rightarrow \infty} \sum_{j=0}^n \left[ -\frac{\partial}{\partial l} \right]^j \int d\mathbf{v} m v_x v_y^{j+1} f_L. \quad (3.6)$$

To evaluate the space derivatives, the expressions of Sec. II are assumed,

$p = \text{const}$ ,

$$\mathbf{U} = [U_x(0) + al] \hat{\mathbf{x}}, \quad (3.7)$$

$$T = T(0) + \epsilon l - (m\gamma/k_B) l^2,$$

where the dimensionless constant  $\gamma(a)$  is given by

$$\gamma(a) \equiv a^2 F_\eta(a) / 5F_\lambda(a). \quad (3.8)$$

It is then straightforward to evaluate the integrals in (3.6) with the result (see Appendix A)

$$t_{xy}^* = -\eta_0(T(y)) F_\eta(a) \frac{\partial U_x}{\partial y}, \quad (3.9)$$

where

$$\begin{aligned} F_\eta(a) &\equiv \lim_{n \rightarrow \infty} \int_0^\infty dt_1 \int_0^\infty dt_2 t_1 t_2 e^{-(t_1+t_2)} \\ &\quad \times \sum_{j=0}^n \frac{(-\gamma t_1^2 t_2^2)^j}{j! 2^j}. \end{aligned} \quad (3.10)$$

This verifies the form assumed in Eqs. (2.9) and (2.10). However, the limit required in Eq. (3.10) does not exist, indicating that the formal solution (3.5) is not uniformly convergent with respect to  $\mathbf{v}$ . To obtain a meaningful form for  $F_\eta$ , it is observed that (3.10) is an asymptotic expansion of the well-defined function

$$F_\eta(a) = \int_0^\infty dt_1 \int_0^\infty dt_2 t_1 t_2 e^{-(t_1+t_2)} e^{-\gamma t_1^2 t_2^2 / 2}. \quad (3.11)$$

We identify (3.11) as the proper definition of  $F_\eta$ .

The integral for the heat flux in Eq. (3.1) can be evaluated in an analogous way, leading to

$$q_y^* = -\lambda_0(T(y)) F_\lambda(a) \frac{\partial T}{\partial y}, \quad (3.12)$$

with

$$F_\lambda(a) = \frac{a^2 F_\eta}{5\gamma} + G(a, \gamma). \quad (3.13)$$

The function  $G(a, \gamma)$  has a representation similar to that of  $F_\eta$ ,

$$\begin{aligned} &-10\gamma^2 G(a, \gamma) \\ &= a^2 - 3\gamma - \int_0^\infty dt_1 \int_0^\infty dt_2 (a^2 - 3\gamma + \gamma^2 t_1^2 t_2^2) \\ &\quad \times e^{-(t_1+t_2)} e^{-\gamma t_1^2 t_2^2 / 2}. \end{aligned} \quad (3.14)$$

The function  $F_\eta$  has been given only implicitly as a function of  $\gamma$ . The dependence of  $\gamma$  on the shear rate  $a$  can be obtained by substitution of (3.8) into (3.13),

$$G(a, \gamma) = 0. \quad (3.15)$$

In summary, the BGK equation with solutions to the hydrodynamic equations of Sec. II leads to fluxes of the assumed form, (2.9) and (2.10). This verifies the internal consistency of the hydrodynamic and kinetic theory descriptions.

#### IV. CALCULATION OF THE FLUXES

The heat and momentum fluxes are given by Fourier's law and Newton's viscosity law with the generalized thermal conductivity and shear viscosity of Eq. (2.10). These differ from the Navier-Stokes order results only by the shear-rate-dependent factors  $F_\eta$  and  $F_\lambda$ . Their relationship can be characterized through a shear-rate-dependent Prandtl number defined by

$$P(a) \equiv \eta c_p / \lambda = 5\gamma(a)/a^2, \quad (4.1)$$

where  $c_p$  is the specific heat. The integral in Eq. (3.11) for  $F_\eta$  exists only if  $\gamma \geq 0$ , indicating that it is not analytic at the origin. For similar reasons (3.15) implies that  $\gamma$  is not analytic in  $a$ . Consequently, the generalized shear viscosity, Prandtl number, and thermal conductivity are nonanalytic functions of the shear rate. A power-series expansion, such as that given by the Chapman-Enskog method, can only be asymptotic at best in this case.

The equation that determines  $\gamma(a)$  can be written in terms of  $F_\eta$  according to

$$2\gamma^2 \frac{d}{d\gamma} \left[ 2\gamma \frac{d}{d\gamma} (\gamma F_\eta) \right] + (3\gamma - a^2) 2\gamma \frac{d}{d\gamma} (\gamma F_\eta) = 0, \quad (4.2)$$

as follows directly from Eq. (3.15) using the defining equations (3.11) and (3.14). To calculate  $F_\eta$  the integral representation can be evaluated directly, but we have found it more convenient to use an expansion about the point at infinity. In Appendix B it is shown that

$$F_\eta = \gamma^{-1} \left[ \frac{1}{2} (\ln \gamma) \sum_{j=0}^{\infty} c_j \gamma^{-j/2} + \sum_{j=0}^{\infty} d_j \gamma^{-j/2} \right], \quad (4.3)$$

where the numerical coefficients  $c_j$  and  $d_j$  are given by Eqs. (B9) and (B10). Then using (4.2),  $\gamma$  is calculated as a function of  $a$ . The result differs from the leading ( $a^2$ ) term in the divergent expansion around the origin by about 20% for  $0.1 \leq a$ . The function  $F_\eta(a)$  for the shear viscosity is shown in Fig. 1, where the monotonic decrease represents shear thinning. The expansion around the origin (Chapman-Enskog result to Burnett order) is

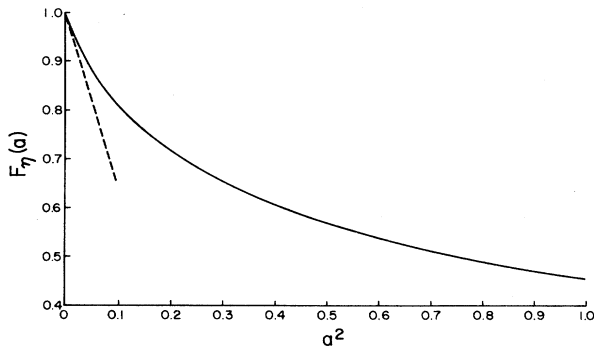


FIG. 1. Reduced shear viscosity,  $F_\eta(a) = \eta(a)/\eta_0$ , as a function of  $a^2$  (—), and its asymptotic form,  $1 - 18a^2/5$  (---).

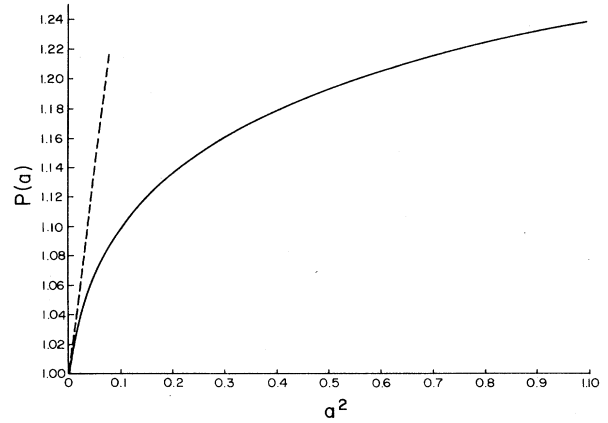


FIG. 2. Prandtl number,  $P(a)$ , as a function of  $a^2$  (—), and its asymptotic form,  $1 + 72a^2/25$  (---).

useful only for very small shear rates. The Prandtl number is shown in Fig. 2, monotonically increasing from 1 to a limiting value of  $\frac{5}{3}$ .

#### V. HYDRODYNAMIC VARIABLES

The shape of the velocity and temperature profiles are given by Eqs. (3.7) and the transformation from  $l$  to  $y$ , Eq. (2.6). The latter is determined by the collision frequency  $\nu[T(y)]$ , whose temperature dependence is determined by the interatomic potential. Also, the profiles depend parametrically on the shear rate  $a$  and the constant  $\epsilon$ . For  $a=0$  (boundaries at rest), the temperature is linear in  $l$  and  $\epsilon$  is a measure of the imposed temperature gradient. The results here agree with those of Ref. 5 in this case. For  $a \neq 0$ , there is a temperature profile even in the absence of a temperature difference at the boundaries, due to viscous heating. The additional effect of an imposed temperature difference is simply to shift this profile by a constant,  $\alpha \equiv k_B \epsilon / (2m\gamma)$ ,

$$U_x = U_x(\alpha) + a\bar{l}, \quad (5.1)$$

$$T = T(\alpha) - (m\gamma/k_B)\bar{l}^2,$$

with  $\bar{l} \equiv l - \alpha$ . This result shows a general relationship of the temperature and velocity profiles,

$$T - T(\alpha) = - \left[ \frac{m\gamma}{K_B a^2} \right] [U_x - U_x(\alpha)]^2. \quad (5.2)$$

This means that a plot of  $T$  versus  $U_x$  gives a parabola no matter what interaction potential is considered. It would be interesting to see if this prediction of the model is verified in actual experiments. It is also interesting to note that the coefficient  $\gamma(a)/a^2$  is quite insensitive to the value of  $a$ .

According to the above discussion we can now restrict our attention to a system with no imposed thermal gradient ( $\epsilon=0$ ), without loss of generality. Let the lower and upper boundaries be located at  $y=0$  and  $y=L$ , respectively, with  $U_x(y=0)=0$  and  $U_x(y=L)=U$ . Also, from Eq. (2.6),

$$y = \int_0^l dl' v^{-1}(T(l')), \quad (5.3)$$

so that  $y=0$  at  $l=0$ . Then Eq. (5.2) gives a relationship among the boundary parameters,

$$\Delta \equiv \frac{T_0 - T_L}{T_L} = \frac{m\gamma(a)U^2}{K_B a^2 T_L}, \quad (5.4)$$

where  $T_0$  and  $T_L$  are the temperatures at the lower and upper boundaries. To proceed further, the temperature dependence of the collision frequency must be specified. As an example, consider Maxwell molecules, for which  $\nu \propto \rho T^{-1}$ , and consequently

$$\nu = \nu_L \frac{T_L}{T}. \quad (5.5)$$

Here  $\nu_L$  is the collision frequency at  $y=L$ . It is now convenient to introduce dimensionless variables defined by

$$y^* = y/L, \quad U_x^* = U_x/U, \quad T^* = T/T_L, \quad l^* = l/U. \quad (5.6)$$

Equations (5.1)–(5.3) then become

$$\begin{aligned} U_x^* &= a l^*, \\ T^* &= 1 + \Delta - \Delta a^2 l^{*2}, \\ y^* &= \frac{U}{\nu_L L} (1 + \Delta - \frac{1}{3} \Delta a^2 l^{*2}) l^*. \end{aligned} \quad (5.7)$$

At  $y^*=1$ ,  $U_x^*=1$ , so

$$\frac{U}{\nu_L L} = a (1 + \frac{2}{3} \Delta)^{-1}. \quad (5.8)$$

Elimination of  $l^*$  in Eqs. (5.7) then yields

$$\begin{aligned} y^* &= U_x^* \frac{1 + \Delta - \frac{1}{3} \Delta U_x^{*2}}{1 + \frac{2}{3} \Delta}, \\ y^* &= \frac{2}{3} \frac{1 + \Delta + \frac{1}{2} T^*}{1 + \frac{2}{3} \Delta} \left[ \frac{1 + \Delta - T^*}{\Delta} \right]^{1/2}. \end{aligned} \quad (5.9)$$

These equations provide the velocity and temperature profiles for the case of Maxwell molecules.

A similar calculation can be carried out for hard spheres with  $\nu \propto \rho T^{-1/2}$ . The result is

$$\begin{aligned} y^* &= \frac{U}{2a\nu_L L} \left[ U_x^* (1 + \Delta - \Delta U_x^{*2})^{1/2} \right. \\ &\quad \left. + \frac{1 + \Delta}{\Delta^{1/2}} \sin^{-1} \left[ \frac{U_x^*}{(1 + \Delta^{-1})^{1/2}} \right] \right], \\ y^* &= \frac{U}{2a\nu_L L} \left\{ \left[ T^* \frac{1 + \Delta - T^*}{\Delta} \right]^{1/2} \right. \\ &\quad \left. + \frac{1 + \Delta}{\Delta^{1/2}} \sin^{-1} \left[ \left[ \frac{1 + \Delta - T^*}{1 + \Delta} \right]^{1/2} \right] \right\}. \end{aligned} \quad (5.10)$$

The boundary conditions now give

$$\frac{U}{\nu_L L} = 2a \left[ 1 + \frac{1 + \Delta}{\Delta^{1/2}} \sin^{-1} \left[ \frac{1}{(1 + \Delta^{-1})^{1/2}} \right] \right]^{-1}. \quad (5.11)$$

In Fig. 3 the velocity and temperature profiles are shown for Maxwell molecules and for hard spheres, corresponding to the values  $\Delta=1$  and 5. The coincidence of the velocity profiles for hard spheres with  $\Delta=5$  coincide accidentally with those for Maxwell molecules with  $\Delta=1$ , and has not been shown. The profiles for the velocity (temperature) are antisymmetric (symmetric) with respect to the vertical axis. The curvature always increases with  $\Delta$ , and, at a given value of  $\Delta$ , it is greater for Maxwell molecules than for hard spheres. In general, the harder the interaction is, the closer the velocity (temperature) profile is to a straight line (parabola). The parameter  $\Delta$  can be understood as a measure of the square of the relative velocity of the two planes enclosing the region under consideration, or as the relative difference in temperature of the planes induced by their motion.

It is possible to establish a simple relationship between the parameter  $a$  and the mean shear rate  $U/L$ . From Eq. (5.7) one gets

$$a = \frac{1}{\bar{v}} \frac{U}{L}, \quad (5.12)$$

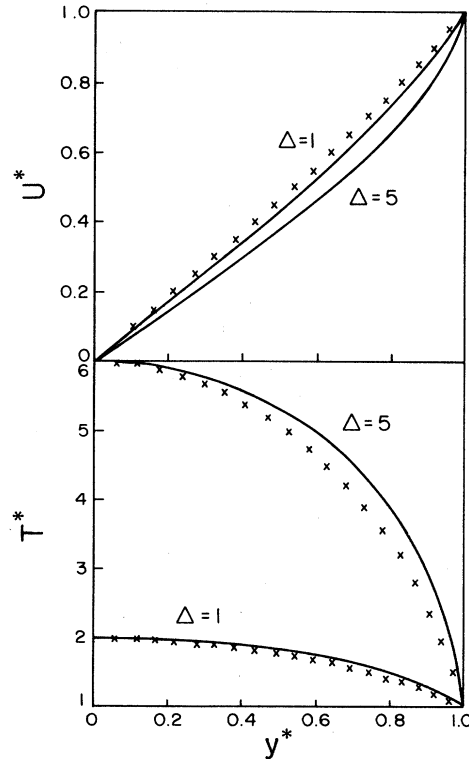


FIG. 3. Velocity (upper) and temperature (lower) profiles for Maxwell molecules (—) and for hard spheres (×) at  $\Delta=1$  and 5 (for  $U^*$  the hard-sphere results at  $\Delta=5$  agree closely with the Maxwell case of  $\Delta=1$ , by accident, and are not shown).

with  $\bar{v}$  being the mean collision frequency,

$$\bar{v} = \frac{1}{L} \int_0^L dy \nu(y). \quad (5.13)$$

## VI. SUMMARY AND CONCLUDING REMARKS

The results of Sec. V completely describe a macroscopic stationary state for heat and momentum transport far from equilibrium. As noted in the Introduction, such descriptions are rare, and progress was possible here due to simplifications of the BGK model. However, a similar analysis of the limit  $a \rightarrow 0$  (pure heat flow) using the BGK model<sup>5</sup> has now been extended to a corresponding solution of the Boltzmann equation for Maxwell molecules.<sup>3</sup> We expect that the macroscopic state described here is also an exact result for the Maxwell-molecules Boltzmann equation, although we have not yet proved this. Also, it is interesting to speculate on the relevance of these low-density gas results for comparison with dense-fluid computer simulations of stationary states.<sup>7</sup> A comparison by Zwanzig of BGK results with computer simulations for uniform shear flow indicates both qualitative and quantitative agreement, with a suitable scaling of the collision frequency  $\nu$ .

It is interesting to contrast the shear flow described here with uniform shear flow.<sup>4</sup> The latter has a spatially constant temperature field that increases with time, while here the temperature field is constant in time, but spatially varying. The velocity profiles are both linear in  $l$ , but the transformation from  $l$  to  $y$  is different because uniform shear flow occurs at constant density instead of constant pressure. One consequence of this is that the shear viscosity of uniform shear flow is analytic in the shear rate for the special case of Maxwell molecules, although nonanalytic otherwise. In contrast, the reduced shear viscosity obtained here,  $F_\eta = \eta(T, a)/\eta_0(T)$ , is a universal nonanalytic function of the shear rate, independent of the potential model. Finally, we note that although both types of shear flow describe exact macroscopic properties of a normal solution to the Boltzmann equation, there are no physically realistic boundary conditions associated with uniform shear flow. However, the normal solution for the flow considered here is expected to result from the usual local boundary conditions (e.g., diffuse, Maxwell, etc.).

A weak point of the analysis in Sec. III is the use of a formal solution to the BGK equation, Eq. (3.5). This leads to a divergent asymptotic series for the heat and momentum fluxes. In effect, we have identified the fluxes with well-defined functions having the same asymptotic series. However, such identification is not unique. For this reason we have used the terminology "consistent with" rather than "derived from" the BGK equation. Further study of this point is required.

The additional main results are summarized as follows.

(1) The stationary profiles with and without an imposed temperature gradient are closely related. This is a consequence of their additive character in the auxiliary variable  $l$ .

(2) The shear viscosity is uniform in space and does not depend on the imposed temperature gradient. Considerations of symmetry alone would allow, for example, contributions of second order in the temperature gradient and third order in the shear rate. Such terms do not occur.

(3) The heat flux obeys a generalized Fourier's law, i.e., it is proportional at each point to the local temperature gradient. The transport coefficient is a function of the shear rate. The ratio between the shear viscosity and the thermal conductivity defines a shear-rate-dependent Prandtl number that turns out to be bounded between 1 (for  $a \rightarrow 0$ ) and  $\frac{5}{3}$  (for  $a \rightarrow \infty$ ).

(4) The natural parameter to carry out a Chapman-Enskog expansion is the reduced shear rate  $a$ , but such an expansion is only asymptotic and diverges very rapidly. A similar result has been found for the uniform-shear-flow problem.<sup>5</sup>

(5) Although the velocity and temperature profiles are not simple, an "equation of state" relating the velocity and the temperature at each point applies. Namely, the temperature is a quadratic function of the velocity with shear-rate-dependent coefficients.

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## APPENDIX A: HEAT AND MOMENTUM FLUXES

The integrals in Eq. (3.6) can be performed to give

$$t_{xy}^* = \lim_{n \rightarrow \infty} 2p \sum_{(j \text{ odd})}^n \left[ -\frac{\partial}{\partial l} \right]^j v_0^{j-1} U_x \frac{j!!}{2^{(j+1)/2}}, \quad (A1)$$

where  $v_0^2 \equiv 2k_B T(l)/m$ . Let  $j \rightarrow 2j+1$ , and  $n \rightarrow 2n+1$ , so

$$t_{xy}^* = \lim_{n \rightarrow \infty} -p \sum_{j=0}^n \frac{(2j+1)!!}{2^j} \left[ U_x \frac{\partial^{2j+1}}{\partial l^{2j+1}} v_0^{2j} + (2j+1)a \frac{\partial^{2j}}{\partial l^{2j}} v_0^{2j} \right]. \quad (A2)$$

The first term in the large parentheses vanishes since  $v_0^{2j}$  is a polynomial in  $l$  of degree  $2j$ . The second term is easily evaluated with the result

$$\begin{aligned} t_{xy}^* &= \lim_{n \rightarrow \infty} -ap \sum_{j=0}^n (2j+1)!(2j+1)!!(-\gamma)^j \\ &= \lim_{n \rightarrow \infty} -ap \sum_{j=0}^n \frac{[(2j+1)!!]^2 (-\gamma)^j}{2^j j!}, \end{aligned} \quad (A3)$$

where  $\gamma$  is defined by Eq. (3.8). The factorials  $(2j+1)!!$  can be represented in integral form using

$$j! = \int_0^\infty dt e^{-t} t^j. \quad (A4)$$

The function  $F_\eta$  in (3.11) can then be identified easily and is given by Eq. (3.10).

Next consider the heat flux, defined by (3.1),

$$\begin{aligned}
q_y^* &= \int d\mathbf{v} v_y \frac{1}{2} m [(v_x - U_x)^2 + v_y^2 + v_z^2] f \\
&= \lim_{n \rightarrow \infty} \left\{ \sum_{j=0}^n \frac{m}{2} \left[ \left[ -\frac{\partial}{\partial l} \right]^j \int d\mathbf{v} v_y^{j+1} v^2 f_L - 2U_x \left[ -\frac{\partial}{\partial l} \right]^j U_x \int d\mathbf{v} v_y^{j+1} f_L \right] \right\} \\
&= \lim_{n \rightarrow \infty} -p \sum_{\substack{j=1 \\ (j \text{ odd})}}^n \left\{ \frac{(j+2)!! + 2(j)!!}{2^{(j+3)/2}} \left[ \frac{\partial}{\partial l} \right]^j v_b^{j+1} + \frac{j!!}{2^{(j+1)/2}} \left[ -2U_x \left[ \frac{\partial}{\partial l} \right]^j v_b^{j-1} U_x + \left[ \frac{\partial}{\partial l} \right]^j v_b^{j-1} U_x^2 \right] \right\}.
\end{aligned}$$

Again changing  $j \rightarrow 2j+1$ ,  $n \rightarrow 2n+1$  gives

$$\begin{aligned}
q_y^* &= \lim_{n \rightarrow \infty} -p \sum_{j=0}^n \frac{(2j+1)!!}{2^{j+2}} \left[ (2j+5) \left[ \frac{\partial}{\partial l} \right]^{2j+1} v_b^{2j+2} + 2a^2(2j+1)2j \left[ \frac{\partial}{\partial l} \right]^{2j-1} v_b^{2j} \right] \\
&= \lim_{n \rightarrow \infty} -\frac{pk_B}{2m} \frac{\partial T}{\partial l} \sum_{j=0}^n (2j+1)!!(2j+1)!(-\gamma)^j \left[ \frac{a^2}{\gamma} + (j+1) \left[ 2j+5 - \frac{a^2}{\gamma} \right] \right] \\
&= \lim_{n \rightarrow \infty} -\frac{pk_B}{2m} \frac{\partial T}{\partial l} \sum_{j=0}^n \frac{[(2j+1)!]^2(-\gamma)^j}{2^{j+1} j!} \left[ \frac{a^2}{\gamma} + (j+1) \left[ 2(j+1) + 3 - \frac{a^2}{\gamma} \right] \right].
\end{aligned}$$

The function  $F_\lambda$  can now be identified in the form (3.13) with

$$\begin{aligned}
G(a, \gamma) &\equiv \lim_{n \rightarrow \infty} \frac{1}{5} \sum_{j=0}^n \frac{[(2j+1)!]^2(-\gamma)^j}{2^{j+1} j!} (j+1) \\
&\quad \times \left[ 2(j+1) + 3 - \frac{a^2}{\gamma} \right]. \quad (\text{A5})
\end{aligned}$$

Changing  $j \rightarrow j-1$  and  $n \rightarrow n-1$  in (A5) leads to

$$\begin{aligned}
F_\eta(\gamma) \equiv \psi(\omega) &= \int_0^\infty dt_1 \int_0^\infty dt_2 e^{-(t_1+t_2)} t_1 t_2 \exp \left[ -\frac{1}{2} \frac{t_1^2 t_2^2}{\omega^2} \right] \\
&= \omega^2 \int_0^\infty du u e^{-u^2} \int_0^\infty dt \frac{1}{t} \exp \left[ -\omega^{1/2} \left[ t + \frac{u}{t} \right] \right]. \quad (\text{B1})
\end{aligned}$$

The last integration in Eq. (B1) can be understood as the Laplace transform  $G(s)$  of the function

$$g(t) = \frac{1}{t} e^{-k^2/4t}, \quad k^2 = 4u\omega^{1/2} \quad (\text{B2})$$

evaluated at  $s = \omega^{1/2}$ . The result is<sup>8</sup>  $2K_0(2\sqrt{u\omega})$ , where  $K_0$  is the zeroth-order modified Bessel function. Therefore,

$$\psi(\omega) = 2\omega^2 \int_0^\infty du u e^{-u^2} K_0(2\sqrt{u\omega}). \quad (\text{B3})$$

The series expansion of  $K_0$  is<sup>8</sup>

$$K_0(x) = -(\ln \frac{1}{2} x) \sum_{q=0}^{\infty} \frac{(x^2/4)^q}{(q!)^2} + \sum_{q=0}^{\infty} \chi(q+1) \frac{(x^2/4)^q}{(q!)^2}, \quad (\text{B4})$$

where

$$\chi(1) = -\gamma_E, \quad (\text{B5}) \quad c_0 = 1, \quad c_1 = (\pi/2)^{1/2}, \quad (\text{B11})$$

$$G(a, \gamma) = \lim_{n \rightarrow \infty} \frac{1}{10} \sum_{j=1}^n \frac{[(2j)!]^2(-\gamma)^{j-1}}{j! 2^j} \left[ 2j + 3 - \frac{a^2}{\gamma} \right]. \quad (\text{A6})$$

The integral representation for  $G(a, \gamma)$  in Eq. (3.4) is obtained from (A6) using the identity (A4).

#### APPENDIX B: REPRESENTATION OF $F_\eta$

In this appendix we are going to derive a representation of the function  $F_\eta$  that is useful for computational purposes. The function  $F_\eta$  is given by Eq. (3.11). By introducing the variable  $\omega \equiv \gamma^{-1/2}$ , we get

$$\chi(\frac{1}{2}) = -2 \ln 2 - \gamma_E, \quad (\text{B6})$$

$$\chi(q+1) = \chi(q) + q^{-1}. \quad (\text{B7})$$

Here,  $\gamma_E = 0.57721\dots$  is the Euler constant. Substitution of Eq. (B4) into Eq. (B3) yields

$$\frac{\psi(\omega)}{\omega^2} = -\ln \omega \sum_{q=0}^{\infty} c_q \omega^q + \sum_{q=0}^{\infty} d_q \omega^q, \quad (\text{B8})$$

with

$$c_q = \frac{\Gamma(q/2+1)}{(q!)^2} 2^{q/2}, \quad (\text{B9})$$

$$d_q = c_q \left\{ 2\chi(q+1) - \frac{1}{2} [\ln 2 + \chi(q/2+1)] \right\}. \quad (\text{B10})$$

These coefficients satisfy the following recurrence relations:

$$c_{q+2} = \frac{c_q}{(q+2)(q+1)^2}, \quad (\text{B12})$$

$$d_0 = -\frac{1}{2}(\ln 2 + 3\gamma_E), \quad d_1 = (\pi/2)^{1/2}(1 + \frac{1}{2}\ln 2 - \frac{3}{2}\gamma_E), \quad (\text{B13})$$

$$d_{q+2} = \frac{d_q}{(q+2)(q+1)^2} + \frac{3q+5}{(q+2)(q+1)}c_{q+2}. \quad (\text{B14})$$

The expansion (B8) is convergent for all values  $\omega > 0$ , and it has been used to evaluate the function  $F_\eta$  in the results reported in the main text.

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