Kinetic model for heat and momentum transport

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(Received 2 March 1994; accepted 30 June 1994)

Expressions for the heat and momentum transport are obtained for a dilute gas in a steady state with both temperature and velocity gradients. The results are derived from a kinetic model recently proposed: the Liu model [Phys. Fluids A **2**, 277 (1990)]. This model improves the well-known Bhatnagar–Gross–Krook (BGK) model equation. At a hydrodynamic level, the solution is characterized by a constant pressure, a linear profile of the flow velocity with respect to a space variable scaled with the local collision frequency, and a parabolic profile of the temperature with respect to the same variable. The shear viscosity and thermal conductivity coefficients are explicitly obtained. They are nonlinear functions of the shear rate and their only dependence on the temperature gradient is through their zero shear-rate values. In addition, the shear-rate dependence of the viscometric functions is also analyzed. A comparison with previous results derived from the BGK equation is carried out.

I. INTRODUCTION

The study of transport phenomena in dilute gases is a subject of great interest. From a theoretical point of view, they are usually analyzed in the framework of the Boltzmann equation.[1] For near equilibrium situations, the Chapman–Enskog expansion[2] provides an approximate method for solving the Boltzmann equation for a general interaction law. From the knowledge of the constitutive equations for the heat and momentum fluxes, one may derive the corresponding hydrodynamic equations in successive approximations. However, because of the mathematical complexity embodied in the Boltzmann collision operator, it is very difficult to obtain explicit results especially in states far from equilibrium. Consequently, several kinetic models have been suggested in the last few years for avoiding the above problem. The general idea is to construct a collision term mathematically simpler than the one corresponding to the Boltzmann equation but preserving its main physical properties, such as the equilibrium solution and the conservation laws.

The most widely used model in the past years has been the nonlinear model proposed by Bhatnagar, Gross, and Krook (BGK).[3] In this model, the Boltzmann collision integral is replaced by an exponential relaxation toward a local equilibrium state with a rate determined by an effective collision frequency. In spite of its simplicity, some results derived from the BGK model in several nonequilibrium problems have been shown to be identical to those obtained from the Boltzmann equation. Therefore, in the uniform shear flow[4] and steady Fourier flow[5] states, the main transport properties given by the BGK equation are the same as those given by the Boltzmann equation for Maxwell molecules[6] if one chooses the BGK-collision frequency to be a particular eigenvalue of the Boltzmann operator. For other interaction potentials, the BGK results exhibit a good agreement with Monte Carlo simulations of the Boltzmann equation.[7]

Nevertheless, the BGK model presents some insufficiencies. In particular, it does not give the correct value of the Prandtl number. For this reason, Liu has recently suggested a novel kinetic model[8] to improve some of the predictions made from the BGK equation. The collision term of the Liu model is constructed by demanding that in the cases of viscous flow and molecular flow, its solutions coincide with those given by the Boltzmann equation. This necessarily implies that the Liu collision term must be proportional to the Chapman–Enskog first approximation of the Boltzmann equation. Beyond the Navier–Stokes regime, recently it has been shown[9] that the Burnett transport coefficients are identical to the ones arising from the Boltzmann equation for some values of the ratio of the two collision frequencies ζ/ν introduced in the Liu model. Consequently, the Burnett transport coefficients obtained from the Liu model are closer to the Boltzmann coefficients than the ones given by the BGK equation[10] for the same choices of the collision frequencies.

The aim of this paper is to describe the transport properties of a dilute gas in a steady state and subject to arbitrarily large velocity and temperature gradients (steady Couette flow). Due to the mathematical difficulties associated with this problem, no solution to the Boltzmann equation has been found. However, an exact description can be given if one uses the BGK equation.[11] Now, our goal is to extend this description by taking the Liu model as the starting point. The main reason for considering the steady Couette flow is that the Liu and BGK models yield the same results in the two limit cases of pure shear flow[4] and pure Fourier flow.[5] For that it is only necessary to choose appropriate values for the ratio ζ/ν. In this way, the results obtained from both kinetic models will be in principle noticeably different in nonequilibrium problems where combined heat and momentum transport takes place in the system. Recent results describing linear heat transport around the uniform shear flow state[12] support the above conjecture.

The organization of the paper is as follows. In Sec. II we give a brief review of the Liu kinetic model for dilute gases. In Sec. III, we construct a consistent solution to the Liu model in the steady Couette flow state. This solution is characterized by a constant pressure and linear velocity and parabolic temperature profiles with respect to a new length scale. The parabolic profile is measured through a shear-rate dependent parameter γ. In contrast to what happens in the BGK solution, there is a critical value of γ beyond which a physical solution fails to exist. The most relevant fluxes are obtained in Sec. IV. In particular, the shear viscosity and thermal conductivity coefficients are highly nonlinear functions of the shear rate. The shear rate dependence of these coefficients and of viscometric functions is illustrated and compared with the one predicted by the BGK equation. Finally, Sec. V offers a brief discussion of the results.

II. LIU KINETIC MODEL FOR DILUTE GASES

The complicated nature of the Boltzmann collision integral has stimulated in the past the search of several kinetic models. The general idea is to replace the exact collision term by a simpler expression keeping the main physical properties. Perhaps, the most elementary model is the single relaxation one proposed by Bhatnagar, Gross, and Krook (BGK).[3] Although it has been shown to be very useful for many purposes, it presents some deficiencies. For example, the BGK model leads to a Prandtl number of 1 instead of the more correct value of 2/3. Subsequently, Gross and Jackson[13] suggested a systematic procedure for constructing more elaborate models for Maxwell molecules. These models improve the predictions made from the BGK equation. The extension of this hierarchy of models to arbitrary molecular force laws as well as mixtures was given later by Sirovich.[13] More recently, a new model kinetic equation has been proposed by Liu.[8] The Liu kinetic model is a version of the nonlinear Boltzmann equation in which the exact Boltzmann operator is substituted by the Chapman–Enskog solution to the linearized Boltzmann equation. Neglecting external forces, the Liu equation can be written in the form:

$$\frac{\partial}{\partial t} f+\mathbf{v}\cdot\nabla f=-\zeta(f-f^{\rm LE})+Af^{\rm LE}\frac{m}{k_{\rm B}T}\left(V_iV_j-\tfrac{1}{3}V^2\delta_{ij}\right)\times\nabla_j u_i+Bf^{\rm LE}\left(\frac{mV^2}{2k_{\rm B}T}-\frac{5}{2}\right)V_i\nabla_i \ln T, \tag{1}$$

where $f(\mathbf{r},\mathbf{v};t)$ is the velocity distribution function, $\zeta(\mathbf{r};t)$ is an effective collision frequency, and $f^{\rm LE}(\mathbf{r},\mathbf{v};t)$ is the local equilibrium velocity distribution function:

$$f^{\rm LE}(\mathbf{r},\mathbf{v};t)=n(\mathbf{r};t)\left(\frac{m}{2\pi k_{\rm B}T(\mathbf{r};t)}\right)^{3/2}\times\exp\left(-\frac{m}{2k_{\rm B}T(\mathbf{r};t)}\mathbf{V}^2(\mathbf{r};t)\right). \tag{2}$$

Here, $k_{\rm B}$ is the Boltzmann constant, m is the mass of a particle, $n(\mathbf{r};t)$ is the local number density, $\mathbf{V}(\mathbf{r};t)=\mathbf{v}-\mathbf{u}(\mathbf{r};t)$, with $\mathbf{u}(\mathbf{r};t)$ being the local flow velocity, and $T(\mathbf{r};t)$ is the local temperature. In terms of the distribution function, these hydrodynamic fields are defined as

$$n=\int d\mathbf{v}\, f, \tag{3}$$

$$n\mathbf{u}=\int d\mathbf{v}\,\mathbf{v}f, \tag{4}$$

$$nk_{\rm B}T=\frac{m}{3}\int d\mathbf{v}\,\mathbf{V}^2 f. \tag{5}$$

Further, Eq. (1) introduces the coefficients

$$A=1-\frac{\zeta\eta_0}{nk_{\rm B}T}, \tag{6}$$

$$B=1-\frac{2}{5}\zeta\lambda_0\frac{m}{nk_{\rm B}^2T}, \tag{7}$$

where $\eta_0=(5/8)(nk_{\rm B}T/\nu)$ and $\lambda_0=(15/4)(k_{\rm B}\eta_0/m)$ are the coefficients of viscosity and thermal conductivity, respectively, obtained from the Chapman–Enskog solution to the Boltzmann equation to first order in the uniformity expansion parameter of the method (Navier–Stokes order). Here, $\nu(\mathbf{r};t)$ is another velocity-independent collision frequency that can depend upon the density and temperature. For instance, for a repulsive potential of the form $r^{-\mu}$, it is $\zeta\propto nT^{\alpha}$ with $\alpha=(1/2)-(2/\mu)$.

As additional interesting features, the Liu model has an H theorem for small deviations from a local Maxwellian and satisfies the conservation laws. Thus, by taking moments in velocity space, Eq. (1) leads to the familiar transport equations

$$\frac{d}{dt}n=-n\nabla_i u_i, \tag{8}$$

$$mn\frac{d}{dt}u_i=-\nabla_i P_{ij}, \tag{9}$$

$$\frac{3}{2}nk_{\rm B}\frac{d}{dt}T=-\nabla_i q_i-P_{ij}\nabla_i u_j, \tag{10}$$

where the transport of momentum and energy are described respectively by the pressure tensor

$$P_{ij}=\int d\mathbf{v}\,mV_iV_jf, \tag{11}$$

and the heat flux

$$q_i=\int d\mathbf{v}\,\frac{m}{2}\mathbf{V}^2V_if. \tag{12}$$

The balance equations (8)–(10) do not constitute a closed set. To complete the derivation of transport equations one needs to know the explicit expressions of the fluxes as functions of the gradients. Since the solution to the general problem is unapproachable, specific situations must be considered. Here, we will restrict ourselves to analyze the steady Couette flow state.

According to the form proposed for the collision term in the Liu equation, it is clear that its Navier–Stokes transport coefficients are identical to the ones calculated from the Boltzmann equation with independence of the value of the ratio ζ/ν. Consequently, it gives the correct value of the Prandtl number. Beyond the Navier–Stokes approximation, the Liu transport coefficients depend on the ratio ζ/ν. Recently, it has been shown that particular choices of this ratio may lead to the same results for the Liu and Boltzmann equations.[9] Therefore, if $\zeta/\nu=8/5$ (for which $A=0$ and η_0 coincides with the BGK-shear viscosity coefficient) the Burnett transport coefficients that appear in the pressure tensor expression are the same as those calculated from the Boltzmann equation. Analogous conclusions for the heat flux are drawn out if one takes $\zeta/\nu=16/15$ (for which $B=0$ and λ_0 coincides with the BGK-thermal conductivity coefficient).

III. HYDRODYNAMIC FIELDS

We consider a dilute gas between two parallel plates maintained at different temperatures and kept in relative motion. Let the x axis be parallel to the direction of motion and the y axis be orthogonal to the walls. We are interested in studying a system in a steady state with velocity and temperature gradients along the y direction. Under these conditions the Liu equation (1) becomes

$$v_y \frac{\partial}{\partial y} f=-\zeta(f-f_0), \tag{13}$$

where

$$f_0=f^{\rm LE}\left[1+A \frac{m}{k_{\rm B}T} \frac{V_xV_y}{\zeta} \frac{\partial}{\partial y} u_x+B \times\left(\frac{mV^2}{2k_{\rm B}T}-\frac{5}{2}\right) \frac{V_y}{\zeta} \frac{\partial}{\partial y} \ln T\right]. \tag{14}$$

In order to solve Eq. (13), one needs to introduce appropriate boundary conditions for obtaining the profiles of the hydrodynamic fields. However, rather than solving the problem numerically,[14] we will follow a different route in the same spirit as in previous works.[5,11] As we are interested in the transport properties in the bulk of the system far away from the boundaries, we first *guess* the profiles and then verify their consistency. Thus, one expects to describe the relevant transport phenomena in the bulk domain by looking for a consistent solution regardless of the details of the boundary conditions.

Now, we will proceed in a heuristic way. First, it must be noticed that the rate at which collisions take place is nonuniform, so that it is not convenient to measure distance in terms of the space variable y. Thus, we take instead the scaled space variable s defined through the relation

$$ds=\zeta(y)dy. \tag{15}$$

This variable measures distance in units of mean-free paths and scales the influence of the interaction potential on the collision frequency ζ. In terms of s, and suggested by the parallel results derived from the BGK model,[11] we assume that the Liu model admits a consistent solution with a uniform pressure p, a linear velocity profile and a parabolic temperature profile, i.e.,

$$p=n(s)k_{\rm B}T(s)\equiv{\rm const}, \tag{16}$$

$$\frac{\partial}{\partial s} u_x=a\equiv{\rm const}, \tag{17}$$

$$\frac{\partial^2}{\partial s^2} T=-\frac{2m}{k_{\rm B}} \gamma(a)\equiv{\rm const}, \tag{18}$$

where a is the reduced shear rate and $\gamma(a)$ is a dimensionless parameter to be determined by consistency. Equations (16)–(18) constitute our guess of hydrodynamic profiles. Obviously, these assumptions must be verified later. Notice that the simplicity of the profiles (17) and (18) is not so apparent if one uses the real space variable y. The relationship of s to the space variable y is obtained from the integration of (15). Since the dependence of the collision frequency ζ on the temperature T depends on the interaction model considered, the velocity and temperature profiles will also have this dependence.

It remains still to check that the solution to Eq. (13) characterized by the profiles (16)–(18) is self-consistent, namely, it reproduces the first five conserved moments:

$$\int d{\bf v}\, \chi_\alpha({\bf v})(f-f_0)=0, \quad \chi_\alpha({\bf v})\leftrightarrow(1,{\bf v},v^2). \tag{19}$$

In order to verify this relation, an explicit expression for the velocity distribution function f must be specified. Here, a formal solution given from a series representation is sufficient for proving (19) and evaluating the fluxes. We rewrite the steady Liu equation as

$$f=\left(1+v_y \frac{\partial}{\partial s}\right)^{-1} f_0=\sum_{k=0}^{\infty} (-v_y)^k \frac{\partial^k}{\partial s^k} f_0. \tag{20}$$

The distribution function $f({\bf v})$ as a function of s is universal, namely, does not depend on the interaction potential. This solution is only formal as f_0 is a nonlinear functional of f. Equation (20) provides an expansion of f in powers of velocity and temperature gradients in the variable s.

The verification of the consistency between the solution (20) and the conditions (19) is made in Appendix A. The consistency condition for the temperature gives the dependence of γ on the shear rate a through the implicit equation:

$$a^2=\gamma \frac{3F_1(\gamma)+2F_2(\gamma)}{F_1(\gamma)-(1/3)F_0(\gamma)}, \tag{21}$$

where the functions $F_r(\gamma)$ are defined in Eq. (A11). The function γ is a measure of the curvature of the parabolic temperature profile. It can be seen as an independent parameter characterizing the departure from equilibrium. For $a=0$ (boundaries at rest), the temperature is linear in s and one recovers the results derived in the pure heat flow problem.[5] In the limit of small shear rates, the (asymptotic) expansion of γ gives

$$\gamma\approx \frac{2}{15} a^2+\frac{12}{125} a^4+\cdots . \tag{22}$$

On the other hand, we observe that a strict limitation on the shear rate appears in the relation (21). There exists a critical value of γ for which (21) has no solution. It corresponds to $\gamma_c\simeq 18.35$. Therefore, we find solutions for $\gamma<\gamma_c$ and unphysical solutions for $\gamma>\gamma_c$. This restriction contrasts with the BGK solution where the ratio γ/a^2 reaches a limiting constant positive value when $a\rightarrow\infty$. The existence of this

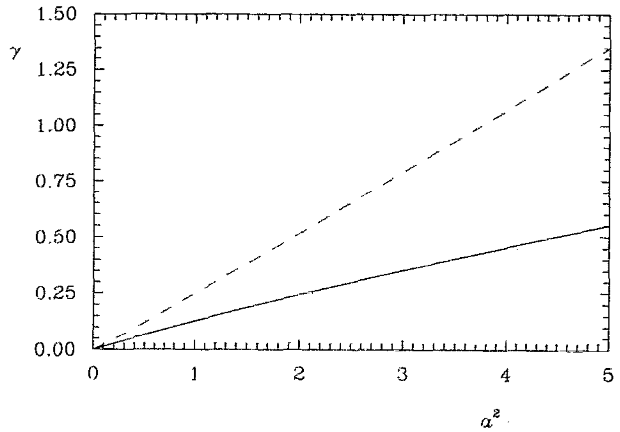

FIG. 1. Shear-rate dependence of the dimensionless function γ. The solid line corresponds to the Liu model and the dashed line refers to the BGK model.

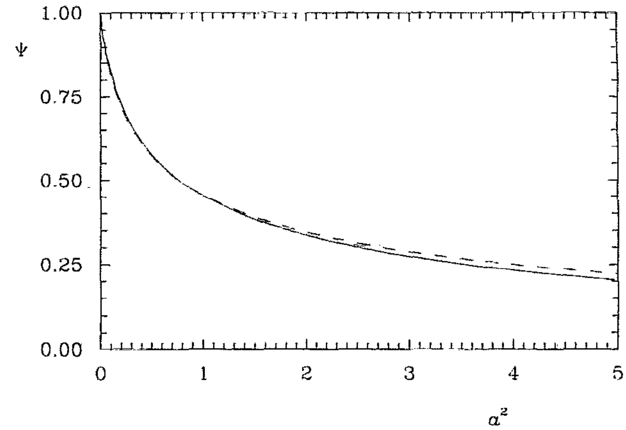

FIG. 2. Reduced shear viscosity Ψ as a function of a^2 for the Liu model (solid line) and for the BGK model (dashed line). Notice that the BGK dimensionless coefficient has been defined from its corresponding equilibrium value.

singularity is probably due to the fact that the velocity distribution function obtained from the Liu model may turn out to be negative. This problem also appears in the previous extensions to the BGK equation proposed by Gross and Jackson and by Sirovich.[13] Therefore, for values of γ larger than γ_c the Liu distribution f can be negative so that our solution becomes physically meaningless. This circumstance limits the description given by the Liu model for the steady Couette flow state.

Nevertheless, and for practical purposes, one may conclude that our solution describes situations reasonably far from the linear regime. In this range of allowed values one may evaluate the relevant transport properties of the system. In Fig. 1 we plot γ versus a^2 from the Liu and BGK results. It is shown that the general shear-rate dependence of γ is similar in both models since γ is a monotonically increasing function. However, for a given shear rate, the value predicted by the Liu model is smaller than the one obtained from the BGK equation. This means that the temperature profile predicted by the BGK model exhibits a curvature more noticeable than the one reported by the Liu model for the same value of the shear rate. Furthermore, it must be emphasized that the implicit equation (21) holds for any value of the ratio ζ/ν.

To sum up, we have proved that there exists a solution to the nonlinear Liu model (13) that is consistent with the hydrodynamic profiles (16)–(18). This solution does not apply for arbitrary values of the parameter γ defined by Eq. (18). This parameter controls the "distance" of the system from equilibrium. Nevertheless, since the corresponding critical value obtained is large, nonlinear effects in the heat and momentum transport will still be significant for $\gamma<\gamma_c$. The examination of this point is the goal of Sec. IV.

IV. TRANSPORT PROPERTIES

In this section we proceed to the calculation of some of the transport properties. They are related with the momentum and heat fluxes. According to the symmetry of the problem, the most relevant transport coefficients are determined from the xy component of the pressure tensor (11) and the y component of the heat flux vector (12). The evaluation of these quantities is rather involved and is made in Appendix B. The results are

$$P_{xy}=-\eta_0[T(y)]\Psi(a)\frac{\partial}{\partial y}u_x, \tag{23}$$

$$q_y=-\lambda_0[T(y)]\Phi(a)\frac{\partial T}{\partial y}, \tag{24}$$

where

$$\Psi(a)=F_0(\gamma)-2\gamma[2F_3(\gamma)+F_2(\gamma)], \tag{25}$$

$$\Phi(a)=\frac{2}{15}\frac{a^2}{\gamma}\Psi(a). \tag{26}$$

Equation (23) is a generalization of Newton's viscosity law where a reduced shear viscosity coefficient $\Psi(a)$ is identified. It is a highly nonlinear function of the shear rate but does not depend on the thermal gradient. Although our description applies for arbitrary temperature gradients, the heat flux happens simply to be proportional to the temperature gradient so that a Fourier's law is verified. The reduced thermal conductivity coefficient $\Phi(a)$ is a function again only of the shear rate. In the limit of small shear rates, their asymptotic forms are $\Psi(a)\approx 1-(16/5)a^2+\cdots$, and $\Phi(a)\approx 1-(98/25)a^2+\cdots$. The shear-rate dependence of both transport coefficients is shown in Figs. 2 and 3. The reduced shear viscosity $\Psi(a)$ monotonically decreases representing shear thinning. Although the numerical values predicted by the Liu and BGK models are very similar, the shear thinning is slightly more noticeable in the Liu results especially for large shear rates. More important discrepancies between the predictions of both models are observed in the case of the reduced thermal conductivity. Figure 3 indicates that the transport of energy along the direction of the thermal gradient is inhibited by the presence of the shear rate. In contrast to what happens in the shear viscosity, this inhibition is more significant in the BGK model. In addition, it must be

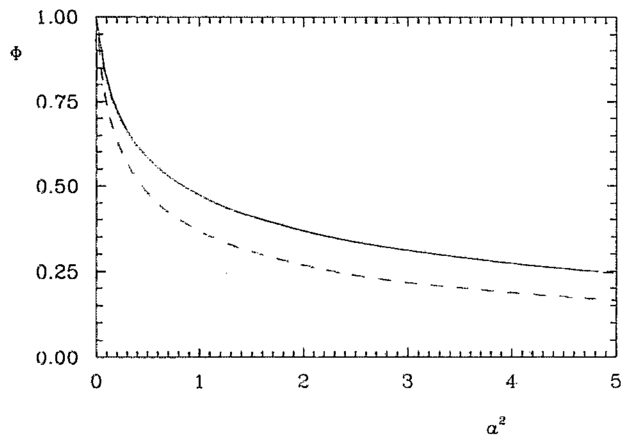

FIG. 3. The same as in Fig. 2, but for the reduced thermal conductivity Φ.

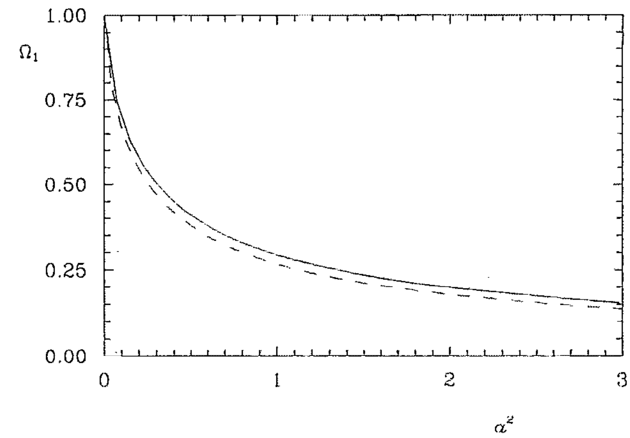

FIG. 4. The same as in Fig. 2, but for the reduced first viscometric function Ω_1.

noticed that both reduced transport coefficients are again independent of the ratio ζ/ν. It is easy to see that this fact is a direct consequence of the consistency of the solution.

The diagonal components of the pressure tensor define the viscometric functions φ_1 and φ_2. These functions characterize normal stresses in a fluid under shear flow. In terms of dimensionless quantities, they can be defined as

$$\varphi_1=-\frac{P_{xx}^*-P_{yy}^*}{a^2}, \tag{27}$$

$$\varphi_2=-\frac{P_{yy}^*-P_{zz}^*}{a^2}, \tag{28}$$

where $P_{ij}^* \equiv P_{ij}/p$. From the explicit expressions of the normal components of P obtained in Appendix B, the first and second viscometric functions can be written, respectively, as

$$\varphi_1(a)=\frac{2\gamma}{a^2}(B-1)[3F_1(\gamma)+4F_2(\gamma)], \tag{29}$$

$$\varphi_2(a)=-\frac{4\gamma}{a^2}(B-1)F_2(\gamma). \tag{30}$$

They depend on the choice of the ratio ζ/ν through the parameter B. The expansion of P_{ij}^* to order a^2 allows identification of the viscometric functions at zero shear rate. For instance, one gets $\varphi_1(0)=(28/15)(B-1)$ and $\varphi_2(0)=-(8/15)(B-1)$. These numerical values coincide with those previously obtained from the Hilbert method in the Burnett approximation.[9] To analyze the shear-rate dependence of the viscometric functions with independence of the value of B, we have considered it adequate to plot the reduced quantities $\Omega_i(a)\equiv\varphi_i(a)/\varphi_i(0)$ in Figs. 4 and 5. Both functions exhibit a similar behavior, namely, they monotonically decrease as a increases. Furthermore, for a given shear rate, the Liu value is greater than the one corresponding to the BGK equation and consequently the anisotropy measured by the normal stress effects becomes more important in the Liu description.

V. CONCLUSIONS

In this paper we have analyzed heat and momentum transport in a dilute gas far from equilibrium. The specific state considered is the steady planar Couette flow, in which the system is enclosed between two parallel plates in relative motion and maintained at different temperatures. Two parameters measure the departure from equilibrium: the shear rate and the thermal gradient. The study was done using a kinetic model of the nonlinear Boltzmann equation recently proposed: the Liu model. This model improves some insufficiencies of the well-known Bhatnagar–Gross–Krook (BGK) model. For example, it provides the correct value of the Prandtl number. Our description is not restricted to small gradients, and progress was possible here due to previous results derived from the simple BGK model.[11]

In the same way as the BGK results, the solution is characterized by a constant pressure, and linear and parabolic profiles for the flow velocity and the temperature, respectively. The linear and parabolic dependencies take place with respect to a space variable conveniently scaled with the local collision frequency. The coefficient γ measuring the curva-

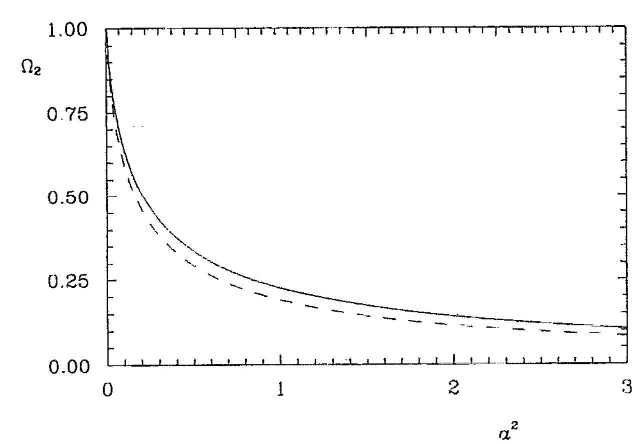

FIG. 5. The same as in Fig. 2, but for the reduced second viscometric function Ω_2.

ture of the temperature profile is related with the shear rate through an implicit equation. In contrast to the BGK description, the physical solution to this equation is restricted to values of γ less than a critical value $\gamma_c \simeq 18.35$. The presence of this singular behavior is most likely due to a failure of the Liu model rather than a physical feature since this model can predict negative values for the distribution function at large values of the curvature parameter γ. Anyway, and from a practical point of view, it is evident that the solution extends over a range of shear rates where nonlinear effects are important. The above drawback could be avoided if one used the so-called ellipsoidal statistical model[13] where the local Maxwellian is replaced by an anisotropic three-dimensional Gaussian. However, such an approach lies beyond the scope of the present paper due to the intricacy of the collision term in this latter model. It appears nevertheless to be an interesting problem which we would like to address in the future.

Once the solution is characterized, the main transport properties were determined: the reduced shear viscosity coefficient Ψ and the reduced thermal conductivity coefficient Φ. Both coefficients are universal functions of the shear rate, independent of the potential model considered. The dependence on the interaction potential appears through the y dependence of ζ, so that to get the real space dependence of the fluxes one needs to consider the relationship between ζ and T. The reduced shear viscosity is a highly nonlinear function of the shear rate but it does not depend on the imposed thermal gradient. The heat flux obeys a generalized Fourier's law with a reduced transport coefficient Φ also a function only of the shear rate. Comparison between the results given by the Liu and BGK models shows a good agreement in the general shear-rate dependence of these coefficients, although important quantitative discrepancies appear especially in the case of Φ. As a matter of fact, the shear-rate-dependent Prandtl number $P_r(a)=\Psi(a)/\Phi(a)$ monotonically decreases in the Liu model whereas it increases as the shear rate increases in the BGK model. This is an important difference between the predictions made by the BGK and Liu models. In addition, the viscometric functions were also calculated. They give a measure of the normal stresses in a fluid under shear flow. In the same way as $\Psi(a)$ and $\Phi(a)$, they decrease as the shear rate increases.

The derivation of explicit expressions for the transport properties involved in a far from equilibrium state may prove to be relevant for analyzing computer simulation results. We expect that the results presented here stimulate the performance of simulations where the combined effect of heat and momentum transport takes place. In the case of dense fluids, recently Liem, Brown, and Clarke[15] have computed shear properties of a Lennard-Jones fluid in steady Couette flow. However, the values of shear rates considered in this simulation are not large enough to appreciate nonlinear effects. On the other hand, we are not aware of the availability of similar simulation results in dilute gases where larger shear rates are possibly not so difficult to achieve. In this way, one could speculate on the relevance of the Liu results for comparison with those directly obtained from the Boltzmann equation by using computer simulations.[16]

ACKNOWLEDGMENTS

We want to thank E. G. D. Cohen for a critical reading of the manuscript and useful suggestions. V. G. thanks the financial support of the Dirección General de Investigación Científica y Técnica (DGICYT) of the Spanish Government through Grant No. PB91-0316. M. L. H. acknowledges the support by PAPIID of DGAPA-UNAM under Project IN-101392.

APPENDIX A: CONSISTENCY CONDITIONS FOR THE HYDRODYNAMIC FIELDS

In this appendix we prove the consistency of the solution given by Eq. (20) with the profiles (16)–(18). For that, it is necessary to verify the relations:

$$\int d\mathbf{v}\, f = \int d\mathbf{v}\, f_0 = n, \tag{A1}$$

$$\int d\mathbf{v}\, \mathbf{v} f = \int d\mathbf{v}\, \mathbf{v} f_0 = n\mathbf{u}, \tag{A2}$$

$$\int d\mathbf{v}\, v^2 f = \int d\mathbf{v}\, v^2 f_0 = n\left(\frac{3k_\mathrm{B}T}{m} + u_x^2\right). \tag{A3}$$

First, from the integration of Eqs. (17) and (18) one gets the dependence of the hydrodynamic fields on s:

$$u_x(s) = u_x(0) + as, \tag{A4}$$

$$T(s) = T(0) + \epsilon s - \frac{m\gamma}{k_\mathrm{B}} s^2, \tag{A5}$$

where a and ϵ are constants fixed by the boundary conditions. Let us start with Eq. (A1). Taking into account the series representation for f, one gets

$$\begin{aligned}\int d\mathbf{v}\, f &= \sum_{k=0}^{\infty} \left(-\frac{\partial}{\partial s}\right)^k \int d\mathbf{v}\, v_y^k f_0 \\ &= \sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k} (2k+1)!!\, n (k_\mathrm{B}T/m)^k - B \\ &\quad \times \sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k+1} k(2k+1)!!\, n(k_\mathrm{B}T/m)^{k+1} \\ &\quad \times \frac{\partial}{\partial s} \ln T = n,\end{aligned} \tag{A6}$$

since, according to the s dependence of the hydrodynamic fields, for $k \geqslant 1$ the order of the derivative $\partial/\partial s$ increases faster that the power of s. This automatically implies the verification of Eq. (A1) as the first term in the second series vanishes. The consistency condition for the x component of the velocity is

$$\int d\mathbf{v}\, v_x f = \sum_{k=0}^{\infty} \left(-\frac{\partial}{\partial s}\right)^k \int d\mathbf{v}\, v_x v_y^k f_0$$

$$= \sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k} (2k+1)!!nu_x(k_{\mathrm{B}}T/m)^k - 4Aa$$

$$\times \sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k+1} (2k+1)!!n(k_{\mathrm{B}}T/m)^{k+1}$$

$$-B\sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k+1} k(2k+1)!!nu_x$$

$$\times (k_{\mathrm{B}}T/m)^{k+1} \frac{\partial}{\partial s} \ln T = nu_x, \tag{A7}$$

where in the last step use has been made of Eqs. (16)–(18). The consistency conditions for the y and z components of the velocity can be similarly verified. The consistency for the temperature imposes the relationship between γ and a. Thus, following similar steps one gets that

$$\int d\mathbf{v}\, v^2 f = \sum_{k=0}^{\infty} \left(-\frac{\partial}{\partial s}\right)^k \int d\mathbf{v}(\mathbf{V}+\mathbf{u})^2 v_y^k f_0$$

$$= n\left(\frac{3k_{\mathrm{B}}T}{m} + u_x^2\right) + \beta(a), \tag{A8}$$

where the function $\beta(a)$ is given by

$$\beta(a) = \sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k} (2k-1)!!n(k_{\mathrm{B}}T/m)^k[(2k+3)(k_{\mathrm{B}}T/m) + u_x^2] - 2A$$

$$\times \sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k+1} (2k+1)!!nu_x(k_{\mathrm{B}}T/m)^{k+1} - B\sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k+1} (k+1)(2k+5)(2k+1)!!n(k_{\mathrm{B}}T/m)^{k+2} \frac{\partial}{\partial s} \ln T - B$$

$$\times \sum_{k=0}^{\infty} \left(\frac{\partial}{\partial s}\right)^{2k+1} k(2k+1)!!nu_x^2(k_{\mathrm{B}}T/m)^{k+1} \frac{\partial}{\partial s} \ln T. \tag{A9}$$

Now, taking into account the s dependence of the velocity and of the temperature, one arrives at the expression:

$$\beta(a) = \frac{p}{m} \sum_{k=0}^{\infty} (2k+2)!(2k+1)!!(-\gamma)^{k+1}\left(2k+5-\frac{a^2}{\gamma}\right) - 2\frac{p}{m}Aa^2 \sum_{k=0}^{\infty} (2k+1)!(2k+1)!!(-\gamma)^k$$

$$-\frac{p}{m}B\sum_{k=0}^{\infty} (2k+2)(2k+5)(2k+1)!(2k+1)!!(-\gamma)^{k+1} - 2\frac{p}{m}Ba^2\sum_{k=0}^{\infty} k(2k+1)!(2k+1)!!(-\gamma)^k. \tag{A10}$$

The function $\beta(a)$ is expressed in terms of asymptotic series. A more adequate representation can be obtained by Borel summations.[11,17] We introduce the auxiliary function

$$F_0(\gamma) = \frac{2}{\gamma} \int_0^{\infty} dt\, t \exp(-t^2/2) K_0(2\gamma^{-1/4} t^{1/2}), \tag{A11}$$

K_0 being the zeroth-order modified Bessel function. From a computational point of view, F_0 can also be represented by a Frobenius series around the point at infinity (γ^{-1}). Its explicit expression has been obtained in Appendix B of Ref. 11 and will not be repeated here. Let us define the functions

$$F_r(\gamma) = \left(\frac{d}{d\gamma}\gamma\right)^r F_0(\gamma). \tag{A12}$$

The expansion of F_0 around $\gamma=0$ is asymptotic.[11] From this expansion, it is straightforward to show that F_r can be written as

$$F_r(\gamma) = \sum_{k=0}^{\infty} (k+1)^r (2k+1)!(2k+1)!!(-\gamma)^k. \tag{A13}$$

Comparison between Eqs. (A3) and (A8) implies that $\beta(a) = 0$. Consequently, in terms of the functions F_r one gets the condition

$$2\gamma(3F_1 + 2F_2)(B-1) = 2a^2[(A-B)F_0 + (B-1)F_1]. \tag{A14}$$

Making use of the identity

$$\frac{A-B}{1-B} = \frac{1}{3}, \tag{A15}$$

Eq. (A14) reduces to the implicit Eq. (21). In this way, we conclude that our solution is self-consistent.

APPENDIX B: CALCULATION OF THE FLUXES

This appendix is concerned with the explicit evaluation of the relevant fluxes. Since the procedures to arrive at explicit expressions for the transport coefficients are identical to the ones employed in Appendix A, we only quote some of the steps here. The reduced shear viscosity $\Psi(a)$ is obtained from the xy component of the pressure tensor. After some algebra, one gets

$$P_{xy}=-pa\sum_{k=0}^{\infty}(2k+1)!(2k+1)!!(-\gamma)^k+paA\sum_{k=0}^{\infty}(2k)!(2k+1)!!(-\gamma)^k+paB\sum_{k=0}^{\infty}2k(2k)!(2k+1)!!(-\gamma)^k$$
$$=-paF_0(\gamma)+paA[1-2\gamma(2F_2(\gamma)+F_1(\gamma))]-4paB\gamma[2F_3(\gamma)+F_2(\gamma)]. \qquad \text{(B1)}$$

The expression of the reduced shear viscosity given by Eq. (25) can be obtained by comparing Eqs. (23) and (B1) and by taking into account the relation (A15) between A and B and Eq. (15).

To evaluate the y component of the heat flux required for the determination of the thermal conductivity, we consider similar arguments as those used in Ref. 11 for the BGK solution. Rather than a direct integration we take into account that the hydrodynamic fields (16)–(18) are exact solutions of the hydrodynamic equations (8)–(10) in the steady Couette flow. As a consequence, the momentum and heat fluxes must necessarily be of the form given by Eqs. (23) and (24), respectively. By insertion of these forms into the conservation equation of the energy (10), one arrives at the expression (26) for the reduced thermal conductivity $\Phi(a)$. It must be emphasized that the fact that the functions (a^2/γ), $\Psi(a)$, and $\Phi(a)$ are independent functions of the ratio ζ/ν is a direct consequence of the consistency of the solution.

Finally, the normal components of the pressure tensor can be evaluated in a similar way. They are given by

$$P_{yy}=\int d\mathbf{v}\; mv_y^2f$$
$$=m\sum_{k=0}^{\infty}\left(\frac{\partial}{\partial s}\right)^{2k}(2k+1)!!n(k_BT/m)^{k+1}-mB\times\sum_{k=0}^{\infty}\left(\frac{\partial}{\partial s}\right)^{2k+1}(k+1)\times(2k+3)!!n(k_BT/m)^{k+2}\frac{\partial}{\partial s}\ln T$$
$$=p[1+2(\gamma-1)(B-1)(F_1(\gamma)+2F_2(\gamma))], \qquad \text{(B2)}$$

$$P_{zz}=\int d\mathbf{v}\; mv_z^2f$$
$$=p+m\sum_{k=1}^{\infty}\left(\frac{\partial}{\partial s}\right)^{2k}(2k-1)!!n(k_BT/m)^{k+1}-mB\times\sum_{k=0}^{\infty}\left(\frac{\partial}{\partial s}\right)^{2k+1}(k+1)\times(2k+1)!!n(k_BT/m)^{k+2}\frac{\partial}{\partial s}\ln T$$
$$=p[1+2\gamma(B-1)F_1(\gamma)], \qquad \text{(B3)}$$

$$P_{xx}=3p-P_{yy}-P_{zz}$$
$$=p[1-4\gamma(B-1)(F_1(\gamma)+F_2(\gamma))]. \qquad \text{(B4)}$$

From these expressions one gets the corresponding expressions for the viscometric functions given by Eqs. (29) and (30).

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