Heat transport in a dilute gas under uniform shear flow

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Energy transport in a dilute gas under a steady shear flow state is analyzed. The physical situation is such that a linear profile of the flow velocity coexists with a weak thermal gradient. The shear rate is arbitrary so that the heat flux is affected by the presence of the shear flow. The results are obtained from the Boltzmann equation for Maxwell molecules. By performing an expansion around the shear flow state, an explicit expression for the shear-rate-dependent thermal conductivity tensor is derived. A comparison with previous results obtained from the Bhatnagar-Gross-Krook kinetic model is carried out.

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I. INTRODUCTION

The theory of linear nonequilibrium thermodynamics establishes that fluxes and forces of different tensorial rank cannot be coupled [1]. In particular, in a physical problem where a fluid is simultaneously subjected to both weak velocity and temperature gradients, the heat flux (vector quantity) is not affected by the presence of the velocity gradient (second-rank tensorial quantity). Consequently, the thermal conductivity coefficient is independent of the strain rate. Beyond the linear regime, this assumption is no longer valid and the energy transport may be disturbed, for instance, by shearing motion.

In order to capture the essential aspects of such a nonlinear problem, a dilute gas with short-range interactions can be chosen as a prototype system. Further, we adopt a kinetic description according to which the state of the system is characterized by the one-particle velocity distribution function. This function obeys the well-known Boltzmann equation [2]. Nevertheless, due to the intricacy of its collision term, only a few solutions are known for spatially inhomogeneous situations far from equilibrium. Perhaps, the so-called uniform shear flow [3] is the most physically relevant solution since rheological properties such as nonlinear shear viscosity and viscometric functions can be exactly computed for all values of the shear rate. This solution is restricted to the particular case of Maxwell molecules, namely, particles interacting via a repulsive potential $\varphi(r) = \phi r^{-4}$.

The aim of this paper is to study a linear energy transport problem in a dilute gas under steady uniform shear flow. As the system is strongly sheared, the heat flux can be modified by the presence of the shear flow. In the limit of small temperature gradients (but arbitrary shear rates), one expects that the heat flux verifies a generalized Fourier law where a shear-rate-dependent thermal conductivity tensor can be identified. Our goal is to get the explicit expression of this tensor in the special case of Maxwell molecules. The search for such expression has been prompted by recent results [4] derived from the Bhatnagar-Gross-Krook (BGK) kinetic model of the Boltzmann equation. According to the results obtained from this model, the thermal conductivity tensor happens to be a highly nonlinear function of the shear rate and its expression is not restricted to any particular interaction potential. The derivation of an *exact* expression for the thermal conductivity also allows us to test the relevance of the results previously derived from the BGK approximation.

In the context of dense gases, Evans [5] has obtained a Green-Kubo formula for the thermal conductivity in fluids subjected to shear flow. In the same way as in the equilibrium description, the thermal conductivity of a shearing steady state is related to fluctuations in steady state heat flux. This formula has been subsequently used to analyze the dependence of the thermal conductivity on the shear rate in a Lennard-Jones fluid by means of computer simulations [6].

The paper is organized as follows. In Sec. II we provide a brief account of uniform shear flow at the level of the Boltzmann equation. The particular case of Maxwell molecules allows one to obtain the velocity moments as functions of the shear rate. Here we consider the first nontrivial moments in the steady state: the second-degree moments, which are directly related to hydrodynamic quantities, and the fourth-degree moments, whose knowledge is necessary to evaluate the heat flux under shear flow. In Sec. III we get the thermal conductivity tensor from a perturbation expansion around the uniform shear flow state. Finally, in Sec. IV the results are discussed and compared with previous works.

II. UNIFORM SHEAR FLOW

From a macroscopic point of view, the uniform shear flow is characterized by constant density n and temperature T and a linear velocity field given by

$$u_i = a_{ij} r_j \ , a_{ij} = a\delta_{ix}\delta_{jy} \ , \qquad (1)$$

where a is the constant shear rate. The shear flow produces viscous heating so that the temperature increases

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monotonically. From a simulation point of view, it is desirable to measure the rheological properties in a steady state. For this reason, a nonconservative external force is included to remove this heating effect. Usually the force is taken to be of the Gaussian form [7]

$$\mathcal{F} = -m\alpha\mathbf{V} \ , \tag{2}$$

where m is the mass of a particle and $\mathbf{V} = \mathbf{v} - \mathbf{u}$ is the peculiar velocity. In our description we will choose α as a function of the shear rate a by the condition that the temperature T reaches a constant value in the long time limit (steady state). In this sense, $\mathcal{F}$ plays the role of a thermostat force.

The uniform shear flow state becomes spatially homogeneous when the velocities of particles are referred to a frame moving with the flow velocity $\mathbf{u}(\mathbf{r})$. Therefore, the distribution function adopts the homogeneous form

$$f(\mathbf{r}, \mathbf{v}, t) = g(\mathbf{V}, t) \tag{3}$$

and the nonlinear Boltzmann equation becomes [8]

$$\frac{\partial}{\partial t}g - \frac{\partial}{\partial V_i}(a_{ij}V_j + \alpha V_i)g$$

$$= \int d\mathbf{V}_1 \int d\Omega |\mathbf{V} - \mathbf{V}_1| \sigma(|\mathbf{V} - \mathbf{V}_1|, \theta)(g'g_1' - gg_1)$$

$$\equiv J[g,g] \ . \tag{4}$$

After a transient period, one expects that the solution to Eq. (3) adopts a *normal* form [2] in which all the time dependence of g appears through the time dependence of T. Consequently, and according to the thermostat choice for α, for large t the distribution g is expected to reach a stationary form. This expectation has been recently discussed elsewhere [9].

In the particular case of Maxwell molecules, Eq. (4) can be exactly solved by the moment method. For this interaction the collision rate $V\sigma$ is independent of V, so that a collisional moment of degree k is a bilinear combination of moments of g of degree equal to or smaller than k, the sum of degrees being equal to k. This property of the collison operator allows one to recursively solve the infinite hierarchy of moment equations. To get the shear-rate dependence of the velocity moments, we introduce the dimensionless moments

$$M_{k_1,k_2,k_3} = \frac{1}{n}\left(\frac{m}{2k_BT}\right)^{(k_1+k_2+k_3)/2} \int d\mathbf{V} V_x^{k_1} V_y^{k_2} V_z^{k_3} g \ , \tag{5}$$

where k_B is the Boltzmann constant. According to the symmetry of the uniform shear flow problem, one expects that the only stationary nonvanishing moments correspond to $k_1 + k_2$ and k_3 even [10].

In the long time limit, the first nonzero moments are the second-degree moments. They are related to the pressure tensor

$$P_{ij} = m \int d\mathbf{V} V_i V_j g \ . \tag{6}$$

Taking moments in Eq. (4), the time evolution of the pressure tensor can be obtained. It is easy to show that all the elements of this tensor reach a stationary form for any value of the shear rate [10]. The corresponding nonzero stationary values of the reduced pressure tensor $P_{ij}^* \equiv P_{ij}/p$ are

$$P_{xx}^* = \frac{1+6\alpha^*}{1+2\alpha^*} \ , \tag{7}$$

$$P_{yy}^* = P_{zz}^* = \frac{1}{1+2\alpha^*} \ , \tag{8}$$

$$P_{xy}^* = P_{yx}^* = -\frac{a^*}{(1+2\alpha^*)^2} \ . \tag{9}$$

Here $p = \frac{1}{3}P_{kk} = nk_BT$ is the hydrostatic pressure, $a^* = a/\nu$, and $\alpha^* = \alpha/\nu$, ν being an effective collision frequency given by

$$\nu = 3nA_2, \tag{10}$$

where the numerical value of A_2 is $A_2 = 1.3703\sqrt{2\phi/m}$ [3]. Equations (7)–(9) provide information on the relevant transport properties of the problem, i.e., the nonlinear shear viscosity and the viscometric functions. The thermostat parameter α^* can be determined consistently from the identity $P_{xx}^* + P_{yy}^* + P_{zz}^* = 3$. This relation leads to the cubic equation

$$3\alpha^*(1+2\alpha^*)^2 = a^{*2} \tag{11}$$

whose real root is

$$\alpha^* = \tfrac{2}{3}\sinh^2[\tfrac{1}{6}\cosh^{-1}(1+9a^{*2})] \ . \tag{12}$$

It is interesting to remark that all these results are the same as those derived from the BGK model [11]. Beyond the second-degree moments, it has been recently shown that the Boltzmann and BGK equations yield quite different results [12].

As the third-degree moments decay to zero in the long-time limit [12], the next nontrivial moments in the uniform shear flow problem are the fourth-degree moments. The explicit knowledge of these moments is necessary to get the shear-rate dependence of the thermal conductivity [4]. There are in principle nine independent fourth-degree moments that do not vanish in the steady state. Nevertheless, the symmetry of this problem restricts the number of relevant moments to eight. As the set of dimensionless moments, we take

$$\{M_{400}, M_{040}, M_{220}, M_{202}, M_{022}, M_{310}, M_{130}, M_{112}\}. \tag{13}$$

Recently, explicit expressions for the set (13) as functions of the shear rate have been derived [10]. It has been shown that a strict limitation on the shear rate appears in the stationary solution to the fourth-degree moments. Specifically, if the shear rate is larger than a certain critical value a_c, the fourth-degree moments do not reach stationary values in the long time limit. Possible implications of this singular behavior have been discussed in Ref. [9]. For shear rates smaller than $a_c^* \simeq 6.845$, one may obtain the steady-state values of these moments. Their explicit forms as functions of the shear rate are given in the Appendix.

Anyway, since the numerical value of a_c is rather large, nonlinear shearing effects will still be significant for $a^* < a_c^*$. In particular, the heat flux must be noticeably affected by the action of the shear flow. The examination of this point is the objective of the next section.

III. LINEAR ENERGY TRANSPORT UNDER SHEAR FLOW

The phenomenological Fourier law establishes a linear relation between the heat flux and the temperature gradient through the thermal conductivity coefficient κ. This law is expected to hold in the limit of small temperature gradients. In the case of a dilute gas, the Chapman-Enskog method [13] provides microscopic expressions for the Navier-Stokes transport coefficients. In particular, the thermal conductivity coefficient for Maxwell molecules is given by

$$\kappa = \frac{15}{4}\frac{pk_B}{m\nu} , \tag{14}$$

where ν is defined by Eq. (10).

The problem we want to address is that of energy transport in a dilute gas that is far from equilibrium. In order to gain some insight into this rather general question, we will consider specifically linear heat transport under uniform shear flow. In this situation, the shear rate is arbitrary and the heat flux may be disturbed by the shearing motion. For small temperature gradients, one expects that the heat flux obeys a generalized Fourier law where, due to the anisotropy of the problem, a thermal conductivity tensor rather than a scalar can be identified. This tensor must be a nonlinear function of the shear rate. The derivation of such an expression for the so-called linear thermal conductivity tensor is the objective of this section.

Let us consider a dilute gas of Maxwell molecules in a stationary shear flow state. We assume that we perturb this state by introducing a weak thermal gradient. The thermal gradient induces a density gradient so that n and T are now inhomogeneous. Here, to parallel the results derived from the BGK model [4], we assume that both gradients are coupled to keep the pressure p constant. Under these conditions, the Boltzmann equation can be written as [8]

$$\frac{\partial}{\partial t}f - \frac{\partial}{\partial V_i}\left(a_{ij}V_j - \frac{F_i}{m}\right)f + (V_i + a_{ij}r_j)\frac{\partial}{\partial r_i}f = J[f,f] , \tag{15}$$

where $\mathbf{F}$ is the total external force acting on each particle. This force is introduced in the system to achieve a steady state. In the absence of thermal gradient, $\mathbf{F}$ is given by the conventional thermostat force (2) used in computer simulations. Nevertheless, when ∇T is not zero, additional external forces must be considered.

In order to get the velocity moments of the velocity distribution function f, we shall use a perturbation expansion around the steady shear flow state g by taking the temperature gradient as the perturbation parameter. The main feature of this scheme is that the different approximations to f retain all the hydrodynamic orders in the shear rate. Therefore, we write

$$f = f^{(0)} + f^{(1)} + \cdots , \tag{16}$$

where $f^{(k)}$ is of order k in ∇T but preserves the full nonlinear dependence on the shear rate. The zeroth-order approximation $f^{(0)}$ corresponds to the uniform shear flow state but taking into account the local dependence of g through the density and temperature. In this paper we will restrict ourselves to first order in the expansion. Consequently, at this level of approximation, the external force can be written as

$$\mathbf{F} = -m\alpha\mathbf{V} + \mathbf{F}^{(1)} , \tag{17}$$

$\mathbf{F}^{(1)}$ being determined from the corresponding balance equations. Assuming that the system reaches a steady state after a transient period, the distribution $f^{(1)}$ verifies the equation

$$-\frac{\partial}{\partial V_i}(\alpha V_i + a_{ij}V_j)f^{(1)} + (V_i + a_{ij}r_j)\frac{\partial}{\partial r_i}f^{(0)} + \frac{\partial}{\partial V_i}\frac{F_i^{(1)}}{m}f^{(0)} = J[f^{(1)},f^{(0)}] + J[f^{(0)},f^{(1)}] , \tag{18}$$

where use has been made of Eq. (4) in the long time limit. It is clear that our description is only valid *a priori* for the range of shear rates below the critical value a_c, in which case the moments (13) reach steady values.

The mass balance equation associated with Eq. (18) implies that $\mathbf{u}\cdot\nabla n = 0$ and consequently $\mathbf{u}\cdot\nabla T = 0$. This means that the thermal gradient must be orthogonal to the direction of the flow velocity. On the other hand, from the momentum balance equation of Eq. (18) it is easy to show that the simplest choice for $\mathbf{F}^{(1)}$ is a constant [4]:

$$F_i^{(1)} = k_B T\frac{\partial}{\partial r_j}P_{ij}^{*(0)} = k_B T\frac{\partial}{\partial T}P_{ij}^{*(0)}\frac{\partial}{\partial r_j}T . \tag{19}$$

Here the nonvanishing elements of $P_{ij}^{*(0)}$ are given by Eqs. (7)–(9) and the operator $T\partial/\partial T$ for Maxwell molecules reads

$$T\frac{\partial}{\partial T} = 2\alpha^*\frac{1+2\alpha^*}{1+6\alpha^*}\frac{\partial}{\partial\alpha^*} + a^*\frac{\partial}{\partial a^*} , \tag{20}$$

when one takes α^* and a^* as independent parameters. The expression of $\mathbf{F}^{(1)}$ is the same as the one obtained from the BGK model [4]. This additional external force (absent in the pure shear flow problem) has not been considered in the computer simulations performed in dense gases [6]. In the absence of $\mathbf{F}^{(1)}$ the stationary velocity field is perturbed by the thermal gradient so that a steady state does not exist. This is an important difference with respect to previous analyses [5,6]. The external force $\mathbf{F}^{(1)}$ exhibits the anisotropy originated in the system by the presence of the shear flow. For small shear rates, their components behave as

$$F_x^{(1)} \approx -k_B \left(1 - 4a^{*2} + \frac{140}{9}a^{*4} - \frac{1072}{27}a^{*6}\right) a^* \frac{\partial T}{\partial y} , \tag{21}$$

$$F_y^{(1)} \approx -\frac{4}{3}k_B \left(1 - 4a^{*2} + \frac{92}{9}a^{*4}\right) a^{*2} \frac{\partial T}{\partial y} , \tag{22}$$

$$F_z^{(1)} \approx -\frac{4}{3}k_B \left(1 - 4a^{*2} + \frac{92}{9}a^{*4}\right) a^{*2} \frac{\partial T}{\partial z} . \tag{23}$$

We are interested in computing the heat flux $\mathbf{q}^{(1)}$ across the system. It is defined by

$$\mathbf{q}^{(1)} = \frac{m}{2} \int d\mathbf{V} V^2 \mathbf{V} f^{(1)}. \tag{24}$$

The heat flux is related to the third-degree moments of the distribution $f^{(1)}$. There are ten independent moments. For computational purposes, we choose the following dimensionless moments [3]:

$$N_{2|i} = \frac{1}{n}\left(\frac{m}{2k_BT}\right)^{3/2} \int d\mathbf{V} Y_{2|i}(\mathbf{V}) f^{(1)} , \tag{25}$$

$$N_{0|ijk} = \frac{1}{n}\left(\frac{m}{2k_BT}\right)^{3/2} \int d\mathbf{V} Y_{0|ijk}(\mathbf{V}) f^{(1)} , \tag{26}$$

where

$$Y_{2|i}(\mathbf{V}) = V^2 V_i , \tag{27}$$

$$Y_{0|ijk}(\mathbf{V}) = V_i V_j V_k - \frac{1}{5}V^2(V_i\delta_{jk} + V_j\delta_{ik} + V_k\delta_{ij}). \tag{28}$$

At this level of approximation, one needs to know their corresponding collisional moments. They are given by [3]

$$\frac{1}{n}\left(\frac{m}{2k_BT}\right)^{3/2} \int d\mathbf{V} Y_{2|i}(\mathbf{V}) \big(J[f^{(1)}, f^{(0)}] + J[f^{(0)}, f^{(1)}]\big) = -\frac{2}{3}\nu N_{2|i} , \tag{29}$$

$$\frac{1}{n}\left(\frac{m}{2k_BT}\right)^{3/2} \int d\mathbf{V} Y_{0|ijk}(\mathbf{V}) \big(J[f^{(1)}, f^{(0)}] + J[f^{(0)}, f^{(1)}]\big) = -\frac{3}{2}\nu N_{0|ijk} . \tag{30}$$

We consider the following set of ten independent moments:

$$\{N_{2|x}, N_{2|y}, N_{2|z}, N_{0|xxy}, N_{0|xxz}, N_{0|xyy}, N_{0|yyz}, N_{0|xzz}, N_{0|yzz}, N_{0|xyz}\}. \tag{31}$$

Taking moments in Eq. (18), one gets a set of ten coupled algebraic equations for the third-degree moments (31). By using matrix notation, it can be written as

$$\mathcal{A}_{\sigma\sigma'}\mathcal{N}_{\sigma'} = \mathcal{B}_\sigma \epsilon_y + \mathcal{C}_\sigma \epsilon_z , \quad \sigma = 1, \ldots, 10. \tag{32}$$

Here $\mathcal{N}$ is the column matrix defined by the set (31), $\mathcal{A}$ is the matrix given by

$$\mathcal{A} = \begin{pmatrix}
c_1 & \frac{7}{5}a^* & 0 & 2a^* & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{2}{5}a^* & c_1 & 0 & 0 & 0 & 2a^* & 0 & 0 & 0 & 0 \\
0 & 0 & c_1 & 0 & 0 & 0 & 0 & 0 & 0 & 2a^* \\
\frac{8}{25}a^* & 0 & 0 & c_2 & 0 & \frac{8}{5}a^* & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & c_2 & 0 & 0 & 0 & 0 & \frac{8}{5}a^* \\
0 & \frac{8}{25}a^* & 0 & -\frac{7}{5}a^* & 0 & c_2 & 0 & 0 & -a^* & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & c_2 & 0 & 0 & -\frac{2}{5}a^* \\
0 & -\frac{2}{25}a^* & 0 & -\frac{2}{5}a^* & 0 & 0 & 0 & c_2 & a^* & 0 \\
-\frac{2}{25}a^* & 0 & 0 & 0 & 0 & -\frac{2}{5}a^* & 0 & 0 & c_2 & 0 \\
0 & 0 & \frac{1}{5}a^* & 0 & 0 & 0 & a^* & 0 & 0 & c_2
\end{pmatrix} , \tag{33}$$

where $c_1 \equiv \frac{2}{3} + 3\alpha^*$ and $c_2 \equiv \frac{3}{2} + 3\alpha^*$, and $\epsilon = \frac{1}{\nu}(2k_BT/m)^{1/2}\nabla \ln T$ is the reduced thermal gradient. The column matrix $\mathcal{B}$ is

$$\mathcal{B} = \begin{pmatrix} R_{102} + R_{120} + R_{300} \\ R_{012} + R_{030} + R_{210} \\ R_{003} + R_{021} + R_{201} \\ \frac{1}{5}(4R_{210} - R_{012} - R_{030}) \\ \frac{1}{5}(4R_{201} - R_{003} - R_{021}) \\ \frac{1}{5}(4R_{120} - R_{102} - R_{300}) \\ \frac{1}{5}(4R_{021} - R_{003} - R_{201}) \\ \frac{1}{5}(4R_{102} - R_{120} - R_{300}) \\ \frac{1}{5}(4R_{012} - R_{030} - R_{210}) \\ R_{111} \end{pmatrix} . \tag{34}$$

with

$$R_{k_1,k_2,k_3} = -\left[\frac{1}{2}(k_1+k_2+k_3-1) + T\frac{\partial}{\partial T}\right] M^{(0)}_{k_1,k_2+1,k_3} + \frac{1}{2}\left[k_1 M^{(0)}_{k_1-1,k_2,k_3} T\frac{\partial}{\partial T}P^{*(0)}_{xy} + k_2 M^{(0)}_{k_1,k_2-1,k_3} T\frac{\partial}{\partial T}P^{*(0)}_{yy}\right] , \tag{35}$$

while the column matrix $\mathcal{C}$ is given by an expression similar to Eq. (34), but with R_{k_1,k_2,k_3} replaced by

$$S_{k_1,k_2,k_3} = -\left[\frac{1}{2}(k_1+k_2+k_3-1) + T\frac{\partial}{\partial T}\right] M^{(0)}_{k_1,k_2,k_3+1} + \frac{1}{2}k_3 M^{(0)}_{k_1,k_2,k_3-1} T\frac{\partial}{\partial T}P^{*(0)}_{zz} , \tag{36}$$

where the elements of $P^{*(0)}_{ij}$ are given by Eqs. (7)–(9) and $M^{(0)}_{k_1,k_2,k_3}$ refers to the fourth-degree moments of g. The right-hand side of the matrix equation (32) also holds for the BGK model equation, although the explicit shear-rate dependence of the fourth-degree moments clearly differs from the Boltzmann ones [12].

The solution to Eq. (32) is

$$\mathcal{N}_\sigma = (\mathcal{A}^{-1})_{\sigma\sigma'}\left(\mathcal{B}_{\sigma'}\epsilon_y + \mathcal{C}_{\sigma'}\epsilon_z\right) . \tag{37}$$

This relation provides an explicit expression for the third-degree moments of the velocity distribution $f^{(1)}$ as functions of the shear rate and the thermal gradient. The heat flux across the system is determined from the first three terms of $\mathcal{N}_\sigma$. According to these expressions, it is easy to show that the heat flux can be cast into the form of a generalized Fourier law

$$q_i^{(1)} = -\kappa\lambda_{ij}(a^*)\frac{\partial T}{\partial r_j} \tag{38}$$

or, equivalently,

$$N_{2|i} = -\frac{15}{8}\lambda_{ij}(a^*)\epsilon_j , \tag{39}$$

where λ_{ij} is the reduced thermal conductivity tensor, which depends on the shear rate. Its nonzero relevant components can be identified from the explicit form of the moments $N_{2|i}$. In terms of the matrices $\mathcal{B}$ and $\mathcal{C}$, and taking into account the symmetry of $M^{(0)}_{k_1,k_2,k_3}$, the above moments can be written as

$$N_{2|x} = \frac{1}{27\alpha^{*2}+46\alpha^*+12}\left[\frac{3}{5}(216\alpha^{*2}+151\alpha^*+30)\mathcal{B}_1 - \frac{27}{5}(24\alpha^*+7)a^*\mathcal{B}_2 + 4\frac{108\alpha^{*2}+23\alpha^*-6}{1+2\alpha^*}a^*\mathcal{B}_4 + 12(54\alpha^*+19)\alpha^*\mathcal{B}_6 + 8\frac{54\alpha^*+19}{1+2\alpha^*}\alpha^* a^*\mathcal{B}_9\right]\epsilon_y, \tag{40}$$

$$N_{2|y} = \frac{1}{27\alpha^{*2}+46\alpha^*+12}\left[-\frac{54}{5}a^*\mathcal{B}_1 + \frac{3}{5}(216\alpha^{*2}+151\alpha^*+30)\mathcal{B}_2 - 24\alpha^*(1+9\alpha^*)\mathcal{B}_4 - 12\frac{9\alpha^*+2}{1+2\alpha^*}a^*\mathcal{B}_6 - 24\alpha^*(9\alpha^*+2)\mathcal{B}_9\right]\epsilon_y, \tag{41}$$

$$N_{2|z} = \frac{1}{23\alpha^*+6}\left[\frac{3}{5}(8\alpha^*+15)\mathcal{C}_3 + 24\alpha^*\mathcal{C}_7 - 12\frac{a^*}{1+2\alpha^*}\mathcal{C}_{10}\right]\epsilon_z. \tag{42}$$

Equations (40)–(42) represent the major result of this paper. They give the explicit expression of the thermal conductivity tensor of a dilute gas of Maxwell molecules under strong shear rates. The components of this tensor provide all the information on the physical mechanisms involved in the energy transport under shear flow.

In the absence of shear field ($a^* = 0$), $N_{2|x} = 0$ and $N_{2|y}/\epsilon_y = N_{2|z}/\epsilon_z = -15/8$, so that $\lambda_{ij} = \delta_{ij}$ and thus one recovers the conventional expression of the thermal conductivity coefficient κ given by the Chapman-Enskog method [13]. Furthermore, according to Eqs. (40)–(42), $\lambda_{xz} = \lambda_{yz} = \lambda_{zy} = 0$, in agreement with the symmetry of the problem. For small shear rates, the behaviors of the nonzero components of the thermal conductivity tensor are $\lambda_{yy} \approx 1 + 3.04a^{*2}$, $\lambda_{zz} \approx 1 - 1.18a^{*2}$, and $\lambda_{xy} \approx -3.90a^*$. The general shear-rate dependence of these components is plotted in Figs. 1–3 for $0 \le a^* \le 1$. In this region the shear thinning is quite important. For $a^* \approx 1$, for example, the shear viscosity is about 46% smaller than its limiting zero shear rate value. We also present the results obtained from the BGK equation. Figure 1 shows that λ_{yy} increases with a^* in the region of shear rates considered. Consequently, the shear flow enhances the transport of energy along the direction of the gradient of the flow velocity (y axis). This conclusion contrasts with the results derived from the BGK model [4], where λ_{yy} decreases as a^* increases, except for very small shear rates. The shear-rate dependence of the diagonal component λ_{zz} is shown in Fig. 2. It always decreases as a^* increases, so that the effect of

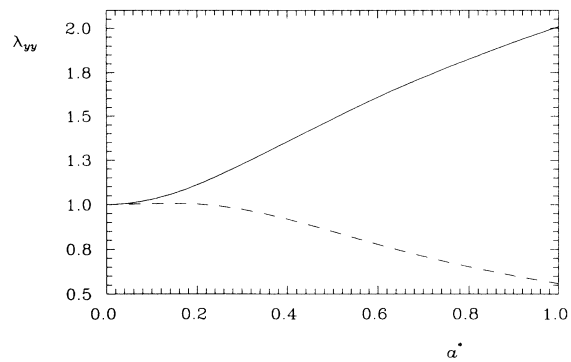

FIG. 1. Shear-rate dependence of λ_{yy} for Maxwell molecules. The solid line corresponds to the Boltzmann equation and the dashed line refers to the BGK model.

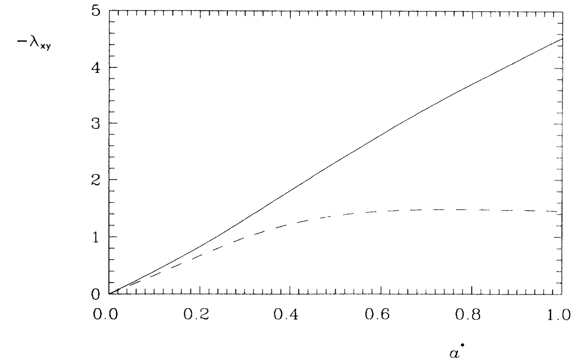

FIG. 3. Same as in Fig. 1, but for $-\lambda_{xy}$.

the shear flow on the heat flux is to inhibit the energy transport along the direction orthogonal to the velocity gradient. This effect is also predicted by the BGK approximation. Further, the BGK model gives a larger deviation from equilibrium for λ_{zz} than the exact Boltzmann value. Anyway, the influence of the shear rate on the zz component is less sensitive than the one observed for the yy component. This may be due to the anisotropy created in the system by the presence of the shear flow. The off-diagonal component λ_{xy} measures cross effects in the thermal conduction. It gives the transport of energy along the x axis due to a thermal gradient parallel to the y axis. This cross coupling does not appear in the linear regime since the heat flux $q_x^{(1)}$ is at least of Burnett order (proportional to $a^*\epsilon_y$). The absolute value of λ_{xy} is plotted in Fig. 3. This component is negative and its absolute value increases with increasing the shear rate. In the region considered, $-\lambda_{xy}$ behaves practically as a linear function of the shear rate. The BGK model underestimates the exact absolute value of λ_{xy}.

The comparison carried out between the Boltzmann and BGK equations for Maxwell molecules at the level of the thermal conductivity tensor indicates that the BGK predictions cannot be considered as reliable, especially at finite shear rates. This is a direct consequence of the different behavior of the fourth-degree moments in the pure shear flow state [12]. In fact, the discrepancies observed here for λ_{ij} are comparable to those observed in Ref. [12] for the fourth-degree moments. In this sense, and for the uniform shear flow state, the BGK model can be used as a good approximation of the Boltzmann equation when one considers the lower-degree moments (related to rheological properties), although it becomes less credible as the degree of the moments increases. A direct consequence of this conclusion is that the BGK distribution does not reproduce well the behavior of the high-velocity population.

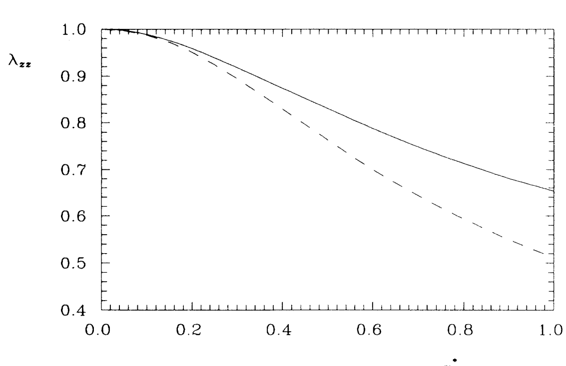

FIG. 2. Same as in Fig. 1, but for λ_{zz}.

IV. DISCUSSION

A linear energy transport problem in a dilute gas under steady uniform shear flow has been analyzed. The system is in a steady inhomogeneous state macroscopically characterized by a constant pressure, a nonuniform temperature, and a flow velocity along the x direction with a constant gradient along the y direction. Since we want to evaluate transport properties in a steady state, external forces are also introduced to control viscous heating. The system is driven out of equilibrium by the action of the shear field as well as the thermal gradient. We are mainly interested in the physical situation where a weak thermal gradient simultaneously coexists with a strong shear flow. Under these conditions, the shear rate *modifies* (but does not create) the heat transport across the system. In a previous paper [4] we used the BGK model kinetic equation to analyze such coupling and found that the energy transport was noticeably disturbed by the presence of the shear flow. Nevertheless, as the BGK equation is a simplified version of the nonlinear Boltzmann equation, no definitive conclusions about the shear-rate dependence of the heat flux were obtained. For this reason the description has now been done from the exact Boltzmann equation in the special case of Maxwell molecules, so that our results are *exact* to all orders in the shear rate.

By assuming that the temperature gradient is weak, a perturbation expansion around the uniform shear flow state with arbitrary shear rate has been carried out. As a consequence, all the different approximations are nonlinear functions of the shear rate. In the case of Maxwell molecules, the hierarchy of moment equations of the Boltzmann equation can be in principle recursively solved at each stage of approximation. Here we have restricted ourselves to the first order in ∇T. At this level of description, the components of the heat flux $\mathbf{q}^{(1)}$ can be expressed as linear functions of the temperature gradient (Fourier's law). Due to the anisotropy of the problem, this law defines the so-called linear thermal conductivity tensor λ_{ij} whose shear rate dependence we aimed at determining. The symmetry of the problem implies that $\lambda_{xz} = \lambda_{yz} = \lambda_{zy} = 0$ while no information for λ_{xx}, λ_{yx}, and λ_{zx} components can be obtained as the thermal gradient must be necessarily orthogonal to the direction of the flow velocity (x axis) to preserve the stationarity of the state. Therefore, the components λ_{xy}, λ_{yy}, and λ_{zz} are the relevant transport coefficients of the problem.

The knowledge of the fourth-degree moments of the distribution function in the pure shear flow state [10] enables one to get an explicit expression for the thermal conductivity tensor. While the diagonal components λ_{yy} and λ_{zz} are even functions of the shear rate, λ_{xy} is an odd function. In general, they exhibit a highly nonlinear dependence on the shear rate. The diagonal components can be interpreted as generalizations of the usual thermal conductivity coefficient since they *conjugate* the ith component of the heat flux vector with the ith component of the temperature gradient. Cross couplings are taken into account through the off-diagonal component, which is a generalization of a nonlinear Burnett coefficient. In the limit of small shear rates, $\lambda_{yy} = \lambda_{zz} \approx 1$ and $\lambda_{xy} \approx -3.90a^*$. From a physical point of view, one expects that the presence of the shear flow does not change the qualitative behavior of the heat flux in the sense that $\lambda_{yy} > 0$, $\lambda_{zz} > 0$, and $\lambda_{xy} < 0$. Otherwise, if there were a critical shear rate for which the diagonal components became negative, the heat would be transferred from the cold wall to the hot wall and an instability would be generated in the system. The results presented in this paper confirm that the transport coefficients maintain the same sign as the shear rate increases. These predictions agree with results obtained in computer simulations [6]. With respect to the quantitative dependence of the thermal conductivity on the shear rate, we observe that the net consequence of the action of the shear flow on the heat transport is to produce an enhancement of the energy transport along the y direction and an inhibition along the z direction. In the case of the x direction, $-\lambda_{xy}$ increases as a^* increases. All these results clearly show that heat conduction under shear flow is a very complex problem due basically to the anisotropy induced by the shear field.

Recently, Daivis and Evans [6] performed computer simulations in a strongly shearing Lennard-Jones fluid to compute the shear-rate-dependent thermal conductivity tensor. Although the Lennard-Jones fluid has an attractive tail (absent in Maxwell molecules), to our knowledge this is the only system for which heat transport under shear flow has been studied. In general, their conclusions agree qualitatively well with our predictions. Nevertheless, as far as quantitative effects are concerned, they observed an influence of a^* on λ_{ij} less noticeable than the one obtained here, especially in the case of the diagonal components. For instance, Daivis and Evans [6] state that the diagonal components are independent of the shear rate up to a certain (finite) value of a^*. Perhaps these quantitative discrepancies are due to the fact that the shear rates considered in the simulation are not large enough to clearly observe nonlinear effects. In fact, by extrapolating our definition of the collision frequency $\nu = (15/4)(pk_B/m\kappa)$ to dense fluids [14], one can estimate that the range of shear rates in Ref. [6] is much smaller than the one considered here.

Finally, we expect that the results presented in this paper will stimulate the performance of simulations in the low-density limit where larger shear rates are possibly not difficult to achieve. In this context, the Monte Carlo simulation method [15] provides a useful tool to obtain numerical solutions of the Boltzmann equation.

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APPENDIX: EXPRESSIONS OF THE FOURTH-DEGREE MOMENTS

In this appendix we give the explicit expressions of the set of dimensionless moments defined in Eq. (13). They can be written as [10]

$$M_{400} = \frac{3}{4}\frac{1}{(1+2\alpha^*)^2}\frac{A_1(\alpha^*)}{\Delta(\alpha^*)}, \tag{A1}$$

$$M_{040} = \frac{3}{4}\frac{1}{(1+2\alpha^*)^2}\frac{A_2(\alpha^*)}{\Delta(\alpha^*)}, \tag{A2}$$

$$M_{220} = \frac{1}{4}\frac{1}{(1+2\alpha^*)^2}\frac{A_3(\alpha^*)}{\Delta(\alpha^*)}, \tag{A3}$$

$$M_{202} = \frac{1}{4}\frac{1}{(1+2\alpha^*)^2}\frac{A_4(\alpha^*)}{\Delta(\alpha^*)}, \tag{A4}$$

$$M_{022} = \frac{1}{4}\frac{1}{(1+2\alpha^*)^2}\frac{A_5(\alpha^*)}{\Delta(\alpha^*)}, \tag{A5}$$

$$M_{310} = -\frac{3}{4}\frac{a^*}{(1+2\alpha^*)^3}\frac{A_6(\alpha^*)}{\Delta(\alpha^*)}, \tag{A6}$$

$$M_{130} = -\frac{3}{4}\frac{a^*}{(1+2\alpha^*)^3}\frac{A_7(\alpha^*)}{\Delta(\alpha^*)}, \tag{A7}$$

$$M_{112} = -\frac{1}{4}\frac{a^*}{(1+2\alpha^*)^3}\frac{A_8(\alpha^*)}{\Delta(\alpha^*)} , \tag{A8}$$

where

$$\Delta(\alpha^*) = 1 + 18.372\alpha^* + 142.83\alpha^{*2} + 608.68\alpha^{*3} + 1524.1\alpha^{*4} + 2166.5\alpha^{*5} + 1310.1\alpha^{*6} - 625.09\alpha^{*7} - 1433.9\alpha^{*8} - 644.27\alpha^{*9} , \tag{A9}$$

$$A_1(\alpha^*) = 1 + 31.631\alpha^* + 452.08\alpha^{*2} + 3723.5\alpha^{*3} + 19401\alpha^{*4} + 66969\alpha^{*5} + 156525\alpha^{*6} + 249212\alpha^{*7} + 269214\alpha^{*8} + 195371\alpha^{*9} + 92180\alpha^{*10} + 23194\alpha^{*11} , \tag{A10}$$

$$A_2(\alpha^*) = 1 + 19.631\alpha^* + 168.85\alpha^{*2} + 831.27\alpha^{*3} + 2568.6\alpha^{*4} + 5142.3\alpha^{*5} + 6669.6\alpha^{*6} + 5464.5\alpha^{*7} + 2669.8\alpha^{*8} + 644.14\alpha^{*9} - 0.0701\alpha^{*10} - 0.1204\alpha^{*11} , \tag{A11}$$

$$A_3(\alpha^*) = 1 + 32.444\alpha^* + 416.36\alpha^{*2} + 2903.9\alpha^{*3} + 12404\alpha^{*4} + 34191\alpha^{*5} + 62004\alpha^{*6} + 74036\alpha^{*7} + 57759\alpha^{*8} + 28795\alpha^{*9} + 7731.5\alpha^{*10} + 0.0706\alpha^{*11} , \tag{A12}$$

$$A_4(\alpha^*) = 1 + 25.380\alpha^* + 281.36\alpha^{*2} + 1780.5\alpha^{*3} + 7085\alpha^{*4} + 18461\alpha^{*5} + 31913\alpha^{*6} + 36521\alpha^{*7} + 27501\alpha^{*8} + 13436\alpha^{*9} + 3615.1\alpha^{*10} + 0.0305\alpha^{*11} , \tag{A13}$$

$$A_5(\alpha^*) = 1 + 20.548\alpha^* + 199.81\alpha^{*2} + 1226.1\alpha^{*3} + 5259.7\alpha^{*4} + 16291\alpha^{*5} + 36364\alpha^{*6} + 57464\alpha^{*7} + 62824\alpha^{*8} + 46488\alpha^{*9} + 22550\alpha^{*10} + 5964.1\alpha^{*11} , \tag{A14}$$

$$A_6(\alpha^*) = 1 + 26.696\alpha^* + 302.6\alpha^{*2} + 1929.0\alpha^{*3} + 7679.5\alpha^{*4} + 19983\alpha^{*5} + 34554\alpha^{*6} + 39717\alpha^{*7} + 30128\alpha^{*8} + 14719\alpha^{*9} + 3865.6\alpha^{*10} , \tag{A15}$$

$$A_7(\alpha^*) = 1 + 19.449\alpha^* + 164.78\alpha^{*2} + 794.47\alpha^{*3} + 2391\alpha^{*4} + 4647\alpha^{*5} + 5864.6\alpha^{*6} + 4757.7\alpha^{*7} + 2410.2\alpha^{*8} + 644.28\alpha^{*9} - 0.0037\alpha^{*10} , \tag{A16}$$

$$A_8(\alpha^*) = 1 + 19.315\alpha^* + 162.54\alpha^{*2} + 777.86\alpha^{*3} + 2321.1\alpha^{*4} + 4464\alpha^{*5} + 5555\alpha^{*6} + 4413.7\alpha^{*7} + 2169.3\alpha^{*8} + 560.76\alpha^{*9} + 0.0110\alpha^{*10} . \tag{A17}$$

From these expressions the shear-rate dependence of the elements of the matrices $\mathcal{B}_\sigma$ and $\mathcal{C}_\sigma$ can be obtained.

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