Heat flux induced by an external force in a strongly shearing dilute gas

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Coupling between energy and momentum transport in a dilute gas subject to uniform shear flow is analyzed. Heat flux is created in the system by the action of a nonconservative external force. The results are obtained by using the Bhatnagar–Gross–Krook kinetic model. The moments of the velocity distribution function are expressed in terms of a perturbation expansion in powers of the heat field strength, the coefficients being highly nonlinear functions of the shear rate. In particular, the thermal conductivity tensor and the shear viscosity coefficient up to second-order approximation are explicitly evaluated. It is shown that the usual choice of the heat field proposed in computer simulations leads to a thermal conductivity tensor different from the one obtained in the thermal gradient problem, confirming previous results. In order to avoid this discrepancy, an alternative external force is proposed.

I. INTRODUCTION

Thermal conductivity is one of the most difficult transport coefficients to calculate. The appropriate laboratory conditions for measuring this coefficient correspond to a system enclosed between two parallel plates at different temperatures. For small temperature gradients, the Fourier law establishes a linear relation between the heat flux and the thermal gradient through the thermal conductivity coefficient.[1] Nevertheless, from a computational point of view, it is more efficient to evaluate this transport coefficient in a homogeneous state where the heat flux is generated by the action of a *fictitious* external force. This method of simulating heat flux in the absence of temperature gradients was proposed independently by Evans[2] and Gillan and Dixon.[3] The technique relies on the introduction of a *heat* field that mimics the macroscopic effect produced by a thermal gradient in a real experiment. The thermal conductivity coefficient is obtained by extrapolating the ratio between the heat flux and the field strength to zero-field limit. This coefficient agrees well with experimental data and with estimates based on alternative inhomogeneous simulation results.[4]

An interesting physical problem is that of linear energy transport in strong shear flows. In this situation, nonlinear effects are important and the heat flux is disturbed by the shearing motion. The anisotropy induced by the shear flow makes the thermal conductivity coefficient become a shear-rate dependent nonsymmetric tensor. Very recently, we have obtained an explicit expression for the thermal conductivity tensor in a dilute gas under uniform shear flow and subject to a weak thermal gradient.[5] This tensor is a highly nonlinear function of the shear rate and its expression is not restricted to any specific interaction potential. Here, our aim is to analyze a similar problem but when the energy flux is generated by a homogeneous external force. As a consequence, unlike real heat flow, no temperature or density gradients appear in the system. The motivation of this work is twofold. First, the analysis of nonequilibrium states induced by external forces is an interesting problem itself because such situations are desirable for practical purposes, especially in molecular dynamics simulations. Second, one can establish the possible equivalence between the resulting transport properties and those driven by means of realistic boundary conditions.

Due to the intricacy embodied in the Boltzmann collision operator, we use again the Bhatnagar–Gross–Krook (BGK) kinetic equation[6] as a model of the Boltzmann equation. The reliance on the BGK model has been shown in the uniform shear flow problem since it leads to moment equations similar to those derived from the exact Boltzmann equation.[7] In this paper, we construct a perturbation solution of the BGK model around the uniform shear flow state by taking the field strength as the perturbation parameter. All the moments of the velocity distribution function are computed. They are nonlinear functions of the shear rate and depend on the external field considered. In particular, we focus on the explicit derivation of the linear thermal conductivity tensor (up to first-order approximation) and the shear viscosity coefficient (up to second order). They are the most relevant transport coefficients of the problem.

In absence of shear flow, the thermal conductivity coefficient obtained from the conventional Evans–Gillan[2,3] method coincides with the one calculated in the presence of a temperature gradient. However, for finite shear rate, we show that both methods lead to different expressions for the thermal conductivity tensor. This confirms the predictions made by Evans *et al.*[8] on the modified Green–Kubo relations for mechanical transport coefficients. Thus, from a practical point of view, the usual choice of the external field used in the Evans–Gillan algorithm cannot be considered as adequate to compute the energy transport under strong shear fields. A similar problem happened in the color field method.[9] In order to avoid the above discrepancy, a modified shear-rate dependent external field is proposed. Comparison between the transport coefficients obtained from the conventional heat field method[2,3] and those derived using this new force is one of the main objectives of this paper.

The organization of the paper is as follows. The physical problem is described in Sec. II. In Sec. III we obtain the successive approximations to the velocity moments in terms of the external force considered. Section IV deals with the explicit calculation of the heat transport. By taking into account the analogies with the usual thermal gradient problem,

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a thermal conductivity tensor is identified. From this expression, the modified external force is obtained. In Sec. V we study the behavior of the shear viscosity coefficient as a function of the heat field up to second-order approximation. Finally, Sec. VI offers a brief discussion of the results.

II. DESCRIPTION OF THE PROBLEM

Let us consider a monatomic dilute gas in a steady uniform shear flow state. This nonequilibrium state is characterized by a linear velocity profile and constant density and temperature[10,11]

$$u_i = a_{ij} r_j, \quad a_{ij} = \delta_{ix}\delta_{jy}, \tag{1}$$

$$n = \text{const.}, \tag{2}$$

$$T = \text{const.}, \tag{3}$$

where a is the constant shear rate. The number density n, the flow velocity $\mathbf{u}$, and the temperature T are defined as moments of the velocity distribution function f as follows:

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

$$n\mathbf{u} = \int d\mathbf{v}\, \mathbf{v} f, \tag{5}$$

$$nk_B T = \tfrac{1}{3}\int d\mathbf{v}\, m\mathbf{V}^2 f. \tag{6}$$

Here, k_B is the Boltzmann constant, m is the mass of a particle and $\mathbf{V} \equiv \mathbf{v} - \mathbf{u}$ is the peculiar velocity. The shearing motion produces viscous heating, so that the temperature tends to increase in time. In order to maintain a steady state, an external drag force must be introduced

$$\mathbf{F} = -\alpha \mathbf{V}, \tag{7}$$

where the thermostat parameter α must be adjusted by consistency. In the uniform shear flow state, the distribution function becomes homogeneous under the change $\mathbf{v} \to \mathbf{V}$, i.e., $f(\mathbf{r},\mathbf{v}) \to f(\mathbf{V})$.[11] Due to this fact, this state has been extensively studied theoretically[7,11] as well as from molecular dynamics simulations.[10]

Since the Boltzmann equation is too difficult to solve far from equilibrium states, we start here from the kinetic model proposed by Bhatnagar, Gross, and Krook (BGK).[6] In this model the Boltzmann collision term is substituted by a single-time relaxation towards the local equilibrium distribution. All the details of the interaction potential are introduced in an effective way through a collision frequency ν, which in general depends on space and time through n and T. In spite of its simplicity, the BGK model yields equivalent results to the ones given by the Boltzmann equation in several nonequilibrium problems. In the case of uniform shear flow, the shear viscosity and the viscometric functions obtained from the BGK equation are the same as those derived from the exact Boltzmann equation for Maxwell molecules if one chooses ν to be a particular eigenvalue of the Boltzmann operator.[7,11] Furthermore, the BGK results present a good agreement with Monte Carlo simulations of the Boltzmann equation in the case of the hard sphere interaction.[12]

We are interested in studying heat transport in a steady shear flow state. According to Curie's principle,[1] in the linear regime, the heat flux cannot be affected by the shear field. Nevertheless, beyond the linear limit, the above principle breaks down and the shear field modifies (but does not generate) the energy transport. In this problem a thermal conductivity tensor rather than a scalar can be identified. Previous studies have dealt with this problem. In the context of dense gases, Evans[13] has obtained a Green–Kubo formula for the thermal conductivity of a strongly shearing fluid. Recently, this formula has been used to compute the linear thermal conductivity by computer simulations.[14] In the low density limit, an explicit expression for the shear-rate dependent thermal conductivity tensor has been found.[5] The results have been derived from the BGK kinetic model and depend on the potential model considered.

The aim of this paper is to analyze energy transport produced by an external force in a dilute gas under uniform shear flow. In the heat field problem, "heat current" is created by the action of an external force in the absence of a temperature gradient. The ratio between the heat current and the field strength in the limit of zero-field strength defines the relevant transport coefficient of the problem. For vanishing shear rate, this coefficient coincides with the usual thermal conductivity coefficient measured in a system in the presence of a thermal gradient. This equivalence allows one to get the thermal conductivity coefficient from the conventional heat field method proposed by Evans–Gillan.[2,3] However, in the non-Newtonian regime, one expects that the heat field exhibits the anisotropy induced in the system by the presence of the shear flow. In this sense, the conventional force used in the Evans–Gillan algorithm does not seem to be the most adequate for calculating nonlinear transport properties. In order to get equivalent results for the thermal conductivity, we assume that each particle in the system is subject to a nonconservative force $\mathcal{F}$

$$\mathcal{F} = -\left(\tfrac{1}{2}m\mathbf{V}^2 - \tfrac{3}{2}k_B T\right)\boldsymbol{\Omega}\cdot\boldsymbol{\epsilon}, \tag{8}$$

where the field strength $\boldsymbol{\epsilon}$ plays the role of a thermal gradient $\nabla T/T$. The tensor $\boldsymbol{\Omega}$ is a dimensionless function of the shear rate to be determined. In the usual heat field method, $\boldsymbol{\Omega}$ is replaced by the unity tensor. For finite shear rate, Eq. (8) takes into account the anisotropy of the problem as $\mathcal{F}$ and $\boldsymbol{\epsilon}$ are no longer parallel. The total force acting on each particle is the sum of $\mathbf{F}$, Eq. (7), and $\mathcal{F}$, Eq. (8).

Under these conditions, the velocity distribution function $f(\mathbf{V})$ verifies the steady BGK equation

$$-\frac{\partial}{\partial V_i}\left(a_{ij}V_j - \frac{F_i + \mathcal{F}_i}{m}\right)f = -\nu(f - f^{\text{LE}}), \tag{9}$$

where

$$f^{\text{LE}}(\mathbf{V}) = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{m}{2k_B T}V^2\right) \tag{10}$$

being the local equilibrium distribution. Conservation of total energy imposes the condition

$$\alpha=-\frac{m}{3p}q_i\Omega_{ij}\epsilon_j-\frac{m}{3p}aP_{xy}. \quad (11)$$

Here, $p=\frac{1}{3}P_{kk}=nk_BT$ is the pressure, P_{xy} is the xy element of the pressure tensor P, where

$$\mathsf{P}=\int d\mathbf{V}\, m\mathbf{V}\mathbf{V}f, \quad (12)$$

and

$$\mathbf{q}=\int d\mathbf{V}\,\frac{m}{2}\,V^2\mathbf{V}f \quad (13)$$

is the heat flux. Equation (11) couples α with the main transport coefficients of the problem, namely, the thermal conductivity tensor $\boldsymbol{\kappa}$ and the shear viscosity coefficient η. They are defined, respectively, by

$$q_i=-\kappa_{ij}T\epsilon_j, \quad (14)$$

$$\eta=-\frac{P_{xy}}{a}. \quad (15)$$

Notice that Eq. (14) has been written taking into account the analogy of this problem with the usual energy gradient problem. In order to evaluate these quantities, we define the dimensionless velocity moments M_{k_1,k_2,k_3} of $f(\mathbf{V})$ as

$$M_{k_1,k_2,k_3}=\frac{1}{n}\left(\frac{m}{2k_BT}\right)^{(k_1+k_2+k_3)/2}\int d\mathbf{V}V_x^{k_1}V_y^{k_2}V_z^{k_3}f(\mathbf{V}). \quad (16)$$

The task now is to get these moments in terms of the shear rate and the field strength. Both parameters measure the departure from equilibrium. This dependence will be analyzed in Sec. III.

III. VELOCITY MOMENTS

By taking moments in the BGK Eq. (9), one gets the following hierarchy for the moments M_{k_1,k_2,k_3}:

$$a^*k_1M_{k_1-1,k_2+1,k_3}+[1+\alpha^*(k_1+k_2+k_3)]M_{k_1,k_2,k_3}=M^{\rm LE}_{k_1,k_2,k_3}+N_{k_1,k_2,k_3}, \quad (17)$$

where

$$M^{\rm LE}_{k_1,k_2,k_3}=\pi^{-3/2}\Gamma\left(\frac{k_1+1}{2}\right)\Gamma\left(\frac{k_2+1}{2}\right)\Gamma\left(\frac{k_3+1}{2}\right) \quad (18)$$

if k_1, k_2, and k_3 are even, being zero otherwise, and

$$N_{k_1,k_2,k_3}=A_{k_1,k_2,k_3}\epsilon_x^*+B_{k_1,k_2,k_3}\epsilon_y^*+C_{k_1,k_2,k_3}\epsilon_z^*, \quad (19)$$

$$A_{k_1,k_2,k_3}=-\frac{k_1}{2}(M_{k_1+1,k_2,k_3}+M_{k_1-1,k_2+2,k_3}+M_{k_1-1,k_2,k_3+2}-\tfrac{3}{2}M_{k_1-1,k_2,k_3}), \quad (20)$$

$$B_{k_1,k_2,k_3}=-\frac{k_2}{2}(M_{k_1+2,k_2-1,k_3}+M_{k_1,k_2+1,k_3}+M_{k_1,k_2-1,k_3+2}-\tfrac{3}{2}M_{k_1,k_2-1,k_3}), \quad (21)$$

$$C_{k_1,k_2,k_3}=-\frac{k_3}{2}(M_{k_1+2,k_2,k_3-1}+M_{k_1,k_2+2,k_3-1}+M_{k_1,k_2,k_3+1}-\tfrac{3}{2}M_{k_1,k_2,k_3-1}). \quad (22)$$

Further, we have introduced the reduced quantities $a^*\equiv a/\nu$, $\alpha^*\equiv\alpha/(m\nu)$, and

$$\epsilon_i^*\equiv\left(\frac{2k_BT}{m}\right)^{1/2}\frac{1}{\nu}\Omega_{ij}\epsilon_j. \quad (23)$$

It must be noticed that in Eq. (17) it is assumed that M is zero if any of its indices is negative. For arbitrary values of $\boldsymbol{\epsilon}^*$, the hierarchy (17) is not closed and cannot be solved. However, in order to obtain the linear thermal conductivity only small values of $\boldsymbol{\epsilon}^*$ need to be retained. On the other hand, it has been shown that the applicability of the heat field method is restricted to small values of field strength since finite values of $\boldsymbol{\epsilon}^*$ leads to an unphysical behavior of the nonlinear thermal conductivity in the homogeneous case.[15] Therefore, we expand the moments in the form

$$M_{k_1,k_2,k_3}=M^{(0)}_{k_1,k_2,k_3}+M^{(1)}_{k_1,k_2,k_3}+\cdots, \quad (24)$$

where the successive approximations $M^{(l)}_{k_1,k_2,k_3}$ are of order l in $\boldsymbol{\epsilon}^*$ but they are nonlinear functions of the reduced shear rate a^*. In the same way, one must carry out an analogous expansion for α^*, i.e., $\alpha^*=\alpha_0^*+\alpha_1^*+\cdots$ Substituting these expansions into Eq. (17), one obtains a set of hierarchies that can be recursively solved. The solution can be written as

$$M^{(l)}_{k_1,k_2,k_3}=\sum_{q=0}^{k_1}(-a^*)^q[1+\alpha_0^*(k_1+k_2+k_3)]^{-(q+1)}\times\frac{k_1!}{(k_1-q)!}R^{(l)}_{k_1-q,k_2+q,k_3}, \quad (25)$$

with

$$R^{(0)}_{k_1,k_2,k_3}=M^{\rm LE}_{k_1,k_2,k_3}, \quad (26)$$

and

$$R^{(l)}_{k_1,k_2,k_3}=A^{(l-1)}_{k_1,k_2,k_3}\epsilon_x^*+B^{(l-1)}_{k_1,k_2,k_3}\epsilon_y^*+C^{(l-1)}_{k_1,k_2,k_3}\epsilon_z^*-(k_1+k_2+k_3)\sum_{r=1}^{l}\alpha_r^*M^{(l-r)}_{k_1,k_2,k_3} \quad (27)$$

for $l\geq1$. The parameters α_r^* can be determined from the relation (11). Equation (25) provides an explicit expression for the velocity moments of f in terms of the reduced shear rate a^* and the reduced field strength $\boldsymbol{\epsilon}^*$. It is not restricted to any specific form of $\boldsymbol{\Omega}$. This expression represents the major result of this paper.

In the zeroth-order approximation, we reobtain the results of the steady uniform shear flow.[16] In particular, the nonzero components of the reduced pressure tensor $P_{ij}^{*(0)}\equiv P_{ij}^{(0)}/p$ are given by

$$P_{xx}^{*(0)}=\frac{1+6\alpha_0^*}{1+2\alpha_0^*}, \quad (28)$$

$$P_{yy}^{*(0)}=P_{zz}^{*(0)}=\frac{1}{1+2\alpha_0^*}, \tag{29}$$

$$P_{xy}^{*(0)}=P_{yx}^{*(0)}=-\frac{a^*}{(1+2\alpha_0^*)^2}. \tag{30}$$

Here, α_0^* is the real root of the cubic equation

$$3\alpha_0^*(1+2\alpha_0^*)^2=a^{*2}. \tag{31}$$

The first and second approximations will be analyzed in Secs. IV and V to get the shear-rate dependence of the linear thermal conductivity tensor and the shear viscosity coefficient.

IV. LINEAR THERMAL CONDUCTIVITY TENSOR

In the first-order approximation, the relation (11) reads

$$\alpha_1^*=-\frac{4}{3}\frac{a^{*2}}{(1+2\alpha_0^*)^3}\alpha_1^*, \tag{32}$$

which implies that $\alpha_1^* = 0$. The heat flux $\mathbf{q}^{(1)}$ across the system can be evaluated from Eq. (25) for $l=1$. After some algebra, $\mathbf{q}^{(1)}$ can be recast into the form (14) where the so-called linear thermal conductivity tensor $\boldsymbol{\kappa}$ is

$$\kappa_{ij}=\frac{5}{2}\frac{nk_B^2T}{m\nu}\Lambda_{ik}\Omega_{kj}, \tag{33}$$

Λ_{ik} being a highly nonlinear function of the shear rate. The expressions of the nonzero elements of the tensor Λ are given in the Appendix. Equation (33) gives the thermal conductivity of a dilute gas under arbitrary shear flow in the limit of zero heat field. In order to analyze its shear-rate dependence specific forms for Ω must be adopted.

The simplest choice corresponds to the one proposed in the Evans–Gillan method,[2,3] in which case Ω is replaced by the unity tensor. With this choice, Λ is the thermal conductivity tensor reduced with respect to its equilibrium value. For $a^*=0$, $\Lambda_{ij}=\delta_{ij}$, and one recovers the well-known expression for the thermal conductivity coefficient given by the BGK model.[15] In this sense, the Evans–Gillan algorithm applied on molecular dynamics simulations is an efficient alternative to simulation methods based on the Green–Kubo formula for measuring the thermal conductivity coefficient. Some elements of Λ are plotted in Fig. 1 as functions of a^*. We observe that the qualitative shear-rate dependence of the diagonal elements Λ_{xx} and Λ_{yy} is very similar. They present a maximum for $a^*\simeq 1.86$ in the case of Λ_{xx} while for Λ_{yy} the maximum is located at $a^*\simeq 1.02$. The element Λ_{zz} exhibits a similar behavior. The xy and yx elements are negative and decrease as the shear rate increases. This dependence on the shear rate is more noticeable in the case of the xy element.

In principle, the heat field method must be distinguished from the familiar heat transport problem. In the latter, energy transport is produced by a temperature gradient instead of an external field. When the system is subject to uniform shear flow, a reduced thermal conductivity tensor λ_{ij} can be defined from a generalized Fourier's law. Very recently, we have obtained an expression of λ_{ij} from a perturbation solution of the BGK model.[5] Comparing the exact results derived

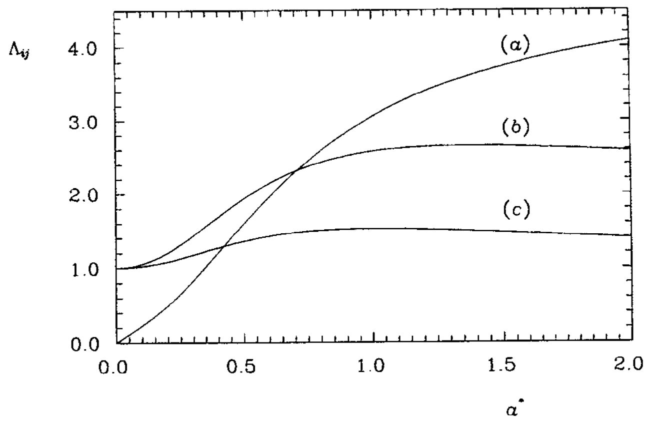

FIG. 1. Shear-rate dependence of some elements of the tensor Λ_{ij}: (a) $-\Lambda_{xy}$, (b) Λ_{xx}, (c) Λ_{yy}.

here and in Ref. 5, we conclude that the tensors Λ_{ij} and λ_{ij} are different. Furthermore, for nonzero shear rates, both tensors have different qualitative features. While the geometry of the heat field problem is arbitrary, the analysis made in Ref. 5 shows that the thermal gradient must be orthogonal to the direction of the flow velocity (x direction) to achieve a steady state. Consequently, the only relevant elements of the thermal conductivity tensor are λ_{yy}, λ_{zz}, and λ_{xy}. On the other hand, λ_{ij} depends on the potential model considered while in our description Λ_{ij} is a universal function independent of the interaction potential. All these considerations show the inadequacy of the conventional Evans–Gillan algorithm to evaluate the linear thermal conductivity tensor under strong shear fields and confirm the general results derived by Evans *et al.*[8] for mechanical transport coefficients. Identical conclusions were obtained in the case of the so-called color field method.[9]

In order to avoid this discrepancy, a different form for Ω must be suggested. By comparing Eq. (33) with Eqs. (16) and (18) of Ref. 5, it is easy to show that the adequate choice is

$$\Omega_{ij}=(\Lambda^{-1})_{ik}\lambda_{kj}, \tag{34}$$

where again we have identified the temperature gradient $\nabla \ln T$ with the field strength $\boldsymbol{\epsilon}$. From this novel external force, the thermal conductivity obtained from the heat field method exactly coincides with the one derived in presence of a temperature gradient. In absence of shear, Eq. (34) reduces to the one proposed in the conventional heat field method. However, for finite shear rate, Ω captures the anisotropy induced by the shear flow. To illustrate the shear-rate dependence of this tensor one needs to know the temperature dependence of the collision frequency. For instance, for $r^{-\mu}$ potentials one has $\nu\propto T^{\gamma-1}$ with $\gamma=1/2-2/\mu$ since p is constant in the energy gradient problem. Figure 2 shows Ω_{yy} vs a^* for three values of γ: $\gamma=0$ (Maxwell gas), $\gamma=\frac{1}{2}$ (hard sphere gas), and $\gamma=1$ [very-hard-particle (VHP) interaction]. We see that the dependence of Ω_{yy} with a^* is similar for the three interaction models considered, as it monotonically decreases as the shear rate increases. For a given value of a^*,

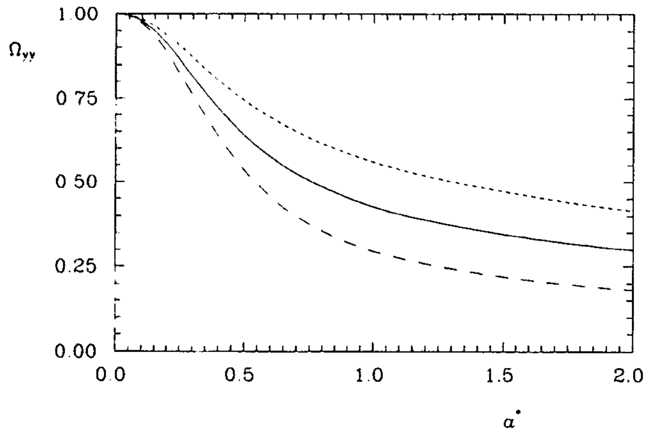

FIG. 2. Plot of Ω_{yy}, as a function of the shear rate for three interaction models: hard-sphere interaction (—), Maxwell interaction (– – –), and VHP interaction (- - -).

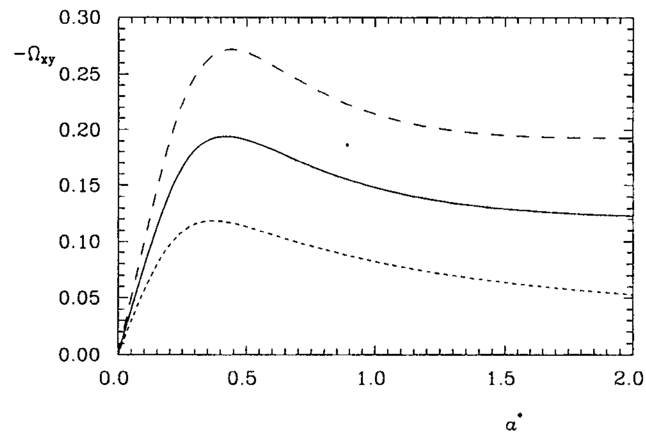

FIG. 3. The same as in Fig. 2, but for $-\Omega_{xy}$.

Ω_{yy} increases as the interaction parameter γ increases. The anistropy of the external force $\mathscr{F}$ is measured by the off-diagonal element Ω_{xy}. It is plotted in Fig. 3. For small shear rates, $-\Omega_{xy}$ increases with a^* while for large shear rates it decreases as a^* increases.

To close this section, it is interesting to perform a more detailed comparison between the thermal conductivity tensors Λ and λ. Specifically, we address our attention to the yy element for which we define the function

$$\Delta_{yy}=\frac{\Lambda_{yy}-\lambda_{yy}}{\Lambda_{yy}}. \tag{35}$$

Here, λ_{yy} refers to the one obtained for the VHP model where ν is also a constant in the thermal gradient problem. This comparison is in the same spirit as the one carried out recently between the color conductivity and self-diffusion tensors.[9] The function Δ_{yy} is plotted in Fig. 4. It is shown that for shear rates not too large, the results derived from both choices of heat field agree qualitatively well. For instance, for shear rates up to $a^*\simeq 0.25$, for which the shear viscosity in the pure shear flow problem is about 8% smaller than its equilibrium value, the relative difference Δ_{yy} is smaller than 7%. For larger values of shear rates, the discrepancies become more significant so that the appropriate external force is the one proposed in Eq. (34).

V. SHEAR VISCOSITY COEFFICIENT

The other relevant physical quantity involved in this problem is the shear viscosity coefficient η, which is defined from Eq. (15). We are interested in exploring the effects of the heat field upon the shear viscosity. For the sake of clarity we restrict our calculations to the second order approximation and we take ϵ parallel to the gradient of the flow velocity, i.e., $\epsilon_x=\epsilon_z=0$. By collecting terms up to ϵ_y^2, it is a simple matter to get the first few terms in the expansion of η. In dimensionless units, the result is

$$\eta^*=\eta/(p/\nu)=\eta_0^*+\frac{53}{6}\frac{k_BT}{m\nu^2}\eta_2^*\epsilon_y^2 \tag{36}$$

with

$$\eta_0^*=(1+2\alpha_0^*)^{-2}, \tag{37}$$

$$\eta_2^*=-\frac{15}{53}\frac{1}{a^*}\frac{2a^*\Lambda_{yy}[a^*+2(1+2\alpha_0^*)(1+3\alpha_0^*)]-3\Lambda_{xy}(1+2\alpha_0^*)^3}{2a^{*3}-2a^{*2}(1+2\alpha_0^*)-3(1+2\alpha_0^*)^4}\Omega_{yy}^2. \tag{38}$$

Equation (36) indicates that the deviation of the shear viscosity coefficient from its pure shear flow η_0^* is at least of second order in the heat field. In the spirit of the Chapman–Enskog method it would correspond to the Burnett hydrodynamic order. The coefficient η_2^* is again a highly nonlinear function of the shear rate. For $a^*=0$, Eq. (36) becomes

$$\eta^*=1+\frac{53}{6}\frac{k_BT}{m\nu^2}\epsilon_y^2, \tag{39}$$

since for $a^*=0$, $\Omega_{yy}=1$. In Fig. 5 we have plotted η_2^* for the same choices of Ω_{yy} as in Sec. IV. We see that both coefficients exhibit different behaviors. In the case of the modified force (34), η_2^* in general monotonically decreases as a^* increases while for the conventional Evans–Gillan choice η_2^* presents a maximum around $a^*\simeq 0.48$. According to these results one could expect that the successive transport coefficients of the problem will be noticeably different when considering both choices of the external force.

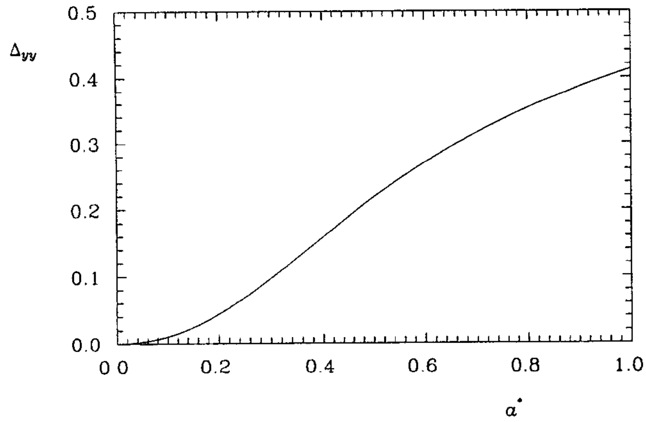

FIG. 4. Plot of the relative difference between Λ_{yy} and λ_{yy} vs the shear rate. Here, λ_{yy} corresponds to the VHP model.

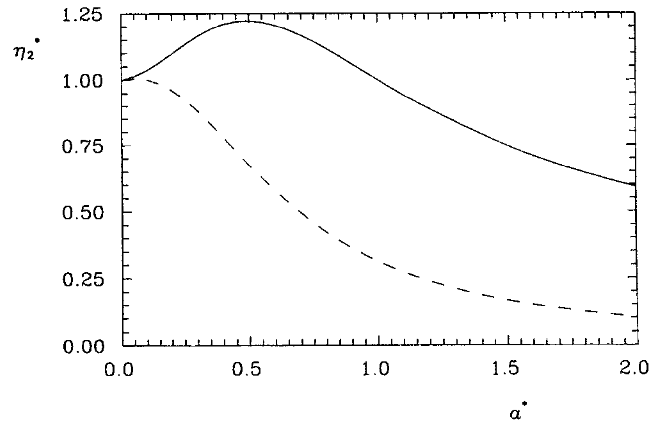

FIG. 5. Shear-rate dependence of the second-order coefficient η_2^* for two choices of Ω_{yy}: $\Omega_{yy}=1$ (solid line) and $\Omega_{yy}=(\Lambda^{-1})_{yk}\lambda_{ky}$ for the VHP interaction (dashed line).

VI. DISCUSSION

In this paper we have analyzed the coupling between heat and momentum transport in a dilute gas described by the BGK kinetic model. The system is in a steady inhomogeneous state (the so-called uniform shear flow) characterized by a constant density and temperature and a local velocity along the x direction with a constant gradient a along the y direction. Further, a nonconservative external force acts on the system producing a *heat current* in spite of the absence of a thermal gradient. A drag force is also included to preserve the stationarity of the state. Therefore, the system is driven out of equilibrium by the shearing motion as well as by the heat field. This method of generating heat flux has been proposed in molecular dynamics simulations[2,3] as a means to evaluate the thermal conductivity coefficient in the zero-field limit.

By assuming that the heat field is weak, the hierarchy of moment equations is solved by means of a perturbation expansion around the uniform shear flow state. Consequently, the different approximations are highly nonlinear functions of the shear rate. All the velocity moments can be obtained in a recursive way. In particular, explicit expressions for the linear thermal conductivity tensor κ_{ij} and the shear viscosity coefficient η up to second-order approximation are derived. These quantities are related, respectively, to the transport of energy and momentum and they are the relevant transport coefficients of the problem.

In absence of shear field ($a=0$), the thermal conductivity coefficient κ reduces to the usual thermal conductivity λ obtained in the thermal gradient problem. This coefficient is defined from the familiar Fourier law and can be evaluated from a Green–Kubo relation. From the computer simulation point of view, the Evans–Gillan algorithm permits a much more efficient calculation of the Navier–Stokes thermal conductivity than a direct calculation of this coefficient from the Green–Kubo formula itself. Unfortunately, and as has been proved recently,[8] this equivalence is not maintained when the system is in a far from equilibrium situation (such as the uniform shear flow state). The exact results derived here and in Ref. 5 for a dilute gas confirm that both thermal conductivity tensors are clearly different for finite values of the shear rates. Nevertheless, for not too large values of $a^*(a^*\simeq 0.25)$, the agreement between both methods is reasonably good.

The above discrepancies can be eliminated by an adequate choice of the external force. By identifying the thermal gradient $\nabla \ln T$ with the field strength $\boldsymbol{\epsilon}$, we have proposed a shear-rate dependent heat field that yields identical expressions for the thermal conductivity tensor. This alternative field takes into account the presence of nonequilibrium normal and shear stresses. Further, its explicit expression depends on the potential model considered through the temperature dependence of the collision frequency.

The use of fictitious fields may prove to be relevant for computing more efficiently linear transport coefficients in computer simulations. In this context, the novel external force suggested in this paper for evaluating the linear thermal conductivity tensor is a nontrivial extension of the conventional Evans–Gillan method and thus represents a step forward. On the other hand, although the results presented here have been obtained from the BGK model, we expect that similar conclusions could be drawn out from the exact Boltzmann equation. Work is in progress along this line.

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APPENDIX: EXPLICIT EXPRESSION OF THE TENSOR Λ

Here we give the list of the nonzero elements of the tensor Λ_{ij}. They can be written in the form

$$\Lambda_{xx}=A_0+A_1a^{*2}+A_2a^{*4}, \tag{A1}$$

$$\Lambda_{xy}=A_3a^*+A_4a^{*3}+A_5a^{*5}, \tag{A2}$$

$$\Lambda_{yx}=A_6a^*+A_7a^{*3}, \tag{A3}$$

$$\Lambda_{yy}=A_0+A_8a^{*2}+A_9a^{*4}, \tag{A4}$$

$$\Lambda_{zz}=A_0+A_{10}a^{*2}+A_{11}a^{*4}, \tag{A5}$$

A_i being nonlinear functions of α_0^*. These quantities are given by

$$A_0=\frac{1-\alpha_0^*}{(1+4\alpha_0^*)(1+3\alpha_0^*)(1+2\alpha_0^*)}, \tag{A6}$$

$$A_1=-\frac{4560\alpha_0^{*5}+3504\alpha_0^{*4}-740\alpha_0^{*3}-1377\alpha_0^{*2}-432\alpha_0^*-43}{5(1+4\alpha_0^*)^3(1+3\alpha_0^*)^3(1+2\alpha_0^*)^3}, \tag{A7}$$

$$A_2=\frac{18}{5}\frac{106\alpha_0^{*2}+65\alpha_0^*+10}{(1+4\alpha_0^*)^5(1+3\alpha_0^*)^3}, \tag{A8}$$

$$A_3=\frac{116\alpha_0^{*3}-6\alpha_0^{*2}-51\alpha_0^*-11}{5(1+4\alpha_0^*)^2(1+3\alpha_0^*)^2(1+2\alpha_0^*)^2}, \tag{A9}$$

$$A_4=\frac{21456\alpha_0^{*6}+13512\alpha_0^{*5}-14348\alpha_0^{*4}-17858\alpha_0^{*3}-7257\alpha_0^{*2}-1318\alpha_0^*-91}{5(1+4\alpha_0^*)^4(1+3\alpha_0^*)^4(1+2\alpha_0^*)^3}, \tag{A10}$$

$$A_5=-\frac{54}{5}\frac{58\alpha_0^{*2}+34\alpha_0^*+5}{(1+4\alpha_0^*)^5(1+3\alpha_0^*)^4}, \tag{A11}$$

$$A_6=\frac{2}{5}\frac{38\alpha_0^{*3}+2\alpha_0^{*2}-13\alpha_0^*-3}{(1+4\alpha_0^*)^2(1+3\alpha_0^*)^2(1+2\alpha_0^*)^2}, \tag{A12}$$

$$A_7=-\frac{6}{5}\frac{13\alpha_0^*+4}{(1+4\alpha_0^*)^4(1+3\alpha_0^*)^2}, \tag{A13}$$

$$A_8=-\frac{1632\alpha_0^{*5}+368\alpha_0^{*4}-1604\alpha_0^{*3}-1233\alpha_0^{*2}-332\alpha_0^*-31}{5(1+4\alpha_0^*)^3(1+3\alpha_0^*)^3(1+2\alpha_0^*)^3}, \tag{A14}$$

$$A_9=\frac{18}{5}\frac{58\alpha_0^{*2}+34\alpha_0^*+5}{(1+4\alpha_0^*)^5(1+3\alpha_0^*)^3}, \tag{A15}$$

$$A_{10}=-\frac{1184\alpha_0^{*5}+440\alpha_0^{*4}-872\alpha_0^{*3}-725\alpha_0^{*2}-200\alpha_0^*-19}{5(1+4\alpha_0^*)^3(1+3\alpha_0^*)^3(1+2\alpha_0^*)^3}, \tag{A16}$$

$$A_{11}=\frac{6}{5}\frac{106\alpha_0^{*2}+65\alpha_0^*+10}{(1+4\alpha_0^*)^5(1+3\alpha_0^*)^3}. \tag{A17}$$

The behavior of α_0^* for small and large shear rates is, respectively,

$$\alpha_0^*\approx\tfrac{1}{3}a^{*2}, \tag{A18}$$

$$\alpha_0^*\approx\tfrac{1}{2}(\tfrac{2}{3})^{1/3}a^{*2/3}. \tag{A19}$$

According to this behavior, for small shear rates one has that $\Lambda_{xx}\approx 1+\frac{79}{15}a^{*2}$, $\Lambda_{xy}\approx-\frac{11}{5}a^*$, $\Lambda_{yx}\approx-\frac{6}{5}a^*$, $\Lambda_{yy}\approx 1+\frac{43}{15}a^{*2}$, and $\Lambda_{zz}\approx 1+\frac{7}{15}a^{*2}$. On the other hand, for large shear rates one gets $\Lambda_{xx}\approx\frac{159}{80}$, $\Lambda_{xy}\approx-\frac{87}{40}(\frac{3}{2})^{1/3}a^{*1/3}$, $\Lambda_{yx}\approx-\frac{13}{40}(\frac{3}{2})^{2/3}a^{*-1/3}$, $\Lambda_{yy}\approx\frac{87}{80}$, and $\Lambda_{zz}\approx\frac{53}{80}$.

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