Thermal transport generated by an external force in a sheared dilute gas

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Energy and momentum transport in a strongly sheared dilute gas is analyzed in the context of the nonlinear Boltzmann equation. Thermal transport is generated in the system by the action of a nonconservative external force which tries to mimick the effects of a temperature gradient. By performing a perturbation expansion in powers of the field strength, we obtain expressions for the field susceptibility tensor and the shear viscosity coefficient up to second order in the force. They are highly nonlinear functions of the shear rate. It is shown that the choice of the heat field used in computer simulations yields a field susceptibility tensor different from the thermal conductivity tensor. In order to get equivalent results, a new shear-rate dependent force is suggested. The calculations presented here extend previous results derived from the Bhatnagar–Gross–Krook approximation [J. Chem. Phys. **101**, 1423 (1994)].

I. INTRODUCTION

The study of transport properties in steady states driven out of equilibrium by the action of external forces is a subject of interest from a theoretical, as well as a computer simulation, point of view. These forces try to mimick the effects produced in the system by the presence of real hydrodynamic gradients. The corresponding transport coefficients, which measure the response of the system, are determined by extrapolating the ratio between the hydrodynamic fluxes and the field strengths to zero-field limit. They exhibit a good agreement with those obtained from computer simulations by using realistic boundary conditions. Some examples of nonequilibrium steady states generated by external forces are the color conductivity[1,2] and the heat conductivity problems.[3–5]

This paper is concerned with the method proposed independently by Evans[3] and Gillan and Dixon[4] to simulate the heat flow. Since this method was developed in nonequilibrium molecular dynamics to measure the thermal conductivity coefficient in the linear regime, it does not work *in principle* once nonlinear effects are present.[6] For instance, when the system is subjected to strong shear flows, it has been shown recently for a low-density gas that the so-called fictitious ''field susceptibility'' tensor (which is defined from the heat flux vector) differs from the thermal conductivity tensor obtained in the presence of a temperature gradient.[7] Although the agreement between both methods is reasonably good for not too large shear rates, the discrepancies increase significantly at finite shear rates. In order to get consistent results, an alternative external force was proposed. The results were derived from the Bhatnagar–Gross–Krook (BGK) kinetic equation as a model of the Boltzmann equation.

Nevertheless, due to the fact that the BGK equation is a simplified version of the exact Boltzmann equation, the results derived in Ref. 7 cannot be taken as conclusive. For instance, recent results[8] obtained for the fourth-degree moments in the uniform shear flow problem show that the BGK predictions are quite different to those given from the Boltzmann equation, especially for large shear rates. For this reason, and since those moments are involved in the evaluation of the field susceptibility, in this paper we extend our previous efforts by carrying out a similar study to that of Ref. 7 but now using the nonlinear Boltzmann equation. The price to be paid is to consider the particular case of Maxwell molecules (repulsive potential of the form r^{-4}), for which an exact solution of the Boltzmann equation in the pure shear flow state is known.[9,10] The underlying purpose of such a study is twofold. On the one hand, we want to analyze the coupling between the shear flow and the conventional heat field suggested in the Evans–Gillan method in order to assess to what extent the previous results derived from the BGK approximation are indicative of what happens in a dilute gas. On the other hand, the study allows us again to propose a new shear-rate dependent heat force that leads to equivalent results as those found from the Boltzmann equation in the thermal gradient problem.[11]

II. DESCRIPTION OF THE PROBLEM

Let us consider a dilute gas under uniform shear flow. At a macroscopic level, this state is characterized by constant density n and temperature T and a linear velocity field of the form $u_x = ay$, where a is the constant shear rate. The shear flow produces viscous heating, so that a thermostat external force is introduced to achieve a stationary state. According to Gauss' principle of least constraint, one selects the force

$$\mathbf{F} = -m\alpha\mathbf{V}, \tag{1}$$

where $\mathbf{V}=\mathbf{v}-\mathbf{u}$ is the peculiar velocity and the thermostat parameter α is determined by consistency. The uniform shear flow is an adequate example for giving a range of validity of the heat field method in the nonlinear regime. It has been extensively used to analyze rheological properties, such as shear thinning and viscometric effects.[12]

We want to analyze a thermal transport problem generated by an external force in a dilute gas under uniform shear flow. Unlike real heat flow, no temperature or density gradients appear in the system. Consequently, two parameters measure the departure from equilibrium: the shear rate and the heat field strength. In the limit of small heat field, but arbitrary shear rate, a field susceptibility tensor rather than a scalar can be identified in the expression of the heat flux. The derivation of such an expression for this tensor is the main goal of this paper. In addition, it is also interesting to study the influence of the nonequilibrium parameters on the nonlinear shear viscosity.

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 way, the isotropic external force used in the conventional Evans–Gillan method cannot be probably the most convenient choice. Here, to parallel the results derived from the BGK model,[7] we assume that the heat field is

$$\mathscr{F}=-\left(\tfrac{1}{2}\,mV^2-\tfrac{3}{2}\,k_BT\right)\Omega\cdot\boldsymbol{\epsilon}, \tag{2}$$

where the field strength $\boldsymbol{\epsilon}$ plays the role of a temperature gradient $\nabla T/T$, and Ω is a shear-rate dependent tensor to be determined. In the usual heat field method, one takes $\Omega_{ij}=\delta_{ij}$. For nonzero shear rates, the force (2) exhibits the anisotropy of the problem since now $\mathscr{F}$ and $\boldsymbol{\epsilon}$ are no longer parallel.

Under the above conditions, the Boltzmann equation reads

$$-\frac{\partial}{\partial V_i}\left(a_{ij}V_j-\frac{F_i+\mathscr{F}_i}{m}\right)f=J[\,f,f\,], \tag{3}$$

where $f(\mathbf{V})$ is the one-particle distribution function and $J[\,f,f\,]$ is the Boltzmann collision operator, which in standard notation reads[13]

$$J[\,f,f\,]=\int d\mathbf{v}_1\int d\hat{\mathbf{n}}|\mathbf{v}-\mathbf{v}_1|\sigma(|\mathbf{v}-\mathbf{v}_1|,\theta)(f'f_1'-ff_1). \tag{4}$$

The parameter α is a function of both the shear rate and the field strength. Conservation of energy

$$\int d\mathbf{V}mV^2J[\,f,f\,]=0 \tag{5}$$

imposes the constraint

$$\alpha=-\frac{1}{3p}\,q_i\Omega_{ij}\epsilon_j-\frac{1}{3p}\,aP_{xy}, \tag{6}$$

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

$$\mathsf{P}=m\int d\mathbf{V}\mathbf{V}\mathbf{V}f, \tag{7}$$

and

$$\mathbf{q}=\frac{m}{2}\int d\mathbf{V}V^2\mathbf{V}f, \tag{8}$$

is the heat flux. Equation (6) couples α with the relevant transport coefficients, namely, the so-called "field susceptibility" tensor

$$\kappa_{ij}=-\frac{1}{T}\frac{q_i}{\epsilon_j}, \tag{9}$$

and the shear viscosity coefficient

$$\eta=-\frac{P_{xy}}{a}. \tag{10}$$

As shown in the BGK description,[7] it is not possible to get these coefficients for arbitrary values of the field strength. Anyway, in order to obtain the shear-rate dependent linear field susceptibility, only terms up to first order in $\boldsymbol{\epsilon}$ need to be retained. Therefore, we construct a solution of Eq. (3) by expanding around the shear flow state, i.e.,

$$f=f_0+f_1+f_2+\cdots, \tag{11}$$

where f_k is of order k in $\boldsymbol{\epsilon}$, but it retains all the hydrodynamic orders in a. In the same way as in Eq. (11), $\alpha=\alpha_0+\alpha_1+\alpha_2\cdots$ and analogous expansions are considered for the momentum and energy fluxes. By introducing these expansions into Eq. (3), one gets a hierarchy of equations for the successive approximations f_k.

At the zeroth-order stage, one gets

$$-\frac{\partial}{\partial V_i}(a_{ij}V_j+\alpha_0V_i)f_0=J[\,f_0,f_0], \tag{12}$$

This equation describes the pure shear flow state. Its solution is necessary to obtain the coefficients (9) and (10). In general, Eq. (12) can only be solved by means of the Chapman–Enskog method,[13] namely, a perturbation expansion around the state of local equilibrium. However, in the special case of Maxwell molecules (repulsive r^{-4} potential), Eq. (12) can be exactly solved by the moment method. In particular, one has[9]

$$\alpha_0=\tfrac{2}{3}\sinh^2[\tfrac{1}{6}\cosh^{-1}(1+9a^2)], \tag{13}$$

$$P_{0,xx}=p\,\frac{1+6\alpha_0}{1+2\alpha_0}, \tag{14}$$

$$P_{0,yy}=P_{0,zz}=p\,\frac{1}{1+2\alpha_0}, \tag{15}$$

$$P_{0,xy}=P_{0,yx}=-p\,\frac{a}{(1+2\alpha_0)^2}. \tag{16}$$

Here, we have chosen $\nu=1$, ν being a convenient collision frequency so that α_0 and a are now dimensionless quantities. Equations (13)–(16) are the same as those derived from the BGK approximation. The next nontrivial moments in the uniform shear flow problem are the fourth-degree moments. Recently, explicit expressions for these moments have been obtained.[10] In contrast to what happens for the pressure tensor, the Boltzmann and BGK equations give quite different results for the above moments.[8] Consequently, the predictions made previously in Ref. 7 for the field susceptibility and the shear viscosity must be reexamined.

III. FIELD SUSCEPTIBILITY AND SHEAR VISCOSITY

In this section we will get the shear-rate dependence of κ_{ij} and η. Concerning the first-order, the corresponding Boltzmann equation is

$$-\frac{\partial}{\partial V_i}(a_{ij}V_j+\alpha_0 V_i)f_1-\alpha_1\frac{\partial}{\partial V_i}V_i f_0-\frac{1}{m}\frac{\partial}{\partial V_i}\left(\frac{m}{2}V^2-\frac{3}{2}k_BT\right)\Omega_{ij}\epsilon_j f_0=J[f_0,f_1]+J[f_1,f_0], \tag{17}$$

where according to Eq. (6), $\alpha_1=-(a/3p)P_{1,xy}$ as $\mathbf{q}_0=\mathbf{0}$ in the pure shear flow state. From Eq. (17) it is easy to show that the pressure tensor is zero in this approximation so that $\alpha_1=0$. The first nontrivial moment is the heat flux

$$\mathbf{q}_1=\frac{m}{2}\int d\mathbf{V}V^2\mathbf{V}f_1, \tag{18}$$

which is related to the third-degree moments of f_1. For the sake of convenience, we choose the following dimensionless moments[9]

$$\{N_{2|i},N_{0|ijk}\}=\frac{1}{n}\left(\frac{m}{2k_BT}\right)^{3/2}\int d\mathbf{V}\{Y_{2|i}(\mathbf{V}),Y_{0|ijk}(\mathbf{V})\}f_1, \tag{19}$$

where

$$Y_{2|i}(\mathbf{V})=V^2V_i, \tag{20}$$

$$Y_{0|ijk}(\mathbf{V})=V_iV_jV_k-\tfrac{1}{5}V^2(V_i\delta_{jk}+V_j\delta_{ik}+V_k\delta_{ij}). \tag{21}$$

In the particular case of Maxwell molecules, the corresponding collisional moments are given by

$$\frac{1}{n}\left(\frac{m}{2k_BT}\right)^{3/2}\int d\mathbf{V}\{Y_{2|i},Y_{0|ijk}\}(J[f_0,f_1]+J[f_1,f_0])=-\{\tfrac{2}{3}N_{2|i},\tfrac{3}{2}N_{0|ijk}\}. \tag{22}$$

Let us consider now the set of ten independent moments

$$\{N_{2|x},N_{2|y},N_{2|z},N_{0|xxy},N_{0|xxz},N_{0|xyy},N_{0|yyz},N_{0|xzz},N_{0|yzz},N_{0|xyz}\} \tag{23}$$

Multiplying Eq. (17) by the polynomials (20) and (21) and integrating over $\mathbf{V}$, one gets the following matrix equation for the third-degree moments (23):

$$\mathscr{M}_{\sigma\sigma'}\mathscr{N}_{\sigma'}=\mathscr{A}_\sigma\epsilon_x^*+\mathscr{B}_\sigma\epsilon_y^*+\mathscr{C}_\sigma\epsilon_z^*,\quad \sigma=1,\ldots,10 \tag{24}$$

where, $\mathscr{N}$ is the column matrix defined by the set (23), and

$$\mathscr{M}=\begin{pmatrix}
c_1 & \frac{7}{5}a & 0 & 2a & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{2}{5}a & c_1 & 0 & 0 & 0 & 2a & 0 & 0 & 0 & 0\\
0 & 0 & c_1 & 0 & 0 & 0 & 0 & 0 & 0 & 2a\\
\frac{8}{25}a & 0 & 0 & c_2 & 0 & \frac{8}{5}a & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & c_2 & 0 & 0 & 0 & 0 & \frac{8}{5}a\\
0 & \frac{8}{25}a & 0 & -\frac{7}{5}a & 0 & c_2 & 0 & 0 & -a & 0\\
0 & 0 & 0 & 0 & 0 & 0 & c_2 & 0 & 0 & -\frac{2}{5}a\\
0 & -\frac{2}{25}a & 0 & -\frac{2}{5}a & 0 & 0 & 0 & c_2 & a & 0\\
-\frac{2}{25}a & 0 & 0 & 0 & 0 & -\frac{2}{5}a & 0 & 0 & c_2 & 0\\
0 & 0 & \frac{1}{5}a & 0 & 0 & 0 & a & 0 & 0 & c_2
\end{pmatrix}. \tag{25}$$

Here, $c_1\equiv\frac{2}{3}+3\alpha_0$, $c_2\equiv\frac{3}{2}+3\alpha_0$, and $\boldsymbol{\epsilon}_{\mathbf{i}}^*=(2k_BT/m)^{1/2}\Omega_{ij}\epsilon_j$. The column matrix $\mathscr{A}$ is

$$\mathscr{A}=\begin{pmatrix} R_{102}+R_{120}+R_{300}\\ R_{012}+R_{030}+R_{210}\\ R_{003}+R_{021}+R_{201}\\ \frac{1}{5}(4R_{210}-R_{012}-R_{030})\\ \frac{1}{5}(4R_{201}-R_{003}-R_{021})\\ \frac{1}{5}(4R_{120}-R_{102}-R_{300})\\ \frac{1}{5}(4R_{021}-R_{003}-R_{201})\\ \frac{1}{5}(4R_{102}-R_{120}-R_{300})\\ \frac{1}{5}(4R_{012}-R_{030}-R_{210})\\ R_{111}\end{pmatrix}, \tag{26}$$

with

$$R_{k_1,k_2,k_3}=-\frac{k_1}{2}(M_{k_1+1,k_2,\,k_3}+M_{k_1-1,k_2+2,k_3}+M_{k_1-1,k_2,k_3+2}-\tfrac{3}{2}M_{k_1-1,k_2,k_3}), \tag{27}$$

and

$$M_{k_1,k_2,k_3}=\frac{1}{n}\left(\frac{m}{2k_BT}\right)^{(k_1+k_2+k_3)/2}\int d\mathbf{V}V_x^{k_1}V_y^{k_2}V_z^{k_3}f_0 \tag{28}$$

are the moments of the shear flow distribution f_0. The column matrices $\mathscr{B}_\sigma$ and $\mathscr{C}_\sigma$ are given by expressions similar to Eq. (26) but with R_{k_1,k_2,k_3} replaced, respectively, by

$$S_{k_1,k_2,k_3}=\frac{k_2}{k_1+1}R_{k_1+1,k_2-1,k_3}, \tag{29}$$

$$T_{k_1,k_2,k_3}=\frac{k_3}{k_1+1}R_{k_1+1,k_2,k_3-1}, \tag{30}$$

According to Eqs. (26)–(28) it is clear that only moments of f_0 up to the fourth degree need to be known. The explicit expressions of these moments can be found in Ref. 10. The right-hand side of the matrix equation (24) also holds for the BGK model equation,[7] although the shear-rate dependence of the fourth-degree moments clearly differs from the Boltzmann ones.[8] The solution to Eq. (24) is

$$\dot{\mathscr{N}}_\sigma=(\mathscr{M}^{-1})_{\sigma\sigma'}(\mathscr{A}_{\sigma'}\epsilon_x^*+\mathscr{B}_{\sigma'}\epsilon_y^*+\mathscr{C}_{\sigma'}\epsilon_z^*). \tag{31}$$

The heat flux across the system is determined from the first three terms of $\dot{\mathscr{N}}_\sigma$, namely, $N_{2|x}, N_{2|y}$, and $N_{2|z}$. They define the components of the field susceptibility tensor κ_{ij}. According to Eq. (9), one gets

$$\kappa_{ij}=\frac{15}{4}\frac{nk_B^2T}{m}\Lambda_{ik}\Omega_{kj}, \tag{32}$$

where the nonzero components of the tensor Λ can be expressed in terms of the matrices $\mathscr{A}_\sigma$, $\mathscr{B}_\sigma$, and $\mathscr{C}_\sigma$. The transport coefficient $\Lambda_{ik}(a)$ measures the *linear* response to the external field (2) of a dilute gas under uniform shear flow, being a nonlinear function of the shear rate. Taking into account the symmetry of M_{k_1,k_2,k_3} (the only nonvanishing moments correspond to k_1+k_2 and k_3 even), the components of Λ can be written in the form $\Lambda_{xx}\equiv F(\mathscr{A})$, $\Lambda_{xy}\equiv F(\mathscr{B})$, $\Lambda_{yx}\equiv G(\mathscr{A})$, $\Lambda_{yy}\equiv G(\mathscr{B})$, and $\Lambda_{zz}\equiv H(\mathscr{C})$, where

$$F(\mathscr{A})=-\frac{8}{15}\frac{1}{27\alpha_0^2+46\alpha_0+12}\left[\frac{3}{5}(216\alpha_0^2+151\alpha_0+30)\mathscr{A}_1-\frac{27}{5}(24\alpha_0+7)a\mathscr{A}_2+4\frac{108\alpha_0^2+23\alpha_0-6}{1+2\alpha_0}a\mathscr{A}_4+12(54\alpha_0+19)\alpha_0\mathscr{A}_6+8\frac{54\alpha_0+19}{1+2\alpha_0}\alpha_0 a\mathscr{A}_9\right], \tag{33}$$

$$G(\mathscr{A})=-\frac{8}{15}\frac{1}{27\alpha_0^2+46\alpha_0+12}\left[-\frac{54}{5}a\mathscr{A}_1+\frac{3}{5}(216\alpha_0^2+151\alpha_0+30)\mathscr{A}_2-24\alpha_0(1+9\alpha_0)\mathscr{A}_4-12\frac{9\alpha_0+2}{1+2\alpha_0}a\mathscr{A}_6-24\alpha_0(9\alpha_0+2)\mathscr{A}_9\right], \tag{34}$$

$$H(\mathscr{C})=-\frac{8}{15}\frac{1}{23\alpha_0+6}\left[\frac{3}{5}(8\alpha_0+15)\mathscr{C}_3+24\alpha_0\mathscr{C}_7-12\frac{a}{1+2\alpha_0}\mathscr{C}_{10}\right]. \tag{35}$$

Equations (32)–(35) provide all the information on the physical mechanisms involved in the thermal transport produced by an external force in a strongly sheared dilute gas. Although these expressions hold in the limit of zero heat field, they have the full nonlinear dependence on the shear rate. In particular, for small shear rates, $\Lambda_{xx}\approx 1+59.4a^2$, $\Lambda_{xy}\approx -2.90a$, $\Lambda_{yx}\approx -1.40a$, $\Lambda_{yy}\approx 1+3.05a^2$, and $\Lambda_{zz}\approx 1+0.72a^2$.

In order to get the explicit shear-rate dependence of the field susceptibility tensor, one needs to consider specific forms of Ω. The simplest choice is the one assumed in the conventional Evans–Gillan method,[3,4] namely $\Omega_{ij}=\delta_{ij}$. In this case, Λ is the field susceptibility tensor reduced with respect to its Navier–Stokes value since for $a=0$, $\Lambda_{ij}=\delta_{ij}$. In this sense, the Evans–Gillan method represents an efficient alternative to methods based on the Green–Kubo formula in the limit of vanishing shear rates. For $a\neq 0$, such an equivalence no longer holds and the predictions based on the conventional heat field method differ from the ones derived from the familiar heat transport problem.[6,7] In the latter case, thermal transport is produced by the presence of a temperature gradient instead of by the action of an external force. A shear-rate-dependent thermal conductivity tensor $\lambda(a)$ can be identified from a generalized Fourier's law. Very recently, we have derived expressions for the xy, yy, and xy components of λ from an exact solution of the Boltzmann equation for Maxwell molecules.[11] Comparison of Λ and λ shows again that both tensors are different. In order to assess such discrepancies, in Fig. 1 we plot Λ_{yy} and

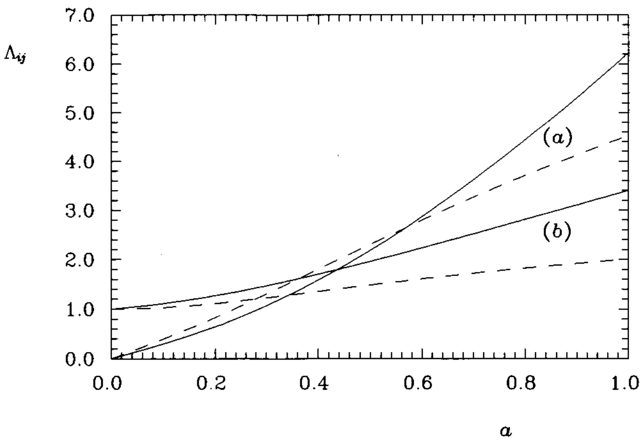

FIG. 1. Shear-rate dependence of some components of the tensor Λ_{ij}: (a) $-\Lambda_{xy}$, (b) Λ_{yy}. The dashed lines refer to their corresponding counterparts in the thermal gradient problem.

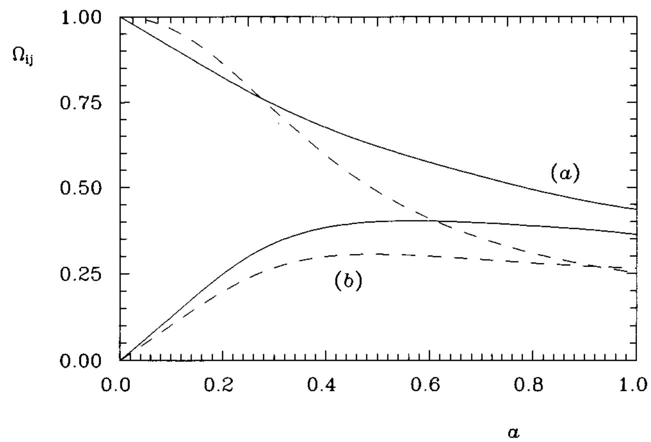

FIG. 2. Plot of some elements of the tensor Ω: (a) Ω_{yy}, (b) $-\Omega_{xy}$. The dashed lines refer to the BGK results.

$-\Lambda_{xy}$ and their corresponding counterparts λ_{yy} and $-\lambda_{xy}$ for $0\leqslant a\leqslant 1$. We see that each couple of coefficients exhibits a qualitative good agreement. As a matter of fact, Λ_{yy} and λ_{yy} increase with the shear rate so that the shear flow enhances the transport of energy along the direction of the gradient of the flow velocity (y axis). With respect to the xy component, it is negative and its magnitude increases as the shear rate increases. At a quantitative level, it is clear that the differences between both methods increase with the shear rate. For instance, for $a\approx 1$ (where the shear viscosity is about twice smaller than its zero shear rate value), the relative difference between the yy components is about 58% while it is about 25% for the xy component. These discrepancies become more significant for the zz component as both methods predict different behaviors. Similar conclusions were obtained in the case of the color-conductivity method.[14]

As said in the Introduction, it is not surprising that the conventional choice for Ω does not lead to consistent results when non-Newtonian effects are taken into account. In fact, this prediction was already stated by the "inventors" of the Evans–Gillan method. Nevertheless, the knowledge of the actual thermal conductivity tensor allows one to eliminate the above discrepancies by introducing a convenient shear-rate-dependent external field. By identifying $\nabla \ln T$ with $\boldsymbol{\epsilon}$ and by comparing Eq. (32) with Eq. (38) of Ref. 11, it is easy to show that the adequate choice is

$$\Omega_{ij}=(\Lambda^{-1})_{ik}\lambda_{kj}. \tag{36}$$

This relation also applies for the BGK model[7] although the shear-rate dependence of Λ and λ clearly differs from the Boltzmann one. It is evident that now the tensor Ω captures the anisotropy induced by the shear field. For $a=0$, it reduces to the one suggested in the Evans-Gillan method. In Fig. 2, we plot Ω_{yy} and $-\Omega_{xy}$ versus a. In general, they exhibit a highly nonlinear dependence on the shear rate. While Ω_{yy} monotonically decreases as the shear rate increases, $-\Omega_{xy}$ has a maximum for $a\approx 0.6$. Furthermore, we see that the BGK predictions cannot be considered as reliable, especially at finite shear rates.

Apart from obtaining the field susceptibility, it is also interesting to get the nonlinear shear viscosity. We are interested in analyzing the influence of the heat field on the shear viscosity in the limit of weak strength fields. In the same way as in Ref. 7, for the sake of clarity we will take $\epsilon_x=\epsilon_z=0$ and we will restrict ourselves to the second order approximation. By following similar mathematical steps as those made in the first order approximation, it is a simple matter of algebra to get the second order contribution to the shear viscosity η. This can be obtained from the xy component of the pressure tensor, whose expression is

$$P_{2,xy}=-\frac{15}{4}\,p\,\frac{k_BT}{m}\,\frac{2a[D\Omega_{yy}(1+6\alpha_0)-2E\Omega_{xy}]-3(1+2\alpha_0)^2(D\Omega_{xy}+E\Omega_{yy})}{4a^2+3(1+2\alpha_0)^3}\,\epsilon_y^2, \tag{37}$$

where

$$D=\Lambda_{yx}\Omega_{xy}+\Lambda_{yy}\Omega_{yy}, \tag{38}$$

$$E=\Lambda_{xx}\Omega_{xy}+\Lambda_{xy}\Omega_{yy}. \tag{39}$$

Taking into account Eqs. (10), (16), and (37), the shear viscosity coefficient can be identified as a function of both the (arbitrary) shear rate and the field strength (up to second order).[15] For $a=0$, $\eta/p=\eta_0/p=1+13.375(k_BT/m)\epsilon_y^2$ in the Evans–Gillan choice while $\eta_0/p=1+20.875(k_BT/m)\epsilon_y^2$ for the choice (36). In Fig. 3, we plot $\eta^*\equiv\eta/\eta_0$ for $\epsilon_y=0.1(m/k_BT)^{1/2}$. We observe that the net consequence of the action of the shear rate and the

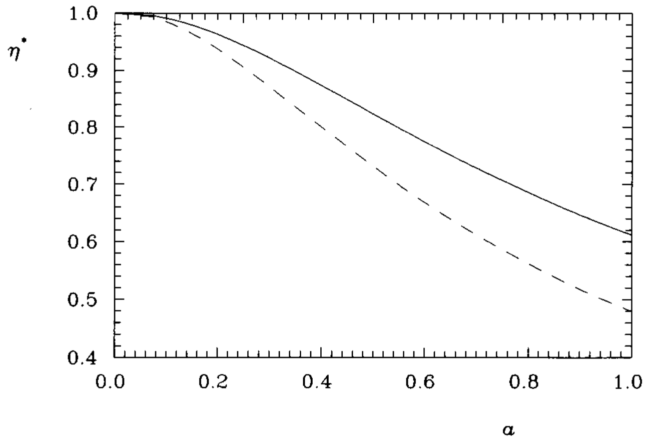

FIG. 3. Shear-rate dependence of the dimensionless shear viscosity $\eta^* \equiv \eta/\eta_0$ for $\epsilon_y = 0.1(m/k_BT)^{1/2}$ and for two choices of Ω_{ij}: $\Omega_{ij} = \delta_{ij}$ (——) and $\Omega_{ij} = (\Lambda^{-1})_{ik}\lambda_{kj}$ (– – –).

heat field is to produce an inhibition of the momentum trans port (shear thinning effect). This inhibition is more significant in the case of the modified force (36).

IV. CONCLUDING REMARKS

Coupling between heat and momentum transport in a dilute gas under uniform shear flow has been analyzed. The system is driven out of equilibrium by the presence of a shear field as well as by the action of a nonconservative external force. The force produces a heat flux in spite of the absence of a temperature gradient. This way of generating energy transport was proposed years ago by Evans[3] and Gillan and Dixon[4] as an efficient tool to study thermal bulk properties. In the limit of weak heat fields, but arbitrary shear rates, the energy transport is modified by the shearing motion. This effect is characterized through a shear-rate-dependent field susceptibility tensor κ, whose expression we aimed at determining. The derivation of such an expression is interesting by itself and also for establishing the possible equivalence with the transport properties obtained by applying more realistic boundary conditions.

A previous study of this problem was already carried out[7] by using the BGK kinetic model. Nevertheless, recent results[11,16] have shown the inadequacies of the BGK approximation to analyze the influence of the shear flow on the thermal conductivity λ in a system subjected to a weak thermal gradient. As a consequence, the conclusions obtained in Ref. 7 should be taken with caution, especially at finite shear rates. For this reason, we have analyzed again the same problem but now starting from the nonlinear Boltzmann equation in the particular case of Maxwell molecules. In this sense, the results presented here are *exact* to all orders in the shear rate.

According to the results derived in this paper for κ and in Ref. 11 for λ, we conclude again that both tensors are different when one uses the conventional choice of the heat field proposed in the Evans-Gillan method. This confirms the predictions made by Evans *et al.*[6] on the modified Green-Kubo relations for mechanical transport coefficients. While the shear-rate dependence of the yy and xy components exhibit a qualitative agreement, the zz component has a very different behavior. As a matter of fact, for small shear rates, one finds that $\Lambda_{yy} \approx 1+3.05a^2$, $\Lambda_{xy} \approx -2.90a$, and $\Lambda_{zz} \approx 1+0.72a^2$, but $\lambda_{yy} \approx 1+3.04a^2$, $\lambda_{xy} \approx -3.90a$, and $\lambda_{zz} \approx 1-1.18a^2$. With respect to the quantitative discrepancies, they become important for shear rates such as $a \simeq 1$.

All these discrepancies between both methods can be avoided by using a convenient heat field. This alternative force is explicitly determined as a function of the shear rate when one identifies the field strength $\boldsymbol{\epsilon}$ with the thermal gradient $\nabla T/T$. The form of the new external field takes into account the anisotropy induced in the system by the action of the shear field. The only obstacle of this new method is that one needs to determine the real thermal conductivity tensor λ, for which an *exact* expression is only known for Maxwell molecules. Nevertheless, beyond this interaction model, it may be expected that the shear-rate dependence of λ is very similar to that of Maxwell molecules.[16] In this context, and from a practical point of view, one could speculate that the heat field algorithm based on the use of the force defined by Eq. (36) could lead to reasonably consistent results for the thermal conductivity even for dense gases. It would be very interesting to perform computer simulations to check the above conjecture.

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