ELSEVIER

Physica A 213 (1995) 409–425

PHYSICA A

Exact moment solution of the Boltzmann equation for uniform shear flow

Andrés Santos, Vicente Garzó
Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain

Received 2 June 1994

Abstract

The Ikenberry-Truesdell exact solution to the Boltzmann equation for Maxwell molecules is revisited. This solution refers to a state characterized by a linear profile of the velocity flow and spatially uniform density and temperature. The solution is extended to include explicit expressions for the fourth-degree moments. It is shown that if the shear rate is larger than a certain critical value, the fourth-degree moments do not reach stationary values, even when the temperature is kept constant. The explicit shear-rate dependence of the moments below this critical value are obtained.

1. Introduction

The so-called uniform shear flow state has been extensively used in computer simulations [1] as well as in theoretical studies [2,3] to analyze rheological properties, i.e. nonlinear shear viscosity and viscometric effects. From a macroscopic point of view, it is characterized by a linear velocity field and uniform density and temperature.

Uniform shear flow is also interesting because it gives rise to one of the rare exact solutions of the Boltzmann equation in non-homogeneous situations, which was obtained almost forty years ago by Ikenberry and Truesdell [4]. This solution is restricted to Maxwell molecules (i.e. particles interacting via a repulsive potential $\varphi(r) \propto r^{-4}$), in which case the infinite hierarchy of velocity moments can be recursively solved. In particular, Ikenberry and Truesdell [4,5] obtained explicit expressions for the second-degree moments (i.e. the elements of the pressure tensor) as functions of time and for arbitrary values of the shear rate. In the long-time limit, the pressure tensor adopts a form consistent with a "normal" solution of the Boltzmann equation. The nonlinear shear-rate dependence of the pressure tensor exactly coincides with the one obtained

Elsevier Science B.V.
SSDI 0378-4371(94)00223-1

from the Bhatnagar-Gross-Krook (BGK) model kinetic equation [6,7]. In addition, the time evolution of the third-degree moments (which vanish in the normal state) have also been obtained [5].

To the best of our knowledge, a study of the fourth-degree moments has not been carried out thus far. Since these moments are not directly related to hydrodynamic quantities, they are apparently less interesting than the lower moments. In our opinion, however, there exist at least three reasons for considering them. First, since the moment method does not provide an explicit expression for the velocity distribution function, one could use the solution of the BGK equation [7] to gain insight into the main features of the exact distribution. Thus, the knowledge of the fourth-degree moments allows one to assess the reliability of the BGK model. Second, fourth-degree moments are necessary [8] to analyze the validity of a variational principle recently proposed for nonequilibrium steady states [9]. The third reason is to investigate whether a normal solution to the Boltzmann equation under uniform shear flow exists arbitrarily far from equilibrium. The fact that moments up to third degree are consistent with a normal state does not imply that the distribution function itself reaches a normal form. In fact, recent results [10] show that the fourth-degree moments do not adopt a normal form beyond a certain critical shear rate.

The aim of this paper is to analyze the time evolution and the shear-rate dependence of the fourth-degree moments. In Section 2 we define the uniform shear flow state from the point of view of the Boltzmann equation. The relevant rheological properties are presented. The third-degree moments are studied in Section 3. It is shown that, when conveniently scaled with the temperature, all of them vanish in the long-time limit. Section 4 contains the original part of the paper. It addresses the derivation of the fourth-degree moments. Finally, the results are discussed in Section 5.

2. Uniform shear flow

In a dilute gas, the time evolution of the velocity distribution function $f(\mathbf{r},\mathbf{v},t)$ is governed by the nonlinear Boltzmann equation. In absence of external forces, it reads [11]:

$$\frac{\partial}{\partial t}f+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}f=\int \mathrm{d}\mathbf{v}_1\int \mathrm{d}\Omega|\mathbf{v}-\mathbf{v}_1|\sigma(|\mathbf{v}-\mathbf{v}_1|,\theta)(f'f_1'-ff_1)$$
$$\equiv J[f,f]\ . \tag{1}$$

This equation must be supplemented with the appropriate initial and boundary conditions.

Let us introduce the velocity field

$$U_i(\mathbf{r})=a_{ij}r_j\ ,\quad a_{ij}=a\delta_{ix}\delta_{jy}\ , \tag{2}$$

where a is a constant shear rate. We define the uniform shear flow (USF) state as the one that is spatially homogeneous when the velocities of particles are referred to a

Lagrangian frame moving with the velocity field $\mathbf{U}(\mathbf{r})$. Consequently, the distribution function has the form

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

where $\mathbf{V} \equiv \mathbf{v} - \mathbf{U}(\mathbf{r})$, and Eq. (1) becomes

$$\frac{\partial}{\partial t} f - \frac{\partial}{\partial V_i} a_{ij} V_j f = J[f,f] . \tag{4}$$

Upon writing Eq. (4), we have assumed that the boundary conditions are consistent with the USF, i.e. initial conditions of the form $f(\mathbf{V},0)$ map into solutions $f(\mathbf{V},t)$ of Eq. (1). The usual boundary conditions used to generate the USF are the Lees-Edwards periodic boundary conditions [12,13]. It is interesting to notice that Eq. (4) can also represent a homogeneous state under the action of the nonconservative external force $F_i = -m a_{ij} V_j$. In addition, Eq. (4) is invariant under the transformations $V_z \to -V_z$, $(V_x, V_y) \to (-V_x, -V_y)$, and $(V_x, a) \to (-V_x, -a)$.

In the particular case of Maxwell molecules, i.e. particles interacting via a potential $\varphi = \kappa r^{-4}$, the collision rate $v\sigma(v,\theta)$ is independent of v. From a mathematical point of view, this makes the Boltzmann collision operator more tractable than for other interaction models. As a matter of fact, Eq. (4) for Maxwell molecules exhibits an interesting scaling property [13]. Let us introduce the scaled quantities

$$\overline{\mathbf{V}} = \mathrm{e}^{-\alpha t} \mathbf{V} , \tag{5}$$

$$\overline{f}(\overline{\mathbf{V}},t) = \mathrm{e}^{3\alpha t} f(\mathbf{V},t) , \tag{6}$$

where α is an arbitrary constant. Then, Eq. (4) reduces to

$$\frac{\partial}{\partial t}\overline{f} - \frac{\partial}{\partial \overline{V}_i}(a_{ij}\overline{V}_j + \alpha \overline{V}_i)\overline{f} = J[\overline{f},\overline{f}] . \tag{7}$$

This equation can be interpreted as the one corresponding to USF in presence of a nonconservative external force $-m\alpha\overline{\mathbf{V}}$. In our description, we will choose α as a function of the shear rate a by the condition that the (scaled) temperature reaches a constant value in the long-time limit, so that the above force plays the role of a thermostat force. This kind of thermostat forces is usually employed in nonequilibrium molecular dynamics simulations [1]. Henceforth, we will adopt the point of view behind Eq. (7) and drop the bars.

It is expected that in the limit of long times, the solution to Eq. (4) or, equivalently, to Eq. (7), reaches a "normal" form [11]. This implies that all the time dependence of f appears through the temperature $T(t)$. Consequently, with the thermostat choice for α, the solution to Eq. (7) is expected to reach a stationary form. As said in the Introduction, one of the motivations to study fourth-degree moments is to check the above expectation.

Although the explicit solution to Eq. (7) is not known, it can be exactly solved by the moment method. This is due to the fact that, in the case of Maxwell molecules, a collisional moment of degree k is a bilinear combination of moments of f of degrees k' and k'', such that $k'+k''=k$ [5]. This allows one, in principle, to solve recursively the hierarchy of moment equations. We will call *asymmetric* moments to those that vanish for solutions exhibiting the same invariance properties than Eq. (4). The rest of the moments will be referred to as *symmetric*. To clarify this point, let us introduce the moments

$$M_{k_1,k_2,k_3}=\frac{1}{n}\int d\mathbf{V}V_x^{k_1}V_y^{k_2}V_z^{k_3}f$$
$$=\langle V_x^{k_1}V_y^{k_2}V_z^{k_3}\rangle . \tag{8}$$

Then, M_{k_1,k_2,k_3} is a symmetric moment if k_1+k_2 and k_3 are even numbers. The degree of the moment M_{k_1,k_2,k_3} is $k=k_1+k_2+k_3$. There are $\frac{1}{2}(k+1)(k+2)$ independent moments of degree k.

Let us start with the first-degree moments

$$n\mathbf{u}=\int d\mathbf{V}\mathbf{V}f , \tag{9}$$

where n is the number density. The vector $\mathbf{u}$ measures the deviation of the local velocity from the linear velocity field $\mathbf{U}$. From Eq. (7) one easily gets

$$u_i(t)=[u_i(0)-a_{ij}u_j(0)t]\,e^{-\alpha t} . \tag{10}$$

This implies that, after a transient period of the order of α^{-1}, the flow velocity is given by the linear field (2).

The second-degree moments are related to the pressure tensor:

$$P_{ij}=m\int d\mathbf{V}V_iV_jf . \tag{11}$$

The temperature T is defined from the trace of this tensor as $nk_BT=p=\frac{1}{3}\mathrm{Tr}P$. Eq. (7) yields [5]

$$\frac{\partial}{\partial t}P_{ij}+(a_{ik}P_{jk}+a_{jk}P_{ik})+2\alpha P_{ij}=-\nu(P_{ij}-p\delta_{ij}) . \tag{12}$$

Here, ν is an effective collision frequency defined as

$$\nu=3nA_2 , \tag{13}$$

where

$$A_n\equiv\int d\Omega\sin^n\frac{\theta}{2}\cos^n\frac{\theta}{2}v\sigma(v,\theta) . \tag{14}$$

The numerical value of A_2 is $A_2\simeq 1.3703\sqrt{2\kappa/m}$ [5]. It is interesting to remark that Eq. (12) coincides with the one derived from the BGK model [7]. It is convenient to choose ν^{-1} as the time unit. This means that we use dimensionless quantities $t^*=\nu t$,

$a^* = a/\nu$, and $\alpha^* = \alpha/\nu$. In the following, these dimensionless quantities will be assumed and we will omit the asterisks.

The two asymmetric moments P_{xz} and P_{yz} are simply given by

$$P_{yz}(t) = P_{yz}(0)\,\mathrm{e}^{-(1+2\alpha)t}, \tag{15}$$

$$P_{xz}(t) = [P_{xz}(0) - atP_{yz}(0)]\,\mathrm{e}^{-(1+2\alpha)t}. \tag{16}$$

The following combination of symmetric moments has a similar time behavior:

$$P_{yy}(t) - P_{zz}(t) = [P_{yy}(0) - P_{zz}(0)]\,\mathrm{e}^{-(1+2\alpha)t}. \tag{17}$$

From Eq. (12) one can get the following closed differential equation for p:

$$\left(\frac{\partial}{\partial t} + 2\alpha\right)\left(\frac{\partial}{\partial t} + 2\alpha + 1\right)^2 p = \tfrac{2}{3}a^2 p. \tag{18}$$

So far, α is arbitrary. The three roots of the characteristic equation of Eq. (18) are

$$\lambda_1 = \lambda - 2\alpha, \tag{19}$$

$$\lambda_{2,3} = -(\tfrac{1}{2}\lambda + 1 + 2\alpha) \pm \mathrm{i}\,\omega, \tag{20}$$

where

$$\lambda = \tfrac{4}{3}\sinh^2[\tfrac{1}{6}\cosh^{-1}(1+9a^2)], \tag{21}$$

$$\omega = [\lambda(\tfrac{3}{4}\lambda + 1)]^{1/2}. \tag{22}$$

As said before, we choose α under the condition that the pressure reaches a stationary value in the long-time limit. Consequently, $\alpha = \lambda/2$. The time evolution of p, P_{yy}, and P_{xy} is then

$$p(t) = A + \mathrm{e}^{-(1+3\alpha)t}(B\cos\omega t + C\sin\omega t), \tag{23}$$

$$P_{yy}(t) = \frac{1}{1+2\alpha}\{A - \tfrac{1}{2}\mathrm{e}^{-(1+3\alpha)t}[(B + \frac{\omega}{\alpha}C)\cos\omega t + (C - \frac{\omega}{\alpha}B)\sin\omega t]\}, \tag{24}$$

$$P_{xy}(t) = -\frac{3}{2a}\{2A\alpha - \mathrm{e}^{-(1+3\alpha)t} \times [((1+\alpha)B - \omega C)\cos\omega t + ((1+\alpha)C + \omega B)\sin\omega t]\}, \tag{25}$$

where A, B, and C are constants given by the initial conditions. The relaxation time of p, P_{yy}, and P_{xy} is $(1+3\alpha)^{-1}$, while the remaining elements of the pressure tensor have a longer relaxation time, namely $(1+2\alpha)^{-1}$.

From a rheological point of view, the most relevant transport properties of the problem are the reduced nonlinear shear viscosity η and viscometric functions Ψ_1 and Ψ_2. They are defined as

$$\eta = -\lim_{t\to\infty}\frac{1}{a}\frac{P_{xy}(t)}{p(t)}, \tag{26}$$

$$\Psi_1 = \lim_{t\to\infty} \frac{1}{a^2} \frac{P_{yy}(t) - P_{xx}(t)}{p(t)} , \tag{27}$$

$$\Psi_2 = \lim_{t\to\infty} \frac{1}{a^2} \frac{P_{zz}(t) - P_{yy}(t)}{p(t)} . \tag{28}$$

From Eqs. (17) and (23)–(25) one gets

$$\eta = (1+2\alpha)^{-2} , \tag{29}$$

$$\Psi_1 = -2(1+2\alpha)^{-3} , \tag{30}$$

$$\Psi_2 = 0 , \tag{31}$$

where we have taken into account that

$$a^2 = 3\alpha(1+2\alpha)^2 . \tag{32}$$

3. Third-degree moments

Now we are going to analyze the time behavior of third-degree moments, i.e. moments of the form (8) with $k_1 + k_2 + k_3 = 3$. There are 10 independent moments. Since all of them are asymmetric, one expects that they go to zero in the long-time limit. For computational purposes, it is convenient to work with the following moments:

$$M_{2|i}(t) = \frac{1}{n} \int d\mathbf{V} Y_{2|i}(\mathbf{V}) f(\mathbf{V},t) , \tag{33}$$

$$M_{0|ijk}(t) = \frac{1}{n} \int d\mathbf{V} Y_{0|ijk}(\mathbf{V}) f(\mathbf{V},t) , \tag{34}$$

where

$$Y_{2|i}(\mathbf{V}) = V^2 V_i , \tag{35}$$

$$Y_{0|ijk}(\mathbf{V}) = V_i V_j V_k - \tfrac{1}{5} V^2 (V_i \delta_{jk} + V_j \delta_{ik} + V_k \delta_{ij}) . \tag{36}$$

The corresponding collisional moments are [5]

$$\frac{1}{n} \int d\mathbf{V} Y_{2|i}(\mathbf{V}) J[f,f] = -\tfrac{2}{3} \nu M_{2|i} , \tag{37}$$

$$\frac{1}{n} \int d\mathbf{V} Y_{0|ijk}(\mathbf{V}) J[f,f] = -\tfrac{3}{2} \nu M_{0|ijk} . \tag{38}$$

As the set of 10 independent third-degree moments, we take

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

Taking moments in Eq. (7), one gets the following set of equations:

$$(D + \tfrac{3}{2} + 3\alpha)(\tfrac{1}{4} M_{0|xxz} + M_{0|yyz}) = 0 , \tag{39}$$

$$(D+\tfrac{3}{2}+3\alpha)(\tfrac{1}{4}M_{0|xxy}+M_{0|yzz})=0\,, \tag{40}$$

$$\begin{pmatrix} D+\frac{2}{3}+3\alpha & 0 & 2a \\ 0 & D+\frac{3}{2}+3\alpha & -\frac{2}{5}a \\ \frac{1}{5}a & a & D+\frac{3}{2}+3\alpha \end{pmatrix}\cdot\begin{pmatrix} M_{2|z} \\ M_{0|yyz} \\ M_{0|xyz} \end{pmatrix}=0\,, \tag{41}$$

$$\begin{pmatrix} D+\frac{2}{3}+3\alpha & \frac{7}{5}a & 2a & 0 \\ \frac{2}{5}a & D+\frac{2}{3}+3\alpha & 0 & 2a \\ \frac{8}{25}a & 0 & D+\frac{3}{2}+3\alpha & \frac{8}{5}a \\ 0 & \frac{8}{25}a & -\frac{23}{20}a & D+\frac{3}{2}+3\alpha \end{pmatrix}\cdot\begin{pmatrix} M_{2|x} \\ M_{2|y} \\ M_{0|xxy} \\ M_{0|xyy} \end{pmatrix}$$
$$=a(\tfrac{1}{4}M_{0|xxy}+M_{0|yzz})\begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}\,, \tag{42}$$

$$(D+\tfrac{3}{2}+3\alpha)M_{0|xzz}=a(\tfrac{2}{5}M_{2|y}+\tfrac{2}{5}M_{0|xxy}-M_{0|yzz})\,. \tag{43}$$

In these equations, $D\equiv d/dt$ and we have again chosen ν^{-1} as the time unit. The characteristic relaxation times are ℓ_σ^{-1}, where ℓ_σ are the roots of the characteristic equations. More specifically, $\ell_1=\ell_2=\ell_3=\frac{3}{2}+3\alpha$, ℓ_{4-6} are the roots of the cubic equation

$$(\tfrac{3}{2}+3\alpha-\ell)^2(\tfrac{2}{3}+3\alpha-\ell)=\tfrac{1}{3}a^2\,, \tag{44}$$

and ℓ_{7-10} are the roots of the quartic equation

$$(\tfrac{3}{2}+3\alpha-\ell)^2(\tfrac{2}{3}+3\alpha-\ell)^2=2a^2(\tfrac{31}{36}+3\alpha-\ell)\,. \tag{45}$$

Fig. 1 shows the shear rate dependence of the real parts of the eigenvalues ℓ_σ. Except ℓ_7, all the eigenvalues increase monotonically with the shear rate. For shear rates smaller than $a\simeq 31$, ℓ_7 remains smaller than its equilibrium value $(\frac{2}{3})$. This means that, if $a<31$, the characteristic relaxation time for some of the third degree moments is longer than that of equilibrium.

For shear rates larger than $a=\sqrt{18/31}$, ℓ_7 is smaller than 3α. This implies that, in absence of thermostat, some of the moments increase in time. Truesdell and Muncaster [5] refer to this behavior as an *instability* in the heat flux solution. However, this is simply a consequence of viscous heating. After scaling the moments with the thermal velocity, all of them decay to zero.

4. Fourth-degree moments

In this Section, we are going to analyze the time evolution of the fourth-degree moments and the shear-rate dependence of their stationary values. To the best of our

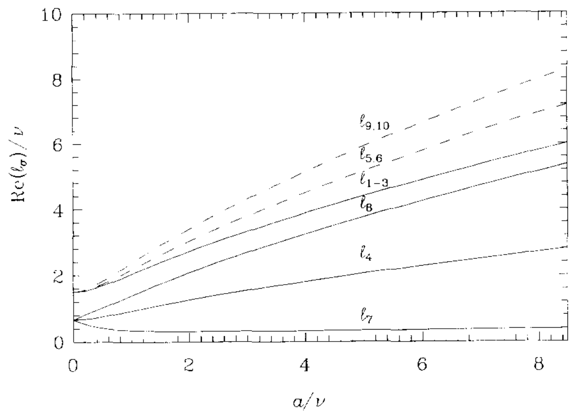

Fig. 1. Shear-rate dependence of the real parts of the eigenvalues corresponding to the evolution of the third-degree moments. The solid (dashed) lines refer to the real (complex) eigenvalues.

knowledge, such an analysis has not been made before, although some results have been used to discuss the existence of a critical shear rate, beyond which a steady state does not exist [10].

We consider the following set of polynomials [5]:

$$Y_{4|0}(\mathbf{V}) = V^4 , \tag{46}$$

$$Y_{2|ij}(\mathbf{V}) = V^2(V_iV_j - \tfrac{1}{3}V^2\delta_{ij}) , \tag{47}$$

$$\begin{aligned} Y_{0|ijkl}(\mathbf{V}) = {} & V_iV_jV_kV_l - \tfrac{1}{7}V^2(V_iV_j\delta_{kl} + V_iV_k\delta_{jl} + V_iV_l\delta_{kj} + V_jV_k\delta_{il} \\ & + V_jV_l\delta_{ik} + V_kV_l\delta_{ij}) + \tfrac{1}{35}V^4(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) . \end{aligned} \tag{48}$$

We denote by $M_{2n|ij\ldots}$ the moments of f corresponding to the polynomials $Y_{2n|ij\ldots}(\mathbf{V})$. Our choice for the 15 independent fourth-degree moments is

$$\{M_{4|0}, M_{2|xx}, M_{2|yy}, M_{2|xy}, M_{2|xz}, M_{2|yz}, M_{0|xxxx}, M_{0|yyyy}, M_{0|zzzz},$$
$$M_{0|xxxy}, M_{0|xxxz}, M_{0|xyyy}, M_{0|xzzz}, M_{0|yyyz}, M_{0|yzzz}\} .$$

The moments of the Boltzmann collision operator for Maxwell molecules are [5]:

$$\frac{1}{n}\int d\mathbf{V} Y_{4|0}(\mathbf{V}) J[f,f] = -\tfrac{2}{3}\nu[M_{4|0} + \frac{1}{n^2m^2}(P_{ij}P_{ij} - 18p^2)] , \tag{49}$$

$$\frac{1}{n}\int \mathrm{d}\mathbf{V} Y_{2|ij}(\mathbf{V})J[f,f] = -\tfrac{7}{6}\nu[M_{2|ij} + \frac{1}{7n^2m^2}(4P_{ik}P_{kj} - 15pP_{ij} - \tfrac{4}{3}P_{kl}P_{kl}\delta_{ij} + 15p^2\delta_{ij})] , \tag{50}$$

$$\frac{1}{n}\int \mathrm{d}\mathbf{V} Y_{0|xxxx}(\mathbf{V})J[f,f] = -\nu' M_{0|xxxx} + \tfrac{3}{35}(2\nu - \nu')\frac{1}{n^2m^2}[8P_{xx}^2 + 3(P_{yy}^2 + P_{zz}^2) + 2P_{yy}P_{zz} - 8P_{xx}(P_{yy} + P_{zz}) - 16(P_{xy}^2 + P_{xz}^2) + 4P_{yz}^2] , \tag{51}$$

$$\frac{1}{n}\int \mathrm{d}\mathbf{V} Y_{0|xxxy}(\mathbf{V})J[f,f] = -\nu' M_{0|xxxy} - \tfrac{3}{7}(2\nu - \nu')\frac{1}{n^2m^2}[2P_{yz}P_{xz} + P_{xy}(3P_{yy} + P_{zz} - 4P_{xx})] . \tag{52}$$

In Eqs. (51) and (52), ν' is given by

$$\nu' = \tfrac{7}{12}(4 - 5\frac{A_4}{A_2})\nu , \tag{53}$$

where the coefficients A_n are defined in Eq. (14). From Ref. [14], one gets $\nu' \simeq 1.873\nu$. In the case of the isotropic scattering model, $\nu' = \frac{7}{4}\nu$. It is clear that from Eqs. (51) and (52), one can obtain similar equations for the remaining moments of the set by adequately changing indices.

Taking velocity moments in Eq. (7), one gets a closed set of equations. For simplicity, we will assume that the second-degree moments P_{ij} take their stationary values. Because of the symmetries of Eq. (7), the symmetric and asymmetric moments are uncoupled. Although the relevant moments are the symmetric ones, we first analyze the time evolution of the asymmetric moments, for the sake of completeness. There are 6 asymmetric moments, which verify the following set of equations:

$$(D + 4\alpha + \nu')(M_{0|yyyz} - M_{0|yzzz}) = 0 , \tag{54}$$

$$\begin{pmatrix} D + 4\alpha + \frac{7}{6} & \frac{9}{7}a & 0 & -2a \\ \frac{2}{7}a & D + 4\alpha + \frac{7}{6} & -2a & 0 \\ 0 & -\frac{12}{49}a & D + 4\alpha + \nu' & -\frac{11}{14}a \\ -\frac{12}{49}a & 0 & \frac{12}{7}a & D + 4\alpha + \nu' \end{pmatrix} \cdot \begin{pmatrix} M_{2|xz} \\ M_{2|yz} \\ M_{0|xxxz} + M_{0|xzzz} \\ M_{0|yyyz} + M_{0|yzzz} \end{pmatrix} = \tfrac{1}{2}a(M_{0|yyyz} - M_{0|yzzz}) \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} , \tag{55}$$

$$(D + 4\alpha + \nu')(M_{0|xxxz} - M_{0|xzzz}) = \tfrac{7}{2}a(M_{0|yyyz} + M_{0|yzzz}) - \tfrac{1}{2}a(M_{0|yyyz} - M_{0|yzzz}) . \tag{56}$$

The eigenvalues are $4\alpha + \nu'$ (double) and the roots of a quartic equation, all of them having a positive real part. Consequently, all the asymmetric moments decay to zero in the long-time limit.

The set of equations for the 9 symmetric moments are given by

$$(D + 4\alpha + \nu')(3M_{0|xxxx} - 4M_{0|yyyy} - 4M_{0|zzzz}) = 0\,, \tag{57}$$

$$(D\delta_{\sigma\sigma'} + \mathcal{L}_{\sigma\sigma'})\mathcal{M}_{\sigma'} = \mathcal{C}_\sigma\,, \quad \sigma = 1, \ldots, 8\,. \tag{58}$$

Here,

$$\mathcal{M} = \begin{pmatrix} M_{4|0} \\ M_{2|xx} \\ M_{2|yy} \\ M_{0|yyyy} \\ M_{0|zzzz} \\ M_{2|xy} \\ M_{0|xxxy} \\ M_{0|xyyy} \end{pmatrix}, \tag{59}$$

$$\mathcal{L} = \begin{pmatrix} 4\alpha + \frac{2}{3} & 0 & 0 & 0 & 0 & 4a & 0 & 0 \\ 0 & 4\alpha + \frac{7}{6} & 0 & 0 & 0 & \frac{32}{21}a & 2a & 0 \\ 0 & 0 & 4\alpha + \frac{7}{6} & 0 & 0 & -\frac{10}{21}a & 0 & 2a \\ 0 & 0 & 0 & 4\alpha + \nu' & 0 & -\frac{96}{245}a & 0 & -\frac{12}{7}a \\ 0 & 0 & 0 & 0 & 4\alpha + \nu' & \frac{24}{245}a & \frac{12}{7}a & \frac{12}{7}a \\ \frac{7}{15}a & \frac{2}{7}a & \frac{9}{7}a & -\frac{7}{3}a & -\frac{1}{3}a & 4\alpha + \nu' & 0 & 0 \\ 0 & \frac{15}{49}a & -\frac{6}{49}a & -\frac{5}{2}a & -\frac{5}{14}a & 0 & 4\alpha + \nu' & 0 \\ 0 & -\frac{6}{49}a & \frac{15}{49}a & 2a & \frac{1}{7}a & 0 & 0 & 4\alpha + \nu' \end{pmatrix}, \tag{60}$$

$$\mathcal{C} = a\mathcal{M}_9 \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{3} \\ \frac{5}{14} \\ -\frac{1}{7} \end{pmatrix} + \frac{(2k_BT/m)^2}{(1+2\alpha)^2} \begin{pmatrix} \frac{1}{2}(5 + 18\alpha + 12\alpha^2) \\ \alpha(1+\alpha) \\ -\frac{1}{4}\alpha(3+2\alpha) \\ -\frac{9}{35}\alpha(4-9\alpha)(2-\nu') \\ \frac{9}{35}\alpha(1+9\alpha)(2-\nu') \\ -\frac{1}{24}a\dfrac{7+6\alpha}{1+2\alpha} \\ -\frac{18}{7}a\dfrac{\alpha}{1+2\alpha}(2-\nu') \\ \frac{27}{14}a\dfrac{\alpha}{1+2\alpha}(2-\nu') \end{pmatrix}. \tag{61}$$

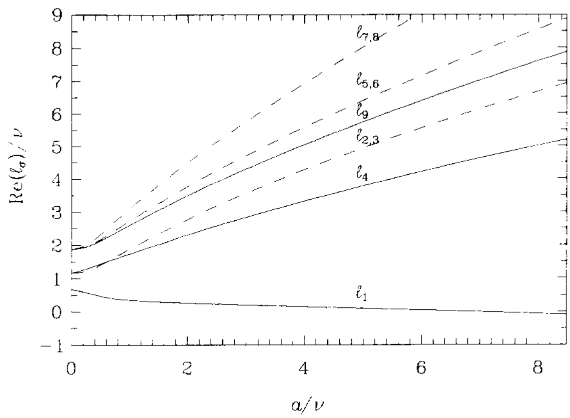

Fig. 2. Shear-rate dependence of the real parts of the eigenvalues corresponding to the evolution of the symmetric fourth-degree moments. The solid (dashed) lines refer to the real (complex) eigenvalues.

Eq. (57) shows that the combination $\mathcal{M}_9 \equiv 3M_{0|xxxx} - 4(M_{0|yyyy} + M_{0|zzzz}) = 6\langle V_y^2 V_z^2\rangle - \langle V_y^4\rangle - \langle V_z^4\rangle$ decays to zero with a characteristic time $(4\alpha + \nu')^{-1}$. This exact behavior is similar to that of $\langle V_y^2\rangle - \langle V_z^2\rangle$. More in general, it can be easily shown that those eigenfunctions of the linearized Boltzmann collision operator that do not depend on V_x give rise to moments decaying to zero. The analysis shows that the only symmetric moment of degree k belonging to the above class is

$$\frac{1}{2}\langle (V_y + \mathrm{i}\, V_z)^k + (V_y - \mathrm{i}\, V_z)^k\rangle = \sum_{q=0}^{k/2} (-1)^q \binom{k}{2q} \langle V_y^{2q} V_z^{k-2q}\rangle . \tag{62}$$

The solution of Eq. (58) can be written as

$$\mathcal{M}(t) = \mathrm{e}^{-\mathcal{L}t} \cdot [\mathcal{M}(0) - \mathcal{M}^{\mathrm{ss}}] + \mathcal{M}^{\mathrm{ss}} , \tag{63}$$

where

$$\mathcal{M}_\sigma^{\mathrm{ss}} = (\mathcal{L}^{-1})_{\sigma\sigma'} \mathcal{C}_{\sigma'} . \tag{64}$$

Upon writing Eq. (63), we have assumed that $\mathcal{M}_9 = 0$, so that $\mathcal{C}_\sigma$ is constant. The time evolution of $\mathcal{M}_\sigma$ is governed by the eigenvalues ℓ_σ of the matrix $\mathcal{L}_{\sigma\sigma'}$. Fig. 2 shows the shear-rate dependence of the real parts of the eigenvalues $\ell_\sigma, \sigma = 1, \ldots, 8$ obtained by numerically solving the corresponding eighth-degree characteristic equation with $\nu' = 1.873$, and of $\ell_9 = 4\alpha + \nu'$. The most remarkable feature of the figure is that the eigenvalue ℓ_1 monotonically decreases with the shear rate and eventually vanishes at a critical shear rate $a_c \simeq 6.845$.

This implies that for shear rates larger than a_c, the fourth-degree moments do not reach stationary values in the long-time limit. As a consequence, the USF velocity distribution function does not adopt the form of a normal solution to the Boltzmann equation. The implications of this singular behavior have been discussed in Ref. [10].

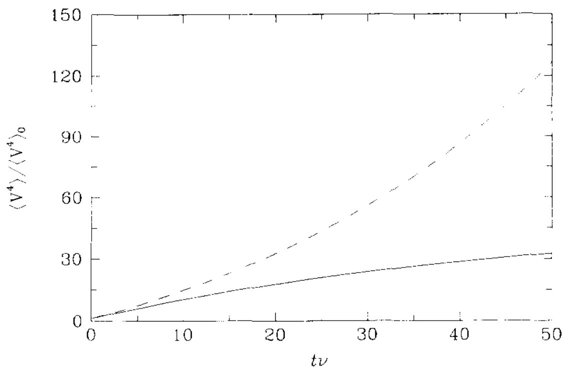

Fig. 3. Time evolution of $\langle V^4\rangle$ relative to its equilibrium value $\langle V^4\rangle_0 = \frac{15}{4}(2k_BT/m)^2$ for two values of the shear rate: $a \simeq 6.45$ (solid line) and $a \simeq 7.33$ (dashed line). In both cases the initial condition is a Gaussian distribution corresponding to the stationary second-degree moments.

Although Eq. (63) gives the full time behavior of m_σ (see Appendix A), for times much larger than $\max\{(\mathrm{Re}\,\ell_\sigma)^{-1}, \sigma = 2\ldots,9\} \leq 6/7$, the asymptotic behavior is

$$\mathcal{M}_\sigma(t) \approx \mathcal{M}_\sigma^{ss} + \mathcal{M}_\sigma^0 \mathrm{e}^{-\ell_1 t}\,, \tag{65}$$

where $\mathcal{M}_\sigma^0$ is a constant depending on the initial conditions. As an illustration, we have plotted in Fig. 3 the time evolution of $\langle V^4\rangle$ relative to its equilibrium value for two values of the shear rate: $a \simeq 6.45$ ($\alpha = \frac{5}{4}$) and $a \simeq 7.33$ ($\alpha = \frac{4}{3}$). While in the first case ($a < a_c$) $\langle V^4\rangle$ reaches a stationary value for times larger than $\ell_1^{-1} \simeq 46.5$, it grows exponentially with a characteristic time $-\ell_1^{-1} \simeq 37.1$ in the second case ($a > a_c$).

For shear rates smaller than a_c, the steady-state values of the moments are given by Eq. (58). Their explicit forms as functions of the shear rate are listed in Appendix B. As said in the Introduction, the derivation of these expressions was one of the main motivations of this paper.

5. Conclusions

In this paper we have revisited the Ikenberry-Truesdell solution of the Boltzmann equation for Maxwell molecules under uniform shear flow. This solution is given in terms of the velocity moments of the distribution function. In particular, Ikenberry and Truesdell [4,5] obtained the explicit nonlinear dependence of the rheological properties (shear viscosity and viscometric functions) on the shear rate. Here we have extended this solution to include the fourth-degree moments. The motivation to consider these moments is not only academic.

Recently, a variational principle for characterizing thermostatted nonequilibrium steady states has been proposed [9]. The knowledge of an exact solution of the Boltzmann equation allows one to test the above variational principle for dilute gases. In order to do that, second-degree moments are not sufficient and the fourth-degree moments are required [8].

A more fundamental question refers to the existence of a normal solution to the Boltzmann equation under *uniform* shear flow far from equilibrium. If such a normal solution exists, then any fourth-degree moment, conveniently scaled with the temperature, should reach in the long-time limit a function of the *reduced* shear rate independently of the initial conditions. Here, we have shown that the above assertion fails if the reduced shear rate is larger than a certain critical value. The possible implications of this fact have been discussed in Ref. [10].

In principle, by following a recursive scheme, one could obtain higher-degree moments. However, a closed expression for the velocity distribution function does not seem attainable. As an alternative, one can start from a simplified kinetic model of the Boltzmann equation and get the corresponding distribution function. In particular, the distribution function obtained from the Bhatnagar-Gross-Krook (BGK) kinetic model is known [7]. The BGK model is interesting because it leads to the same second-degree moments as the Ikenberry-Truesdell solution of the Boltzmann equation. The comparison of the fourth-degree moments obtained from the BGK equation with those derived here can be used to assess the reliability of the BGK model. This comparison is the subject of the subsequent paper [15].

Acknowledgements

We are grateful to Drs. J.J. Brey and J.W. Dufty for discussions about the topic of this paper. This work has been supported by the Dirección General de Investigación Científica y Técnica (Spain) though Grant No. PB91-0316.

Appendix A. Time evolution of the fourth-degree moments

In order to get the explicit time-dependence of the fourth-degree moments from Eq. (63), it is convenient to diagonalize the matrix $\mathcal{L}$. Let us denote by $\{x_\sigma, \sigma = 1, \dots, 8\}$ the eigenvectors of $\mathcal{L}$. Since the matrix $\mathcal{L}$ is not Hermitian, their eigenvectors do not form an orthogonal set. The matrix of change of basis is $\mathcal{U}$, where $\mathcal{U}_{\sigma'\sigma}$ is the σ'-component of x_σ. Consequently,

$$\mathrm{e}^{-\mathcal{L}t} = \mathcal{U} \cdot \mathcal{D}(t) \cdot \mathcal{U}^{-1} , \tag{A.1}$$

where $\mathcal{D}(t)$ is a diagonal matrix whose σ-element is $\mathrm{e}^{-\ell_\sigma t}$.

As an application, we consider the cases $\alpha = \frac{5}{4}$ and $\alpha = \frac{4}{3}$, which according to Eq. (32) correspond to shear rates $a \simeq 6.45$ and $a \simeq 7.33$, respectively. After calculating the corresponding eigenvalues and eigenvectors, one gets the following expressions for $\langle V^4 \rangle$:

$$
\begin{aligned}
(2k_BT/m)^{-2}\langle V^4\rangle = {} & 182.7 - 178.2\,\mathrm{e}^{-0.0215t} \\
& + \mathrm{e}^{-5.82t}[0.46\cos(2.83t) + 3.03\sin(2.83t)] \\
& -0.014\,\mathrm{e}^{-4.40t} - \mathrm{e}^{-7.48t}[0.012\cos(1.75t) + 0.011\sin(1.75t)] \\
& + \mathrm{e}^{-9.52t}[0.64\cos(4.65t) - 0.42\sin(4.65t)]\,,
\end{aligned} \tag{A.2}
$$

$$
\begin{aligned}
(2k_BT/m)^{-2}\langle V^4\rangle = {} & -160.4 + 164.8\,\mathrm{e}^{0.0270t} \\
& + \mathrm{e}^{-6.31t}[0.51\cos(3.21t) + 3.24\sin(3.21t)] \\
& -0.013\,\mathrm{e}^{-4.76t} - \mathrm{e}^{-8.10t}[0.010\cos(1.91t) + 0.011\sin(1.91t)] \\
& + \mathrm{e}^{-10.38t}[0.73\cos(5.05t) - 0.46\sin(5.05t)]\,.
\end{aligned} \tag{A.3}
$$

Here, Eq. (A.1) refers to $\alpha = \frac{5}{4}$ and Eq. (A.3) to $\alpha = \frac{4}{3}$. In both cases, we have taken the Gaussian distribution consistent with the stationary pressure tensor as the initial condition [15].

Appendix B. Steady-state values of the fourth-degree moments

In this Appendix we give the explicit shear-rate dependence of the stationary fourth-degree moments. Let us start by considering the expansion in powers of the shear rate for arbitrary ν'. Up to super-Burnett hydrodynamic order (a^3), the result is

$$
\mathcal{M}^{\mathrm{ss}} = \left(\frac{2k_BT}{m}\right)^2 \left(\mathcal{M}^{(0)} + \mathcal{M}^{(1)}a + \mathcal{M}^{(2)}a^2 + \mathcal{M}^{(3)}a^3 + \cdots\right)\,, \tag{B.1}
$$

where

$$
\mathcal{M}^{(0)} = \begin{pmatrix} \frac{15}{4} \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{B.2}
$$

$$
\mathcal{M}^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -\frac{7}{4} \\ 0 \\ 0 \end{pmatrix}, \tag{B.3}
$$

$$\mathcal{M}^{(2)} = \begin{pmatrix} \frac{5}{2} \\ \frac{18}{7} \\ -\frac{13}{14} \\ -\frac{12}{35}\frac{4-\nu'}{\nu'} \\ \frac{3}{35}\frac{4-\nu'}{\nu'} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \tag{B.4}$$

$$\mathcal{M}^{(3)} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \frac{4259\nu' - 4536}{1715\nu'} \\ -3\frac{756 + 409\nu' - 196\nu'^2}{686\nu'^2} \\ 3\frac{616 + 277\nu' - 147\nu'^2}{686\nu'^2} \end{pmatrix}. \tag{B.5}$$

The full nonlinear dependence on the shear rate for arbitrary ν' can also be obtained, but it is too complicated and not very illuminating. Here we list the full shear-rate dependence for the value $\nu' = 1.873$ obtained by numerical integration in Ref. [14]. They are given by

$$M_{4|0} = \left(\frac{2k_BT}{m}\right)^2 \frac{15}{4}\frac{1}{(1+2\alpha)^2}\frac{N_1(\alpha)}{\Delta(\alpha)}, \tag{B.6}$$

$$M_{2|xx} = \left(\frac{2k_BT}{m}\right)^2 \frac{54}{7}\frac{\alpha}{(1+2\alpha)^2}\frac{N_2(\alpha)}{\Delta(\alpha)}, \tag{B.7}$$

$$M_{2|yy} = -\left(\frac{2k_BT}{m}\right)^2 \frac{39}{14}\frac{\alpha}{(1+2\alpha)^2}\frac{N_3(\alpha)}{\Delta(\alpha)}, \tag{B.8}$$

$$M_{0|yyyy} = -\left(\frac{2k_BT}{m}\right)^2 \frac{\alpha}{(1+2\alpha)^2}\frac{N_4(\alpha)}{\Delta(\alpha)}, \tag{B.9}$$

$$M_{0|zzzz} = \left(\frac{2k_BT}{m}\right)^2 \frac{1}{4}\frac{\alpha}{(1+2\alpha)^2}\frac{N_5(\alpha)}{\Delta(\alpha)}, \tag{B.10}$$

$$M_{2|xy} = -\left(\frac{2k_BT}{m}\right)^2 \frac{7}{4} \frac{a}{(1+2\alpha)^3} \frac{N_6(\alpha)}{\Delta(\alpha)} , \tag{B.11}$$

$$M_{0|xxxy} = -\left(\frac{2k_BT}{m}\right)^2 \frac{a\alpha}{(1+2\alpha)^3} \frac{N_7(\alpha)}{\Delta(\alpha)} , \tag{B.12}$$

$$M_{0|xyyy} = \left(\frac{2k_BT}{m}\right)^2 \frac{a\alpha}{(1+2\alpha)^3} \frac{N_8(\alpha)}{\Delta(\alpha)} , \tag{B.13}$$

where

$$\begin{aligned}\Delta(\alpha) = 1 &+ 18.37\alpha + 142.8\alpha^2 + 608.7\alpha^3 + 1524\alpha^4 + 2167\alpha^5 + 1310\alpha^6 \\ &-625.1\alpha^7 - 1433\alpha^8 - 644.3\alpha^9 ,\end{aligned} \tag{B.14}$$

$$\begin{aligned}N_1(\alpha) = 1 &+ 24.37\alpha + 271.2\alpha^2 + 1796\alpha^3 + 7777\alpha^4 + 22968\alpha^5 + 47063\alpha^6 \\ &+67138\alpha^7 + 66381\alpha^8 + 44959\alpha^9 + 19949\alpha^{10} + 4639\alpha^{11} ,\end{aligned} \tag{B.15}$$

$$\begin{aligned}N_2(\alpha) = 1 &+ 22.61\alpha + 222.8\alpha^2 + 1258\alpha^3 + 4496\alpha^4 + 10636\alpha^5 + 16933\alpha^6 \\ &+18181\alpha^7 + 13078\alpha^8 + 6097\alpha^9 + 1503\alpha^{10} ,\end{aligned} \tag{B.16}$$

$$\begin{aligned}N_3(\alpha) = 1 &+ 24.11\alpha + 249.6\alpha^2 + 1466\alpha^3 + 5423\alpha^4 + 13213\alpha^5 + 21581\alpha^6 \\ &+23687\alpha^7 + 17374\alpha^8 + 8258\alpha^9 + 2081\alpha^{10} ,\end{aligned} \tag{B.17}$$

$$\begin{aligned}N_4(\alpha) = 1.168 &+ 19.22\alpha + 127.3\alpha^2 + 404.7\alpha^3 + 419.2\alpha^4 - 1255\alpha^5 - 5274\alpha^6 \\ &-8776\alpha^7 - 8248\alpha^8 - 4755\alpha^9 - 1491\alpha^{10} ,\end{aligned} \tag{B.18}$$

$$\begin{aligned}N_5(\alpha) = 1.168 &+ 35.20\alpha + 426.4\alpha^2 + 2825\alpha^3 + 11503\alpha^4 + 30298\alpha^5 + 52674\alpha^6 \\ &+60630\alpha^7 + 46012\alpha^8 + 22550\alpha^9 + 5964\alpha^{10} ,\end{aligned} \tag{B.19}$$

$$\begin{aligned}N_6(\alpha) = 1 &+ 22.54\alpha + 223.5\alpha^2 + 1278\alpha^3 + 4648\alpha^4 + 11194\alpha^5 + 18116\alpha^6 \\ &+19691\alpha^7 + 14255\alpha^8 + 6664\alpha^9 + 1657\alpha^{10} ,\end{aligned} \tag{B.20}$$

$$\begin{aligned}N_7(\alpha) = 3.120 &+ 59.31\alpha + 488.0\alpha^2 + 2274\alpha^3 + 6592\alpha^4 + 12329\alpha^5 + 15019\alpha^6 \\ &+11905\alpha^7 + 6041\alpha^8 + 1657\alpha^9 ,\end{aligned} \tag{B.21}$$

$$\begin{aligned}N_8(\alpha) = 2.315 &+ 44.06\alpha + 362.9\alpha^2 + 1692\alpha^3 + 4910\alpha^4 + 9188\alpha^5 + 11200\alpha^6 \\ &+8884\alpha^7 + 4515\alpha^8 + 1242\alpha^9 ,\end{aligned} \tag{B.22}$$

References

[1] W.G. Hoover, Annu. Rev. Phys. Chem. 34 (1983) 103;
D.J. Evans and G.P. Morriss, Comput. Phys. Rep. 1 (1984) 299.
[2] K. Kawasaki and J.D. Gunton, Phys. Rev. A 8 (1972) 2048.
[3] J.W. Dufty, J.J. Brey and A. Santos, in: Molecular-Dynamics Simulations of Statistical-Mechanical Systems, G. Ciccotti and W.G. Hoover, eds. (North-Holland, Amsterdam, 1986) pp. 294–303.
[4] E. Ikenberry and C. Truesdell, J. Rat. Mech. Anal. 5 (1956) 1;
C. Truesdell, J. Rat. Mech. Anal. 5 (1956) 55.
[5] C. Truesdell and R.G. Muncaster, Fundamentals of Maxwell's Kinetic Theory of a Simple Monatomic Gas (Academic Press, New York, 1980).
[6] R. Zwanzig, J. Chem. Phys. 71 (1979) 4416.
[7] A. Santos and J.J. Brey, Physica A 174 (1991) 355.
[8] J.J. Brey, A. Santos and V. Garzó, Phys. Rev. Lett. 70 (1993) 2730.
[9] D.J. Evans and A. Baranyai, Phys, Rev. Lett. 67 (1991) 2597.
[10] A. Santos, V. Garzó, J.J. Brey and J.W. Dufty, Phys. Rev. Lett. 71 (1993) 3971; 72 (1994) 1392 (Erratum).
[11] J.R. Dorfman and H. van Beijeren, in: Statistical Mechanics, Part B: Time-Dependent Processes, B.J. Berne, ed. (Plenum, New York, 1977) pp. 65–179.
[12] A. Lees and S.F. Edwards, J. Phys. C 5 (1972) 1921.
[13] J.W. Dufty, A. Santos, J.J. Brey and R.F. Rodríguez, Phys. Rev. A 33 (1986) 459.
[14] Z. Alterman, K. Frankowski and C.L. Pekeris, Astrophys. J., Supplement Series 7 (1962/3) 291.
[15] V. Garzó and A. Santos, Comparison between the Boltzmann and BGK equations for uniform shear flow, Physica A 213 (1995) 426, subsequent paper.