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Singular behavior of the velocity moments of a dilute gas under uniform shear flow

J. M. Montanero, A. Santos, and V. Garzó
Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain
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The hierarchy of moment equations derived from the nonlinear Boltzmann equation describing uniform shear flow is analyzed. It is shown that all the moments of order $k \geq 4$ diverge in time for shear rates larger than a critical value $a_c^{(k)}$, which decreases as k increases. Furthermore, the results suggest an asymptotic behavior of the form $a_c^{(k)} \sim k^{-\mu}$ for large k. Consequently, even for very small shear rates, either a stationary solution fails to exist (which implies the absence of a normal solution) or a stationary solution exists but with only a finite number of convergent moments. Although the uniform shear flow may be experimentally unrealizable for large shear rates, the above conclusions can be of interest for more realistic flows.

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I. INTRODUCTION

The understanding of physical phenomena in fluids far from equilibrium still remains an open problem. The effort is usually focused on nonlinear transport properties, which are related to the population of molecules with energies of the order of or less than the mean kinetic energy. However, much less is known about the high-energy population in nonequilibrium steady states. This population plays a crucial role in processes such as chemical reactions with a high activation energy or the controlled thermonuclear fusion of a confined hydrogen plasma.

Since a general description of the high-energy population does not seem feasible, it is convenient to gain insight by considering particular states. Perhaps one of the most extensively studied states is the so-called uniform shear flow (USF) [1]. At a macroscopic level, it is characterized by a constant density n, a uniform temperature T, and a linear profile of the x component of the flow velocity along the y direction, i.e., $u_x(y) = ay$, a being the constant (positive) shear rate. At a microscopic level [2], the USF is described by a solution of the Liouville equation with Lees-Edwards boundary conditions [3], which can be seen as periodic boundary conditions in the *local* rest frame. These conditions assure the consistency of uniform shear, density, and temperature, even far from equilibrium. In fact, this state has been used to study rheological properties, such as shear thinning and viscometric effects. In addition, a lot of interest was stimulated by the discovery by Erpenbeck [4] of a transition from USF to an ordered state. On the other hand, it is worthwhile to stress the distinction between the USF and the steady planar Couette flow. In the latter, the shearing is produced by walls in relative motion and the boundary conditions correspond to particles interacting with the walls. Consequently, boundary effects are present and also the shear rate, density, and temperature are local quantities. Far from equilibrium, the rheological properties of the Couette flow differ from those of the USF [5].

In general, no rigorous theory based on first principles exists for the USF state. However, if one selects the nonlinear Boltzmann equation as a secure basis for nonequilibrium phenomena in dilute gases, it is possible to derive some exact results. In the case of USF, the time evolution of moments of second [6] and fourth order [7,8] has been obtained for Maxwell molecules. In contrast to what happens for the second order moments, the fourth order moments do not reach stationary values for shear rates larger than a certain critical value. It is clear that moments of fourth order are not sufficient to infer the high-velocity behavior of the distribution function for a given shear rate. The problem we want to address in this paper is the analysis of higher-order moments. In particular, we investigate whether higher-order moments diverge for smaller values of the critical shear rate and whether there exists a finite range of shear rates for which *all* the moments adopt a stationary form. These points can also shed light on the possible implications discussed in Ref. [4].

II. RESULTS

In the case of a low-density gas, the statistical-mechanical description in terms of the phase-space probability density $\rho(\Gamma, t)$ can be replaced by a kinetic description in terms of the one-particle velocity distribution function $f(\mathbf{r}, \mathbf{v}; t)$. The master equation for this function is the Boltzmann equation [9]

$$\frac{\partial}{\partial t} f + \mathbf{v} \cdot \nabla_r f + \nabla_v \cdot (m^{-1} \mathbf{F}_{\text{ext}} f) = J[f, f] , \quad (1)$$

where $\mathbf{F}_{\text{ext}}$ is an external force and $J[f, f]$ is the collision operator. For USF, the distribution function adopts the form [10] $f(\mathbf{r}, \mathbf{v}; t) = f(\boldsymbol{\xi}, t)$, where $\boldsymbol{\xi} \equiv \mathbf{v} - \mathbf{u}(\mathbf{r})$ is the peculiar velocity. The external force is chosen to control the viscous heating, so that the temperature remains constant. The simplest choice is the thermostat force derived from Gauss's principle of least constraint, namely, $\mathbf{F}_{\text{ext}} = -m\alpha\boldsymbol{\xi}$. Under these conditions, Eq. (1) becomes

$$\frac{\partial}{\partial t} f - a\, \xi_y \frac{\partial}{\partial \xi_x} f - \alpha \frac{\partial}{\partial \boldsymbol{\xi}} \cdot \boldsymbol{\xi} f = J[f, f] . \quad (2)$$

The general solution of this equation is not known. Nevertheless, the associated hierarchy of moment equations can be recursively solved in the special case of Maxwell molecules, namely, particles interacting via an r^{-4} potential [11].

About forty years ago, Ikenberry and Truesdell [6] obtained the time evolution of the second order moments, namely, the pressure tensor, for arbitrary values of the shear rate. In the long-time limit, the pressure tensor reaches a stationary form, which defines the nonlinear shear viscosity and normal stresses. In that limit, the thermostat parameter α is given as a function of the shear rate by

$$\alpha = \frac{2}{3}\,\nu\,\sinh^2\left[\frac{1}{6}\cosh^{-1}\left(1+9\frac{a^2}{\nu^2}\right)\right] , \tag{3}$$

where $\nu \equiv n\lambda_{02}^0$ is an effective collision frequency, λ_{02}^0 being an eigenvalue of the linearized Boltzmann collision operator. The third degree moments (e.g., the heat flux) decay exponentially in time [6,8], so that they vanish in the steady state. According to the concept of normal solution [12], if Eq. (2) admits a normal solution, it must necessarily be stationary. To investigate this point, we now consider the velocity moments of the distribution function.

Let us introduce the polynomials [12]

$$\Psi_{r\ell m}(\boldsymbol{\xi}) = N_{r\ell}\,\xi^\ell\,L_r^{(\ell+\frac{1}{2})}(\xi^2)\,Y_\ell^m(\hat{\boldsymbol{\xi}}) , \tag{4}$$

with

$$N_{r\ell} = \left[2\pi^{3/2}\frac{r!}{\Gamma(r+\ell+\frac{3}{2})}\right]^{1/2} . \tag{5}$$

The polynomials $\{\Psi_{\mathbf{k}}(\boldsymbol{\xi}),\ \mathbf{k} \equiv (r,\ell,m)\}$ constitute a complete set of orthonormal functions with the inner product

$$\langle\Phi|\chi\rangle = \pi^{-3/2}\int d\boldsymbol{\xi}\; e^{-\xi^2}\;\Phi^*(\boldsymbol{\xi})\;\chi(\boldsymbol{\xi}) . \tag{6}$$

Here and in the following we take $(2k_BT/m)^{1/2}=1$ and $n=1$. Due to the invariance properties of uniform shear flow, we can restrict ourselves to the subset $\{\Psi_{\mathbf{k}}\}$ with $k \equiv 2r+\ell =$ even and $m =$even. In this subset, there exist $(\frac{k}{2}+1)^2$ independent polynomials of degree k. Let us assume that the velocity distribution function can be represented in terms of the set $\{\Psi_{\mathbf{k}}\}$, i.e.,

$$f(\boldsymbol{\xi},t) = \pi^{-3/2}e^{-\xi^2}\sum_{\mathbf{k}} M_{\mathbf{k}}(t)\Psi_{\mathbf{k}}(\boldsymbol{\xi}) , \tag{7}$$

where the moments $M_{\mathbf{k}}(t)$ are defined as

$$M_{\mathbf{k}}(t) = \int d\boldsymbol{\xi}\;\Psi_{\mathbf{k}}^*(\boldsymbol{\xi})\;f(\boldsymbol{\xi},t) . \tag{8}$$

Taking moments in Eq. (2) for Maxwell molecules one arrives at the following hierarchy:

$$\frac{\partial}{\partial t}M_{\mathbf{k}} + a\sum_{\mathbf{k}'}\left\langle\Psi_{\mathbf{k}'}\left|\xi_y\frac{\partial}{\partial\xi_x}\right|\Psi_{\mathbf{k}}\right\rangle^* M_{\mathbf{k}'} +\alpha\sum_{\mathbf{k}'}\left\langle\Psi_{\mathbf{k}'}\left|\boldsymbol{\xi}\cdot\frac{\partial}{\partial\boldsymbol{\xi}}\right|\Psi_{\mathbf{k}}\right\rangle^* M_{\mathbf{k}'} = -\lambda_{\mathbf{k}}^0 M_{\mathbf{k}} + \sum_{\mathbf{k}',\mathbf{k}''}{}^{\dagger} J_{\mathbf{k}\mathbf{k}'\mathbf{k}''}\;M_{\mathbf{k}'}\;M_{\mathbf{k}''} . \tag{9}$$

Here,

$$\lambda_{\mathbf{k}}^0 \equiv \lambda_{r\ell}^0 = 2\pi\int d\theta\;\sin(\theta)\;\sigma(\cos\theta) \times\left[1+\delta_{r0}\delta_{\ell 0} - \cos^{2r+\ell}\left(\frac{\theta}{2}\right)\;P_\ell\left(\cos\frac{\theta}{2}\right) - \sin^{2r+\ell}\left(\frac{\theta}{2}\right)\;P_\ell\left(\sin\frac{\theta}{2}\right)\right] \tag{10}$$

are the eigenvalues of the linearized collision operator [12,13], $\sigma(\cos\theta)$ being the collision rate. The dagger in the last summation of Eq. (9) denotes the restrictions $k'+k''=k$ and $k',k''>0$. The explicit expression for the coefficients $J_{\mathbf{k}\mathbf{k}'\mathbf{k}''}$ is known [12] but it will not be needed in our discussion.

The brackets appearing in Eq. (9) are zero if $k'>k$. Consequently, the hierarchy (9) can be recast into the form

$$\frac{\partial}{\partial t}M_{\mathbf{k}} + \sum_{\substack{\mathbf{k}'\\(k'=k)}}\mathcal{L}_{\mathbf{k}\mathbf{k}'}M_{\mathbf{k}'} = B_{\mathbf{k}} , \tag{11}$$

where, for a given order k, $\mathcal{L}_{\mathbf{k}\mathbf{k}'}$ is a $(\frac{k}{2}+1)^2\times(\frac{k}{2}+1)^2$ square matrix given by

$$\mathcal{L}_{\mathbf{k}\mathbf{k}'} = (\lambda_{\mathbf{k}}^0 + k\alpha)\delta_{\mathbf{k}\mathbf{k}'} + a\left\langle\Psi_{\mathbf{k}'}\left|\xi_y\frac{\partial}{\partial\xi_x}\right|\Psi_{\mathbf{k}}\right\rangle^* \tag{12}$$

and $B_{\mathbf{k}}$ is a combination of moments of order *less* than k. A tedious but standard calculation yields, for $2r'+\ell'=2r+\ell$,

$$\left\langle\Psi_{r'\ell'm'}\left|\xi_y\frac{\partial}{\partial\xi_x}\right|\Psi_{r\ell m}\right\rangle = R_{r\ell m}\delta_{\ell'\ell}\delta_{m,m'-2} + R^*_{r'\ell'm'}\delta_{\ell'\ell}\delta_{m',m-2} + S_{r\ell m}\delta_{\ell,\ell'-2}\delta_{m,m'-2} + S^*_{r'\ell'm'}\delta_{\ell',\ell-2}\delta_{m',m-2} +S_{r\ell-m}\delta_{\ell,\ell'-2}\delta_{m,m'+2} + S^*_{r'\ell'-m'}\delta_{\ell',\ell-2}\delta_{m',m+2} + i\frac{m}{2}\delta_{\ell'\ell}\delta_{m'm} , \tag{13}$$

where

$$R_{r\ell m} = \frac{i}{2}\frac{2r+\ell+\frac{3}{2}}{(2\ell+3)(2\ell-1)}\left[\frac{(\ell+m+2)!(\ell-m)!}{(\ell+m)!(\ell-m-2)!}\right]^{1/2} , \tag{14}$$

$$S_{r\ell m} = \frac{i}{2}\frac{1}{2\ell+3}\left[\frac{r(r+\ell+\frac{3}{2})(\ell+m+4)!}{(2\ell+1)(2\ell+5)(\ell+m)!}\right]^{1/2} . \tag{15}$$

The time evolution of all the moments $M_{\mathbf{k}}$ of the same order k is described by the corresponding eigenvalues $\lambda_{\mathbf{k}}(a)$ of the matrix $\mathcal{L}_{\mathbf{k}\mathbf{k}'}$. Obviously, $\lambda_{\mathbf{k}}(0)=\lambda_{\mathbf{k}}^0$. The behavior of $M_{\mathbf{k}}$ in the long-time limit is governed by the eigenvalue with the smallest real part. Such an eigenvalue turns out to be $\lambda_{\frac{k}{2}0}(a)$. Consequently, the moments of order k diverge to infinity when $\lambda_{\frac{k}{2}0}(a)$ becomes negative.

We have evaluated $\lambda_{\frac{k}{2}0}(a)$ for $k = 4, 6, \ldots, 36$ by using the table of λ^0_{rl} reported in Ref. [13]. Figure 1 shows $\lambda_{\frac{k}{2}0}$ as a function of the shear rate for $k = 4, 6, 8$, and 20. In the following, we take $\lambda^0_{02} = 1$, so that ν^{-1} is the time unit. The eigenvalue $\lambda_{\frac{k}{2}0}(a)$ monotonically decreases as the shear rate increases and eventually changes sign at a certain critical value $a_c^{(k)}$. This extends the results already obtained for $k = 4$ [7,8]. Table I gives the numerical values of $a_c^{(k)}$ for $k = 4, 6, \ldots, 36$. In addition to actual Maxwell molecules we have also considered the isotropic Maxwell model [14], for which $\sigma(\cos\theta) = \text{const}$. We observe that the value of $a_c^{(k)}$ decreases as the order k increases. This means that if $a \geq a_c^{(k)}$ all the moments of order equal to or greater than k diverge as $t \to \infty$. On the other hand, if $a < a_c^{(k)}$ all the moments of order less than k reach stationary values in the long-time limit.

The relevant question now is whether there exists a nonzero lower bound for the set $\{a_c^{(k)}, k \geq 4\}$. In other words, is $\lim_{k\to\infty} a_c^{(k)} \equiv a_c^{(\infty)}$ different from zero? If that were the case, all the moments would reach stationary values for shear rates smaller than $a_c^{(\infty)}$. In order to clarify this question, we have plotted $\ln a_c^{(k)}$ versus $\ln k$ in Fig. 2. We see that the points corresponding to the largest values of k tend to align. This suggests that the asymptotic behavior of $a_c^{(k)}$ for large k is of the form

$$a_c^{(k)} \sim k^{-\mu} \,. \tag{16}$$

A linear fit gives $\mu \simeq 0.91$ for actual Maxwell molecules and $\mu \simeq 1.14$ for the isotropic model. We must emphasize that no rigorous proof of the law (16) has been given, although it is strongly supported by the results presented in Table I. In this context, Eq. (16) implies that $a_c^{(\infty)} = 0$.

TABLE I. Values of the critical shear rate $a_c^{(k)}$ associated with moments of order $k = 4, 6, \ldots, 36$.

k	$a_c^{(k)}$ Actual scattering	$a_c^{(k)}$ Isotropic scattering
4	6.846	7.746
6	2.346	3.344
8	1.450	1.667
10	0.817	0.940
12	0.618	0.633
14	0.502	0.479
16	0.427	0.388
18	0.373	0.327
20	0.333	0.283
22	0.301	0.250
24	0.276	0.224
26	0.255	0.202
28	0.238	0.185
30	0.223	0.171
32	0.210	0.158
34	0.199	0.147
36	0.189	0.138

III. CONCLUSIONS

In summary, we have analyzed the time evolution of the velocity moments from the Boltzmann equation for Maxwell molecules under uniform shear flow (USF). The results obtained here allow us to conclude that (i) all the moments of order $k \geq 4$ grow exponentially in time for shear rates larger than a certain critical value $a_c^{(k)}$, (ii) the numerical value of $a_c^{(k)}$ monotonically decreases as k increases, and (iii) $\lim_{k\to\infty} a_c^{(k)} = 0$. This implies that, for *any* value of the shear rate, there exists a value of k such that *all* the moments of order equal to or larger than k diverge as $t \to \infty$. Further, (iv) the results sup-

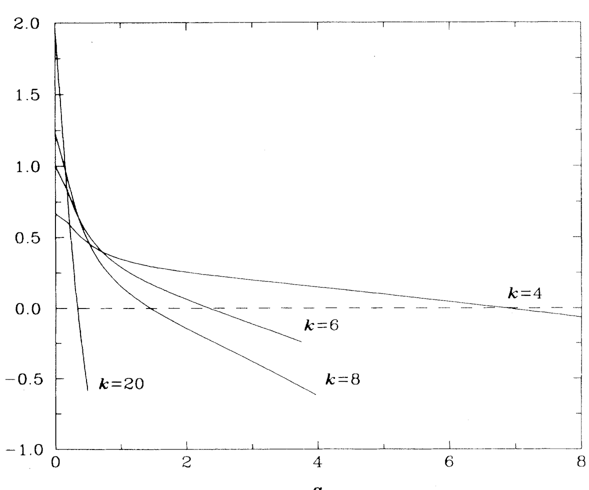

FIG. 1. Shear-rate dependence of the smallest eigenvalue, $\lambda_{\frac{k}{2}0}(a)$, for $k = 4, 6, 8$, and 20, and for the actual scattering model.

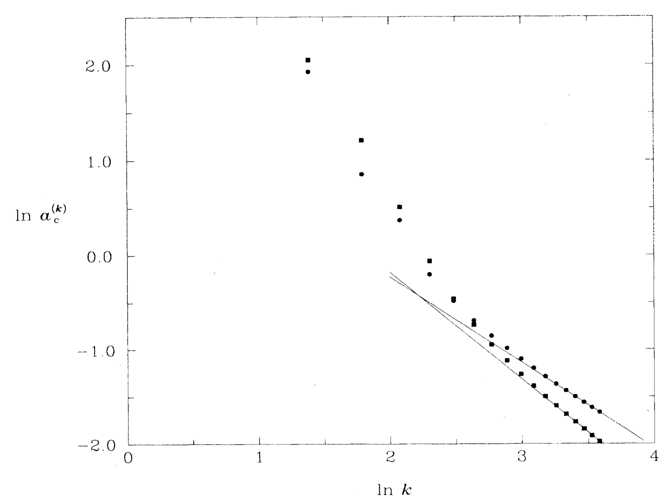

FIG. 2. Log-log plot of $a_c^{(k)}$ versus k for the actual scattering model (circles) and the isotropic scattering model (squares). The straight lines are linear fits of the last four points.

port the conjecture that the asymptotic behavior of $a_c^{(k)}$ for large k is of the form (16). The above conclusions seem to be independent of the scattering model chosen for Maxwell molecules. The apparent influence of the scattering model on the value of μ might be due to the fact that the values of k considered here are not sufficiently large. From that point of view, one is tempted to conjecture that $\mu = 1$ for Maxwell molecules, regardless of the details of the scattering model.

The analysis carried out here has been concentrated on the hierarchy of moments, Eq. (9), rather than on the Boltzmann equation itself, Eq. (2). In this sense, we only have *indirect* information about the time evolution of the distribution function. In principle, there are two possibilities: (a) a stationary solution of the Boltzmann equation does not exist; (b) a stationary solution exists but with a *finite* number (depending on the value of the shear rate) of convergent moments. The possibility (a) means that Eq. (2) does not admit a normal solution, in the sense of kinetic theory [12]. A solution of the Boltzmann equation is called normal when its whole time and space dependence is contained in a functional dependence of f on n, $\mathbf{u}$, and T. Most of the treatments and applications of the Boltzmann equation, such as the Chapman-Enskog expansion, are based on the existence of a normal solution for times sufficiently long and points sufficiently far from the boundaries. The fact that, according to the possibility (a), a normal solution fails to exist for shear rates arbitrarily small would have important physical consequences regarding our understanding of nonequilibrium phenomena. A normal solution does exist in the case (b), but with a high-velocity population decaying more slowly than a certain power, even for small shear rates. A possible scenario for the case (b) is an asymptotic behavior $f(\boldsymbol{\xi}) \sim \xi^{-5-\sigma(a)}$ for large ξ, where $\lim_{a\to\infty}\sigma(a) = 0$ and $\sigma(a) \sim a^{-1/\mu}$ for small shear rates; the critical shear rate $a_c^{(k)}$ would be then the solution of $\sigma(a_c^{(k)}) = k - 2$. Recent simulation results [15] give support to this speculation. The long tail in velocity space of the distribution function would have an important influence on those processes (such as certain chemical or thermonuclear reactions) which are extremely sensitive to the fraction of particles with a sufficiently high energy. A small increase in the shear rate would give rise to a large increase in the occurrence of those events. Elucidation of these points requires further investigation, from both analytical and simulation points of view. In either way, even for small shear rates, the velocity distribution function differs appreciably from the equilibrium distribution for high velocities, so that a linearization around equilibrium is not justified for those velocities.

In Ref. [7] it was suggested that the singular behavior of the fourth order moments might be related to the transition from USF to an ordered state observed in dense fluids [4]. However, the fact that the singularity appears even for arbitrarily small shear rates seems to preclude that possibility. In addition, Monte Carlo simulations of the Boltzmann equation [16] show that the USF is stable. Finally, it is worthwhile to mention that Monte Carlo simulations indicate that a behavior similar to the one reported here for Maxwell molecules can be extended to other repulsive potentials.

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