HIGH-VELOCITY TAIL IN A DILUTE GAS UNDER SHEAR

J. M. Montanero, V. Garzó, A. Santos
(Departamento de Física, Universidad de Extremadura
E-06071 Badajoz, Spain)

ABSTRACT: An overview of recent work concerning the high-velocity tail in a dilute gas under shear flow is presented. In the case of Maxwell molecules, an exact analysis of the hierarchy of moment equations of the Boltzmann equation shows that, for any value of the shear rate, all the moments beyond a certain degree are divergent. This is consistent with an algebraic tail for the distribution function, which is confirmed by Monte Carlo simulations. For non-Maxwell molecules, simulation results suggest that the above singular behavior for the velocity moments is also present although the phenomenon is less notorious as the interaction becomes harder. On the other hand, the transport coefficients are hardly sensitive to the interaction.

1 INTRODUCTION

The high-velocity population in a gas plays a crucial role in phenomena with a high activation energy, such as chemical reactions or the thermonuclear fusion in a plasma. Nevertheless, it is in general very difficult to get information on the high-velocity tail of the distribution function from the Boltzmann equation. In the case of homogeneous and isotropic situations, a lot of work[1] was stimulated by the discovery of the so-called BKW mode. On the other hand, much less is known about the high-velocity tail in inhomogeneous situations. A rare case that lends itself to a detailed analysis is the uniform shear flow for Maxwell molecules. In this state, the only non-zero hydrodynamic gradient is $\partial u_x/\partial y = a$, where $\mathbf{u}$ is the flow velocity and a is the constant shear rate. In the special case of Maxwell molecules, the hierarchy of moment equations derived from the Boltzmann equation can be recursively solved for arbitrary shear rate. Forty years ago, Ikenberry and Truesdell[2] obtained explicit expressions for the second degree moments. These quantities provide the rheological properties of the fluid (nonlinear shear viscosity and viscometric functions), but they do not give enough information about the distribution of velocities much larger than thermal velocities. In order to obtain this information one needs to consider higher degree velocity moments.

In this paper we offer an overview of recent advances on this subject. The Boltzmann equation for uniform shear flow and the corresponding hierarchy of moment equations are worked out in Sec. 2 in the particular case of Maxwell molecules. It is shown that all the moments of degree $k \geq 4$ diverge in time if the shear rate is larger than a certain critical value $a_c^{(k)}$, where $a_c^{(4)} > a_c^{(6)} > a_c^{(8)} > \cdots > 0$. This is consistent with an algebraic tail of the form $f(\mathbf{V}) \sim V^{-(d+2+\sigma(a))}$, where d is the dimensionality of the system and $\sigma(a)$ is a decreasing function of the shear rate. This behavior is confirmed by Monte Carlo simulations for $d = 2$. In Sec. 3 we present simulation results for non-Maxwell interaction potentials. They suggest that the above singular behavior for the velocity moments is also present, but it becomes less significant as the interaction is harder and seems to disappear in the limit of hard spheres.

2 UNIFORM SHEAR FLOW FOR MAXWELL MOLECULES

As said in the Introduction, the uniform shear flow is characterized by a uniform density n and temperature T, and a linear velocity profile: $\mathbf{u}(\mathbf{r}) = ay\widehat{\mathbf{x}}$. As a counterpart of this simplicity, the temperature grows in time. A detailed description of this state can be obtained for a dilute gas of Maxwell molecules[1], namely particles interacting via a repulsive potential of the form $r^{-2(d-1)}$. In this case, the dominant long-time behavior of the temperature is[3,4] $T(t) \sim e^{2\alpha(a)t}$, where $\alpha(a)$ is the real root of the cubic equation $d\alpha(\nu+2\alpha)^2 = \nu a^2$, i.e. $\alpha(a) = \frac{2}{3}\nu \sinh^2[\frac{1}{6}\cosh^{-1}(1+27a^2/d\nu^2)]$. Here, $\nu \equiv n\lambda^0$ is an effective collision frequency, where λ^0 is an eigenvalue of the linearized Boltzmann collision operator[5,6]. It is convenient to introduce the peculiar velocity relative to the thermal velocity: $\mathbf{V} = [\mathbf{v}-\mathbf{u}(\mathbf{r})]/\sqrt{2k_BT(t)/m}$. In terms of this variable, the Boltzmann equation for Maxwell molecules reads

$$\frac{\partial}{\partial t}f - a\, V_y\frac{\partial}{\partial V_x}f - \alpha\frac{\partial}{\partial \mathbf{V}}\cdot\mathbf{V}f = J[f,f]\,, \tag{1}$$

where $J[f,f]$ is the nonlinear Boltzmann collision operator. Henceforth, we will take $\nu = 1$, what defines the time unit. It is worthwhile to note that the third term on the left-hand side of Eq. (1) can be interpreted as arising from a drag force $\mathbf{F} = -m\alpha\mathbf{V}$ that controls the viscous heating. Therefore, there exists an exact equivalence between the uniform shear flow with and without a thermostat force[7]. Nevertheless, this equivalence does not apply for non-Maxwell molecules.

The solution of Eq. (1) is not known. On the other hand, its hierarchy of moment equations can be recursively solved for Maxwell molecules[8]. Let $\{\Psi_{\mathsf{k}}(\mathbf{V})\}$ (k denoting a set of d indices) be a complete set of orthonormal polynomials with the inner product

$$\langle\phi|\chi\rangle = \pi^{-d/2}\int d\mathbf{V}e^{-V^2}\phi^*(\mathbf{V})\chi(\mathbf{V})\,. \tag{2}$$

We define the moments

$$M_{\mathsf{k}}(t) = \int d\mathbf{V}\ \Psi_{\mathsf{k}}^*(\mathbf{V})\ f(\mathbf{V},t)\,. \tag{3}$$

Equation (1) is invariant under the transformations $(V_x, V_y) \to (-V_x, -V_y)$ and $V_i \to -V_i\,(i \neq x, y)$. Here we focus on solutions consistent with the above invariance properties. It is then possible to prove that the moments of degree k = odd vanish and the number of independent moments of degree k = even is $(k+d-1)(k/2+d-2)!/(k/2)!(d-1)!$. For the sake of convenience, we choose $\{\Psi_{\mathsf{k}}(\mathbf{V})\}$ as the set of eigenfunctions of the linearized Boltzmann operator and denote by λ_{k}^0 their corresponding eigenvalues. Taking moments in Eq. (1) we arrive at

$$\frac{\partial}{\partial t}M_{\mathsf{k}} + \sum_{\mathsf{k}'}{}^{\dagger}\mathcal{L}_{\mathsf{kk}'}M_{\mathsf{k}'} = B_{\mathsf{k}}\,, \tag{4}$$

where the dagger means that the summation is restricted to the moments of the *same* degree (k) as M_{k}. The square matrix $\mathcal{L}_{\mathsf{kk}'}$ is

$$\mathcal{L}_{\mathsf{kk}'} = (\lambda_{\mathsf{k}}^0 + k\alpha)\delta_{\mathsf{kk}'} + a\langle\Psi_{\mathsf{k}'}|V_y\frac{\partial}{\partial V_x}|\Psi_{\mathsf{k}}\rangle^* \tag{5}$$

and B_k is a linear and bilinear combination of moments of order *less* than k. The time evolution of the moments $\{M_k\}$ of a given degree k is governed by the eigenvalues $\lambda_k(a)$ of the matrix $\mathcal{L}_{kk'}$. Let us call $\widetilde{\lambda}_k(a)$ the eigenvalue of $\mathcal{L}_{kk'}$ with the smallest real part. A necessary condition for the moments of degree k to reach stationary values is $\mathrm{Re}\widetilde{\lambda}_k(a) > 0$. On the other hand, if $\mathrm{Re}\widetilde{\lambda}_k(a) \leq 0$ then the moments of degree k diverge in time.

We have obtained the eigenvalues of $\mathcal{L}_{kk'}$ through $k = 240$ for $d = 2$ and $k = 36$ for $d = 3$. It turns out[9–11] that $\widetilde{\lambda}_k(a)$ is a real number that becomes negative if the shear rate is larger than a threshold value $a_c^{(k)}$, which monotonically decreases as $k \geq 4$ increases. For instance, if the scattering is isotropic, $a_c^{(4)} = 5.847$ and 7.746 for $d = 2$ and 3, respectively. For shear rates larger than $a_c^{(4)}$ the only non-diverging moments are those of degree 2. Conversely, if $a < a_c^{(k)}$ *all* the moments of degree smaller than or equal to k reach stationary values. The shear-rate dependence of the steady-state values of the fourth degree moments (for $d = 3$) is given in Ref. [4]. In addition, the results indicate that there is no lower bound of $a_c^{(k)}$ and $a_c^{(k)} \sim k^{-1}$ for large k.

The above results for the velocity moments are consistent with a stationary solution of Eq. (1) exhibiting a high-velocity tail of the form $f(\mathbf{V}) \sim V^{-(d+2+\sigma(a))}$ for *any* value of the shear rate a. This would imply that the moments of degree $k \geq \sigma + 2$ diverge. Although the shear-rate dependence of σ is unknown, the analysis of the moments shows that $\sigma = k - 2$ at $a = a_c^{(k)}$ and $\sigma(a) \sim a^{-1}$ for small a. In the opposite limit, it is tempting to speculate that $\lim_{a\to\infty} \sigma(a) = 0$. Since the velocity moments provide only an indirect information about the velocity distribution function, we have resorted to the direct simulation Monte Carlo (DSMC) method[12] to analyze the behavior of $f(\mathbf{V})$ in the case of $d = 2$. At $a = a_c^{(k)}$ we have confirmed[11] that $V^{k+2} f(\mathbf{V})$ reaches a stationary value that is independent of V, for sufficiently large velocities. Furthermore, the relaxation time increases as V increases.

3 MONTE CARLO SIMULATION FOR NON-MAXWELL MOLECULES

So far, the results have been restricted to the special case of Maxwell molecules. A natural question is whether the above high-velocity behavior is also present in other interaction potentials. For non-Maxwell molecules the moment hierarchy cannot be solved recursively, so that no analytical results are known. Although the exact solution of the BGK kinetic model for uniform shear flow with a general interaction is known[13,14], it is not reliable for velocities beyond the thermal domain. Therefore, we have studied the problem by means of the DSMC method[12]. In particular, we have considered repulsive potentials of the form $r^{-\mu}$ with (a) $\mu = 4$, (b) $\mu = 6$, (c) $\mu = 8$, (d) $\mu = 12$, and (e) $\mu = \infty$, for $d = 3$. Now the thermostat coefficient α in Eq. (1) is unknown and is determined by requiring that the temperature remains constant.

The second degree moments are mainly related to the distribution of thermal velocities ($V \sim 1$) and do not provide much information about the high-velocity tail. However, they are worth to study since they give the rheological properties. Figures 1–3 show the time evolution of the reduced shear viscosity $\eta^* = -P_{xy}/(nk_BTa)$ and the reduced viscometric functions $\Psi_1^* = (P_{yy} - P_{xx})/(nk_BTa^2)$, $\Psi_2^* = (P_{zz} - P_{yy})/(nk_BTa^2)$ at $a = 6$, where $P_{ij} = m\int d\mathbf{V} V_i V_j f$ is the pressure tensor. The dashed lines represent the exact solution for Maxwell molecules ($\mu = 4$). We observe that the influence of the interaction is quite small. The value of η^* for hard spheres ($\mu = \infty$) is about 1.5% larger than that for Maxwell molecules ($\mu = 4$). As μ increases, the difference $P_{xx} - P_{yy}$ decreases and the (much smaller) difference $P_{zz} - P_{yy}$ increases. Non-Newtonian effects are clearly present at $a = 6$, since $\eta^* = 1$, $\psi_1^* \simeq -2$ and $\psi_2^* \simeq 0.17$ (for hard spheres) when $a \to 0$. To assess the distortion

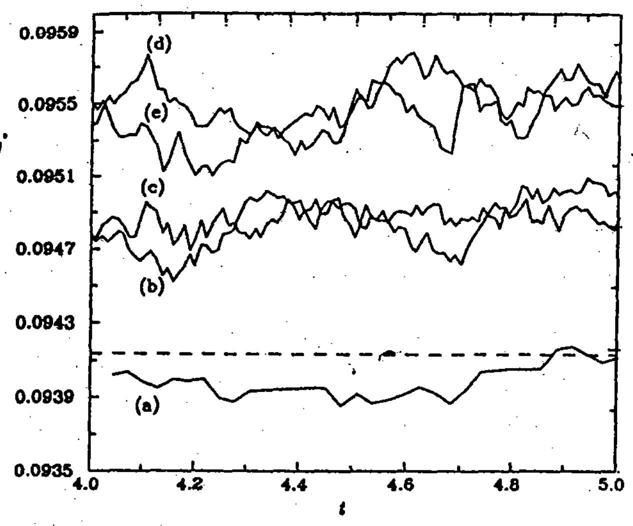

Fig. 1 Reduced shear viscosity η^* at $a = 6$.

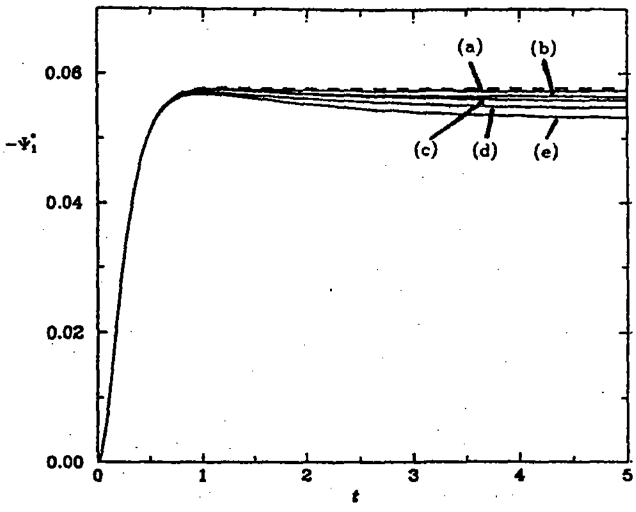

Fig. 2 Reduced first viscometric function Ψ_1^* at $a = 6$.

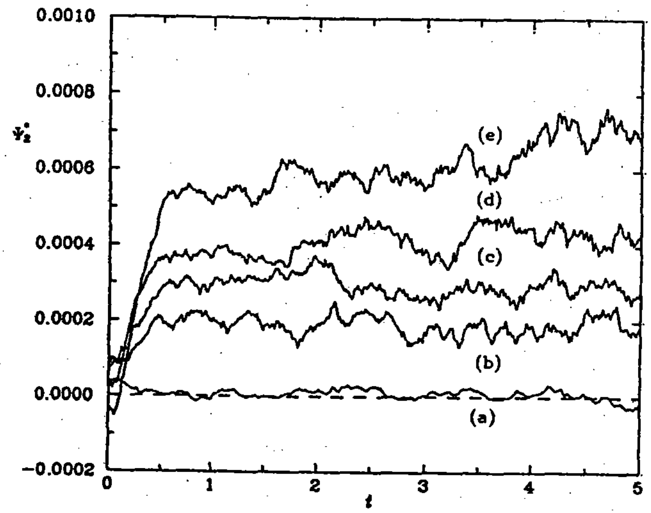

Fig. 3 Reduced second viscometric function Ψ_2^* at $a = 6$.

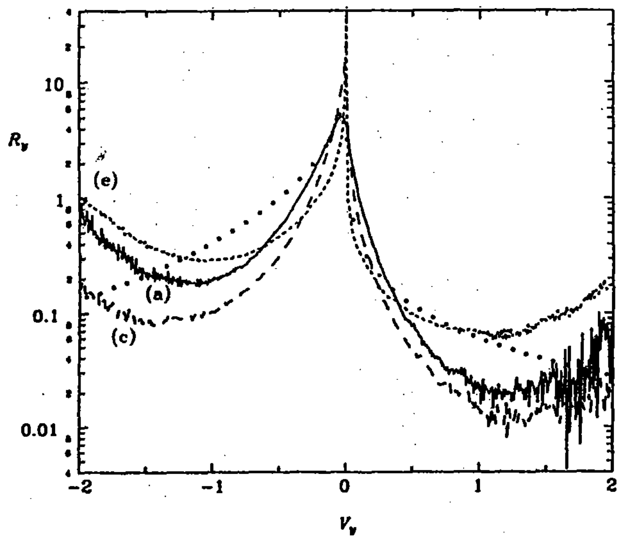

Fig. 4 Reduced velocity distribution function $R_y(V_y)$ at $a = 7.33$.

from local equilibrium, we have computed $R_y(V_y)$ (the number of particles moving with $V_x > 0$ and a given value of V_y, relative to the number at local equilibrium). Figure 4 shows $R_y(V_y)$ at $a = 7.33$ for (a) $\mu = 4$, (c) $\mu = 8$, and (e) $\mu = \infty$. The exact solution of the BGK kinetic equation[13] has also been included (dotted line). It is interesting to note that, despite of the similarity of the second degree moments for different interactions (cf. Figs. 1–3), the velocity distribution is clearly influenced by the interaction.

While the rheological properties are hardly sensitive to the interaction potential considered, the moments of degree four and higher are influenced by the value of μ[15]. On the one hand, the simulation results indicate that the divergence of moments at sufficiently large shear rates can be extended to potentials harder than the Maxwell one. On the other hand, the strength of this phenomenon diminishes as the repulsion becomes harder. In fact, it seems to disappear in the limit of hard spheres ($\mu \to \infty$). A possible explanation is as follows. Although the thermostat controls the *average* kinetic energy per particle, the *relatively small* high-velocity population may increase in time due to viscous heating. This increase is partly inhibited if those particles collide frequently, this effect being more notorious for harder repulsions. This picture is consistent with an asymptotic distribution $f(\mathbf{V}) \sim V^{-(d+2+\sigma(a,\mu))}$, where $\sigma(a,\mu)$ depends on the shear rate in a similar way as for Maxwell molecules $[\mu = 2(d-1)]$ and is an increasing function of μ, so that $\lim_{\mu\to\infty} \sigma = \infty$.

This research has been supported by the DGICYT (Spain) and by the Junta de Extremadura (Fondo Social Europeo) through Grants Nos. PB94-1021 and EIA94-39, respectively.

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