Velocity Distribution Function of a Gas under Shear Flow

Andres Santos

Departamento de Física,
Universidad de Extremadura,
06071 Badajoz, Spain

J. Javier Brey

Física Teórica,
Universidad de Sevilla,
Apdo. 1065, 41080 Sevilla, Spain

The main aim of this paper is to obtain the velocity distribution function of a dilute gas far from equilibrium. Two shear flows with the same geometry are considered: stationary Couette flow and uniform shear flow. Explicit expressions for the normal solution to the nonlinear Bhatnagar-Gross-Krook kinetic equation are derived. In the stationary Couette flow, the distribution function is a universal nonanalytic function of the reduced shear rate and thermal gradient. In the uniform shear flow, the dependence on the shear rate is analytic only in the case of Maxwell molecules.

1. INTRODUCTION

While the statistical-mechanical description of transport phenomena in states near equilibrium is sufficiently well-posed, the situation is much more complicated far from equilibrium. A great deal of the studies about this states come from nonequilibrium molecular dynamics simulations,[1-3] some of them lacking a deep justification.[4,5] On the other hand, theoretical advances are not yet significant enough to allow for a complete understanding of the problems involved.

All of this prompts the consideration of a monatomic, dilute gas with a short-range interaction as a prototype system for the study of transport properties. Rather than a detailed description in terms of the phase-space probability density, it is preferable to use kinetic theory and characterize the state of the system by means of the one-particle velocity distribution function (VDF) $f(\vec{r},\vec{v};t)$. This function is obtained as the solution to the Boltzmann equation (BE)[6]

$$\frac{\partial}{\partial t} f + \vec{v}.\nabla f = \int d\vec{v}_1 \int_0^\infty db \int_0^{2\pi} d\varepsilon \; |\vec{v}-\vec{v}_1| \; b \; (f' f_1' - f f_1)$$

$$\equiv J[f,f], \qquad (1)$$

subject to appropriate initial and boundary conditions. From a hydrodynamic point of view, one is mainly interested in the so-called normal solution, that is expected to apply for times much longer than the mean free time and for distances from the walls much larger than the mean free path.[6] The normal solution is characterized by the fact that all the space and time dependence enters through a functional dependence on the hydrodynamic fields, namely the local particle density

$$n(\vec{r},t) = \int d\vec{v}\, f, \tag{2}$$

the local velocity

$$\vec{u}(\vec{r},t) = \frac{1}{n}\int d\vec{v}\, \vec{v}\, f, \tag{3}$$

and the local temperature

$$T(\vec{r},t) = \frac{m}{3nk}\int d\vec{v}\, (\vec{v}-\vec{u})^2\, f. \tag{4}$$

In Eq. (4), m is the mass of a particle and k is the Boltzmann constant. The standard method to construct the normal solution is given by the Chapman-Enskog (C-E) theory,[7] which consists of an expansion of the VDF in powers of gradients of n, $\vec{u}$, and T:

$$f = f_0 + \mu f_1 + \mu^2 f_2 + \dots \tag{5}$$

Here, μ is called the uniformity parameter and is defined as the ratio between the mean free path and the hydrodynamic length scale over which the quantities n, $\vec{u}$, or T change in space.[6] Thus, μ is of first order in the gradients of those quantities. The C-E method leads to the Navier-Stokes equations (first order in μ) and provides expressions for the transport coefficients in terms of the interaction potential.[6,7] Beyond the scope of the Navier-Stokes order, however, the usefulness of the C-E method is not free of problems.

In an attempt to clarify some of these points, the following questions will be addressed in this paper: (i) Does the C-E expansion converge? (ii) Does there exist a normal solution beyond the range of applicability of the C-E expansion? (iii) Which are the qualitative features of the VDF far from equilibrium? (iv) Does the interaction law play a relevant role in the answers to the above questions? Among the wide diversity of possible nonequilibrium situations, we shall restrict ourselves here to two different states: stationary Couette flow (SCF) and uniform shear flow (USF). In both cases the system is sheared in such a way that it moves along the x-direction with a flow velocity depending on y. Otherwise, they are quite different. In the first case, the system is driven to a nonequilibrium steady state by walls in relative motion, so that the existence of boundary layers is in principle expected. Also, the velocity gradient induces a nonlinear temperature profile. In the case of USF, however, the velocity is the only inhomogeneous field. The state is time-dependent, but no boundary effects exist.

In problems directly related to transport processes, the only exact solutions to the BE we are aware of are those obtained by means of the moment method.[8,9] Since we are mainly interested in obtaining explicit expressions for the VDF, we shall use the well-known Bhatnagar-Gross-Krook (BGK) kinetic equation as a model of the BE.[10] In this model, the Boltzmann collision term is approximated by a single-time relaxation towards the local equilibrium distribution:

$$\frac{\partial}{\partial t} f + \vec{v}.\nabla f = -\nu\,(f - f_{LE}), \tag{6}$$

where

$$f_{LE}(\vec{r},\vec{v};t) = n\left(\frac{m}{2\pi kT}\right)^{3/2} e^{-m(\vec{v}-\vec{u})^2/2kT} \tag{7}$$

is the local equilibrium VDF and $\nu(\vec{r},t)$ is the collision frequency. The latter is proportional to the density n and depends on the temperature T according to the interaction law. For instance, for repulsive potentials of the form $V(r)\sim r^{-b}$, the collision frequency is

$$\nu \propto n\, T^{\alpha}, \quad \alpha = \frac{1}{2} - \frac{2}{\delta} . \tag{8}$$

The BGK equation retains the main physical properties of the BE: verification of an H-theorem and conservation of mass, momentum, and energy.[10] Moreover, some transport properties predicted by the BGK equation agree reasonably well with simulation results.[3,11]

In the next Section, an exact normal solution to the BGK equation is derived for the SCF. First, a formal solution is obtained for boundary conditions such that the Knudsen number vanishes near the walls, eliminating the boundary layer. Next, the symmetry of the problem is used to "guess" the appropriate hydrodynamic fields and the consistency of the resulting VDF is verified. In Section 3, the solution of the BGK equation for the USF is addressed. In this case, the temperature increases in time, so that the collision frequency is not a constant, except for Maxwell molecules. As a consequence, a normal state in a strong sense is restricted to local equilibrium. However, a far from equilibrium normal state can be identified if a weaker condition is adopted. Finally, the conclusions are summarized in Section 4.

2. STATIONARY COUETTE FLOW (SCF)

In the SCF, a gas enclosed between two infinite, parallel plates (orthogonal to the y-axis) reaches a steady state. The plates are kept in relative motion and, generally, at different temperatures, so that a velocity profile $\vec{u}=u(y)\hat{x}$ and a temperature profile $T(y)$ exist. A qualitative picture of the expected profiles is provided by the Navier-Stokes equations, yielding $p=nkT=const.$ and[12]

$$\frac{\partial^2 u}{\partial \ell^2} = 0, \tag{9}$$

$$\frac{\partial^2 T}{\partial \ell^2} = -(\eta_0/\kappa_0)\left(\frac{\partial u}{\partial \ell}\right)^2, \tag{10}$$

where η_0 and κ_0 are the shear viscosity and the thermal conductivity, respectively, and ℓ is a new length scale defined by

$$d\ell = \nu(y)\, dy. \tag{11}$$

Thus, in the Navier-Stokes order u is linear in ℓ and T is a parabola.

In the case of SCF, Eq. (6) becomes

$$v_y \frac{\partial}{\partial \ell} f = -(f - f_{LE}). \tag{12}$$

Equation (12) must be supplemented with appropriate boundary conditions. In the special case of diffuse boundary conditions, the half distributions for velocities directed off the walls are expressed in terms of moments of the corresponding distributions directed into the walls.[13] Since we are interested here in the normal state, a different approach will be taken. The formal solution to Eq. (12) is

$$f(\ell,\vec{v}) = e^{-(\ell-\ell_0)/v_y} f(\ell_0,\vec{v}) + \frac{1}{v_y}\int_{\ell_0}^{\ell} d\ell'\, e^{-(\ell-\ell')/v_y} f_{LE}(\ell',\vec{v}), \tag{13}$$

where ℓ_0 is an arbitrary point. Now, we keep in mind the assumption that the distance between the plates is so large that the temperatures at the walls are negligible as compared to the temperature in the bulk of the system. More explicitly, we choose ℓ_0 as the point where $T=0$

and impose the boundary condition

$$f_+(\ell_0,\vec{v}) = 0, \tag{14}$$

where we have introduced the half distributions $f_\pm=\theta(\pm v_y)f$.

In order to have an explicit expression for the VDF, one needs to insert the space dependence of the fields $n(\ell)$, $u(\ell)$, and $T(\ell)$ into the right side of Eq. (13). The form of the profiles in Navier-Stokes order, Eqs. (9) and (10), suggests to guess that

$$p = const., \tag{15}$$

$$\frac{\partial u}{\partial \ell} = a = const., \tag{16}$$

$$\frac{\partial^2 T}{\partial \ell^2} = -(2m/k)\,\gamma(a) = const. \tag{17}$$

In Eq. (17), $\gamma(a)$ is a dimensionless function of the shear rate a to be determined by consistency. After some algebra, insertion into Eq. (13) of the profiles given by Eqs. (15)-(17) yields[14]

$$f_+/f_{LE} = \frac{2\beta(1+\beta)^{3/2}}{\varepsilon\,\xi_y}\, e^{\xi^2}\int_0^1 dt\; [2t-(1-\beta)t^2]^{-5/2}$$

$$\times\, e^{-2\beta(1-t)/\varepsilon\xi_y(1+\beta)}\, \exp\left\{-\frac{1+\beta}{2t-(1-\beta)t^2}\left[\xi_y^2+\xi_z^2+\left(\xi_x+\frac{2a\beta}{\varepsilon(1+\beta)}(1-t)\right)^2\right]\right\}, \tag{18}$$

where $t\equiv(\ell'-\ell_0)/(\ell-\ell_0)$. In this equation,

$$\vec{\xi} \equiv (\vec{v}-\vec{u})/\sqrt{2kT/m} \tag{19}$$

is the peculiar velocity relative to the thermal speed,

$$\varepsilon \equiv \sqrt{2k/mT}\,(\partial T/\partial \ell) \tag{20}$$

is the (reduced) local thermal gradient, and $\beta\equiv\varepsilon/(\varepsilon^2+8\gamma)^{1/2}$. Both a and ε play the role of independent uniformity parameters, quantitatively measuring the separation from equilibrium.

The other half distribution f_- is obtained by making the changes $\vec{\xi}\to-\vec{\xi}$, $\varepsilon\to-\varepsilon$, $\beta\to-\beta$ in the right side of Eq. (18). The VDF obtained in this way represents the normal solution to the BGK equation, valid in the bulk limit of the SCF state. It remains to verify the consistency of the assumptions (15)-(17). Equations (2) and (3) are identically satisfied with independence of the relationship between a and γ. However, Eq. (4) only holds if $\gamma(a)$ is given by the implicit equation[12,14]

$$a^2 = \gamma\left[5 + 2\frac{d}{d\gamma}\ln\left[\frac{d}{d\gamma}(\gamma F)\right]\right] \tag{21}$$

where

$$F(\gamma) = \frac{2}{\gamma}\int_0^\infty dw\; w\, e^{-w^2/2} K_0(2w^{1/2}/\gamma^{1/4}), \tag{22}$$

K_0 being the zeroth-order modified Bessel function.[15] With the VDF known, all properties of interest can be calculated by quadratures. In particular, the fluxes of momentum,

$$P_{ij} = m \int d\vec{v}\, (v_i - u_i)(v_j - u_j)\, f, \tag{23}$$

and kinetic energy,

$$\vec{q} = \frac{m}{2} \int d\vec{v}\, (\vec{v}-\vec{u})^2\, (\vec{v}-\vec{u})\, f, \tag{24}$$

are easily obtained. If one defines generalized shear viscosity η and thermal conductivity $\varkappa$ by

$$P_{xy} = -\eta\, \partial u/\partial y, \tag{25}$$

$$q_y = -\varkappa\, \partial T/\partial y, \tag{26}$$

then one gets

$$\eta/\eta_0 = F, \tag{27}$$

$$\varkappa/\varkappa_0 = (\alpha^2/5\gamma)\, F. \tag{28}$$

In the limit $\alpha \to 0$, $\gamma \simeq \alpha^2/5$ and $F \simeq 1$, so that the Navier-Stokes transport coefficients are recovered. However, Eqs. (21) and (22) show that F and γ are nonanalytic at $\alpha=0$. Therefore, the VDF is nonanalytic at $\alpha=0$ and also at $\varepsilon=0$. Consequently, a series expansion of f in powers of α and ε (C-E expansion) is only asymptotic. Yet, it is worth mentioning that no dependence with ε occurs in Eq. (28). This means that the heat flux is exactly linear in ε (generalized Fourier's law), although with an α-dependent conductivity coefficient.

3. UNIFORM SHEAR FLOW (USF)

In contrast to the SCF, the USF is characterized by only one nonzero gradient:

$$n = const., \quad \nabla T = 0, \quad \partial u/\partial y = \omega = const. \tag{29}$$

Nevertheless, the total energy cannot be kept fixed, so that the temperature monotonically increases in time (viscous heating). Although external drag forces have been proposed to account for this effect and get a stationary state,[1] they will not be considered here. This state can be generated in the computer by applying generalized periodic boundary conditions, without any reference to rigid walls in relative motion. Thus, there are no boundary layers, but an initial layer is present.

In the USF, the VDF becomes spatially uniform when it is expressed in terms of the peculiar velocity $\vec{V}=\vec{v}-\vec{u}$. Thus, the BGK equation reads

$$\frac{\partial}{\partial s} f + \alpha V_y \frac{\partial}{\partial V_x} f = -(f - f_{LE}), \tag{30}$$

where s is a new time scale given by

$$ds = \nu(t)\, dt. \tag{31}$$

and the shear rate α is defined as in Eq. (16):

$$\alpha = \omega/\nu. \tag{32}$$

This is now the only uniformity parameter in the problem. As a consequence of the time-dependence of temperature, the reduced shear rate α also changes in time. In the case of repulsive potentials for which Eq. (8) holds, $\alpha \propto T^{-\bar{\alpha}}$. Here, we shall restrict ourselves to this

type of interaction, with α ranging from 0 (Maxwell molecules) to $1/2$ (hard spheres). Taking moments in Eq. (30), one gets a closed set of equations for the pressure tensor:

$$\frac{\partial}{\partial s} P_{ij} + \alpha \left(P_{iy}\delta_{jx} + P_{jy}\delta_{ix}\right) = -\left(P_{ij} - p\delta_{ij}\right). \tag{33}$$

In the case of Maxwell molecules, α is independent of s and Eq. (33) becomes linear. In the long time limit (normal state), $p \propto \exp(\lambda s)$, where[16,17]

$$\lambda(\alpha) = \frac{4}{3} \sinh^2\left[\frac{1}{6} \cosh^{-1}(1+9\alpha^2)\right]. \tag{34}$$

The normal solution to Eq. (30) is then[17]

$$f/f_{LE} = e^{\xi^2} \int_0^\infty ds\, e^{-s}\, e^{3\lambda(\alpha)s/2}\, e^{\alpha s \xi_y \partial/\partial \xi_x} \exp\left[-e^{\lambda(\alpha)s}\, \xi^2\right]. \tag{35}$$

The generalized shear viscosity defined by Eq. (24) turns out to be[16]

$$\eta/\eta_0 = \frac{3}{2} \lambda(\alpha)/\alpha^2. \tag{36}$$

The VDF (35) is an analytic function at $\alpha=0$. Consequently, the C-E expansion in this case is convergent (for $|\alpha|<\sqrt{2}/3$). However, the shape of f is greatly distorted far from equilibrium. In particular, if $\alpha \geq 5/3$, f diverges when $\xi \to 0$.[17]

In the more general case ($0<\alpha\leq 1/2$) the uniformity parameter α goes to zero in the long time limit $s\to\infty$. According to this, the normal solution is, strictly speaking, restricted to local equilibrium ($\alpha=0$). However, we shall adopt a weaker criterion and a normal state will be obtained in the limit of $t\to\infty$, but s (and α) finite. This can be accomplished by taking an initial condition corresponding to (formally) a zero temperature. The technical steps are described elsewhere[17] and here we only quote the final result:

$$f/f_{LE} = e^{-\sigma/\alpha}\, \pi^{3/2}\, \delta(\xi) + \frac{e^{\xi^2}}{\alpha} \int_0^\sigma d\sigma'\, e^{-(\sigma-\sigma')/\alpha} \left[\frac{\alpha'}{\alpha}\right]^{3/2\alpha}$$
$$\times e^{\frac{\tau-\tau'}{\alpha} \xi_y \partial/\partial \xi_x} \exp\left[-\left[\frac{\alpha'}{\alpha}\right]^{1/\alpha} \xi^2\right], \tag{37}$$

where σ and τ are functions of α given by the differential equations

$$\frac{\partial \alpha}{\partial \sigma} = -\frac{2}{3} \alpha^3\, \psi(\alpha), \tag{38}$$

$$\frac{\partial \tau}{\partial \sigma} = \alpha, \tag{39}$$

and $\psi(\alpha)\equiv\eta/\eta_0$ is the solution to a second order nonlinear differential equation[16] with the boundary condition $\psi(\alpha)\to 0$ when $\alpha\to\infty$. This function is nonanalytic at $\alpha=0$ as long as $\alpha>0$.[17,18] In consequence, the C-E expansion of the VDF given by Eq. (37) is only asymptotic. Despite this fact, the shear viscosity $\psi(\alpha)$ for hard spheres ($\alpha=1/2$) is quantitatively very close to the one for Maxwell molecules, Eqs. (36) and (34).

The main qualitative difference between the VDF of Maxwell molecules, Eq. (35) and that of more general potentials, Eq. (37), is the presence of the delta term in the latter. It represents the contribution to the VDF of those particles that have not collided yet after a time equivalent to $s=\sigma/\alpha$ collisions per particle. In order to show up the main features of Eq. (37) and see how it reduces to Eq. (35) in the limit $\alpha\to 0$, it is convenient to construct a caricatured

model of Eq. (37). Following steps inspired in the saddle-point method, one finally arrives to[17]

$$f/f_{LE} = e^{-\tilde{\sigma}/\alpha}\,\pi^{3/2}\,\delta(\vec{\xi}) + e^{\xi^2}\int_0^{\tilde{\sigma}/\alpha} ds\, e^{-s}\, e^{3\lambda(\alpha)s/2} \times e^{s\xi_y \partial/\partial\xi_x}\, \exp[-e^{\lambda(\alpha)s}\,\xi^2], \qquad (40)$$

where $\tilde{\sigma}\equiv 1/2\lambda+\ln(1+1/\lambda)$. The dependence on both α and α is now made explicit. Since $\tilde{\sigma}\approx 3/4\alpha^2$ for small α, it is evident that the VDF given by Eq. (40) has an essential singularity at $\alpha=0$. As a function of α, it also has an essential singularity at $\alpha=0$. Both singularities are coupled and in the limit $\alpha\to 0$ Eq. (40) becomes Eq. (35), which is regular at $\alpha=0$.

4. CONCLUDING REMARKS

The two cases of a gas under shear that we have considered complement each other. In the stationary Couette flow (SCF), the system reaches a steady state, but the hydrodynamic profiles are not simple. On the other hand, the hydrodynamic fields are either constant (n, T) or linear ($\vec{u}$) in the uniform shear flow (USF), which otherwise is a time-dependent state. In both cases, normal solutions to the BGK equation arbitrarily far from equilibrium have been obtained by imposing idealized boundary (SCF: zero wall temperature) or initial (USF: zero initial temperature) conditions. The velocity profiles are in both cases linear in the variable ℓ given by Eq. (11), but the transformation from ℓ to y is not the same, since the collision frequency ν depends on y and t for SCF and USF, respectively.

The normal solution corresponding to the SCF is a universal nonanalytic function of the two independent uniformity parameters: reduced shear rate (α) and thermal gradient (ε). In the USF, the detailed dependence of the normal VDF on the only uniformity parameter (α) is different for each interaction potential. In the case of repulsive power-law potentials, that dependence is nonanalytic, except for Maxwell molecules. This shows that the Chapman-Enskog (C-E) expansion has generally an asymptotic character, except for special interactions in special states.

Far from equilibrium, the VDF is quite different from what one could anticipate on the basis of the first terms of the C-E expansion. Even when such an expansion converges (Maxwell molecules, USF), highly nonlinear effects, such as the divergence of the VDF at zero velocity, emerge for sufficiently large shear rates.

Although the analysis has been carried out on the BGK kinetic model, it is reasonable to expect that the above remarks essentially hold in the case of the Boltzmann equation (BE). This is supported by several facts. The shear viscosity obtained from the BE for Maxwell molecules under USF[8] is identical to that of the BGK equation. A similar connection exists in the steady Fourier flow.[9,19] Moreover, Monte Carlo numerical simulations of the BE agree fairly well with BGK predictions.[3,11]

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