Velocity distribution for a gas with steady heat flow

A. Santos and J. J. Brey

Departamento de Física Teórica, Universidad de Sevilla, Apartado Correos 1065, Sector Sur, E-41080 Sevilla, Spain

C. S. Kim and J. W. Dufty

Department of Physics, University of Florida, Gainesville, Florida 32611 (Received 27 April 1988)

An exact solution to the nonlinear Bhatnagar-Gross-Krook kinetic equation representing heat transport in one direction is obtained. The velocity distribution function is given explicitly and illustrated for both small and large temperature gradients. The Chapman-Enskog expansion for this function is proved to be divergent but asymptotic. Also, the relationship of this solution to infinite hierarchies of moment equations is discussed. In the following paper this special solution is analyzed in the context of more physical boundary-value problems.

I. INTRODUCTION

Recently, it was shown that the nonlinear Bhatnagar-Gross-Krook (BGK) kinetic equation admits a solution corresponding to steady heat flow with a temperature profile that is linear in the appropriate coordinate. 1 The heat flux in this nonequilibrium state is given exactly by Fourier's law, even for large temperature gradients. Other macroscopic properties were also found to be structurally simple. For example, the velocity moments of the distribution function are polynomials in the temperature gradient. These results were deduced from properties of a formal representation of the velocity distribution function, although the distribution function itself was not constructed. The objective here is to remove this formal element of Ref. 1 by giving explicitly the exact distribution function for this state. Consequently, a complete description is obtained for an inhomogeneous steady state arbitrarily far from equilibrium. Since exact solutions for inhomogeneous states are rare,² it is instructive to explore in some detail their properties in each case.

The usual method to describe nonequilibrium phenomena is by the Chapman-Enskog expansion for the distribution function.³ This generates a sequence of approximations to a solution as an expansion in the hydrodynamic gradients. Such an expansion presumes a solution whose space and time dependence is entirely characterized through the hydrodynamic variables, generally known as a Hilbert-class or "normal" solution. ⁴ The special solution given here is also normal in this sense, and the Chapman-Enskog series can be obtained from it by a direct expansion in the temperature gradient. It is proved in Sec. III that this series is divergent but asymptotic. Its domain of utility is illustrated by comparison with the exact solution over a range of velocities, for several values of the temperature gradient. Even for small gradients, deviations from the leading Chapman-Enskog order can be significant, particularly for larger velocities directed along the temperature gradient. A second method for describing nonequilibrium states is to solve (approximately) an infinite hierarchy of equations for the velocity moments of the distribution.⁵ An exact solution to this hierarchy is also given here and the results are shown to be equivalent to the moments obtained directly from the distribution function. The technical problem of determining this function from the moments is discussed briefly. For large values of the temperature gradient (far from equilibrium) neither the Chapman-Enskog expansion nor low-order moments are adequate to characterize the nonequilibrium state.

The special normal solution described here is an idealized one in the sense that it applies globally. In general, it is expected that there should be boundary layers and that the normal solution would apply only locally in regions far from these boundary layers. The relationship of this idealized solution to those with more physical boundary conditions is established in the following paper.

II. SOLUTION TO THE BGK EQUATION

The physical system considered is a low-density gas in a stationary state with a nonuniform temperature. It is assumed that the external sources responsible for this state have a geometry leading to spatial variations only along the x axis. An appropriate theoretical description is provided by the nonlinear Boltzmann equation for the distribution of velocities at each position, $f(x, \mathbf{v})$. Here we use instead the BGK equation which is obtained by replacing the Boltzmann collision operator with an effective single relaxation time model. Although approximate, the BGK equation preserves the most important qualitative features of macroscopic transport. For the stationary conditions considered it has the form

$$v_x \frac{\partial f}{\partial x} = -v(x)(f - f_L) , \qquad (1)$$

where v(x) is an average collision frequency whose x dependence occurs only through a given functional dependence of v on the density, n(x), and temperature, T(x) [the specific form of v(T,n) depends on the interatomic force law considered]. The macroscopic state is characterized by the temperature, density, and local flow

39

velocity $\mathbf{U}(x)$. These fields are the parameters of the usual local equilibrium distribution function f_L in Eq. (1) and are defined by

$$n(x) = \int d\mathbf{v} f(x, \mathbf{v}) ,$$

$$n(x)\mathbf{U}(x) = \int d\mathbf{v} \mathbf{v} f(x, \mathbf{v}) ,$$

$$n(x)T(x) = \frac{1}{3} \int d\mathbf{v} [\mathbf{v} - \mathbf{U}(x)]^2 f(x, \mathbf{v}) .$$
(2)

(The mass and Boltzmann's constant have been set equal to 1.) Since the local equilibrium distribution is specified by these macroscopic fields, Eqs. (1) and (2) must be solved self-consistently.

Although simple in structure, these equations are highly nonlinear due to the coupling of (1) and (2) and, in general, it is necessary to employ numerical methods. Here, however, the simplicity of steady heat flow suggests that it may be possible to "guess" the form of n(x), T(x), and U(x). With these known, Eq. (1) becomes a linear problem whose solution is straightforward. Of course, it is then necessary to verify the guess a posteriori by showing that Eqs. (2) are satisfied. This is the procedure followed here. As in Ref. 1, we note that the space dependence of the coefficients of f in Eq. (1) can be eliminated by the change of variables

$$d\sigma = v(x)dx . (3)$$

Next, we look for a normal solution, i.e., one for which the dependence of $f(\sigma, \mathbf{v})$ on σ occurs only through n, T, and \mathbf{U} . It seems physically reasonable to expect heat transport at uniform pressure, $p \equiv n(x)T(x)$, and with the local flow velocity equal to zero. Then the distribution function depends on σ only through the temperature field, and the simplest form for the temperature is assumed, i.e., a linear function of the variable σ . In summary, we look for solutions with the following properties:

$$f(\sigma, \mathbf{v}) = f(T(\sigma), \mathbf{v}) , \qquad (4)$$

$$\mathbf{U}(\sigma) = 0 , \qquad (5)$$

$$p(\sigma) = \text{const}$$
, (6)

$$\frac{\partial T(\sigma)}{\partial \sigma} = \epsilon = \text{const} \tag{7}$$

[for simplicity, we have used the notation $T(x(\sigma)) \rightarrow T(\sigma)$, etc.] The BGK equation then can be written in the simple form

$$\left[\frac{\partial}{\partial T} + \alpha\right] f(T) = \alpha f_L(T), \quad \alpha \equiv (\epsilon v_x)^{-1}, \quad (8)$$

where the velocity dependence of f and f_L has been suppressed. The solution for $\epsilon=0$ or $v_x=0$ is the local equilibrium distribution $f=f_L$. For finite α , the boundary conditions are imposed on the half distributions, 3,6

$$f^{\pm} \equiv \Theta(\pm v_x) f , \qquad (9)$$

where Θ is the Heaviside unit step function. Then Eq. (8) can be integrated to give the general solution,

$$f^{\pm}(T) = e^{-\alpha(T-T_{\pm})} f^{\pm}(T_{\pm}) + \int_{T_{\pm}}^{T} dt \ e^{-\alpha(T-t)} \alpha f_{L}^{\pm}(t) , \qquad (10)$$

where T_+ and T_- are the values of T at which the boundary conditions are to be specified. Since the temperature profile has been assumed linear it has the domain $0 < T < \infty$ for an infinite system, and it is possible to specify the boundary conditions on the distribution of particles entering the system at the end points, $(T_+ = 0, T_- = \infty)$. We choose

$$f^{+}(T=0)=0=f^{-}(T=\infty)$$
 (11)

The first condition indicates a "freezing" of the particles at the surface with T=0, while the second result is due to vanishing density at high temperature and constant pressure. The solution is now completely specified,

$$f^{+}(T) = \int_{0}^{T} dt \ e^{-\alpha(T-t)} \alpha f_{L}^{+}(t) ,$$

$$f^{-}(T) = -\int_{T}^{\infty} dt \ e^{-\alpha(T-t)} \alpha f_{L}^{-}(t) .$$
(12)

The simplicity of this result is due to the assumptions (4)-(7), so the crucial step to establish it as a solution is the verification of Eqs. (2) using (7) and (12). To do so, it is convenient to introduce a dimensionless function ϕ by

$$f \equiv f_L \phi(\epsilon^*, \xi) ,$$

$$\epsilon^*(\sigma) \equiv \epsilon \sqrt{2/T(\sigma)}, \quad \xi \equiv \mathbf{v}/\sqrt{2T(\sigma)} .$$
(13)

Equation (12) now leads to

$$\phi(\epsilon^*, \xi) = (\epsilon^* |\xi_x|)^{-1} \int_0^\infty dt \ \Theta((1-t) \operatorname{sgn} \xi_x) t^{-5/2} \\ \times \exp\{(t-1)[(\epsilon^* \xi_x)^{-1} \\ + \xi^2 t^{-1}]\} \ . \tag{14}$$

In terms of ϕ the consistency conditions (2) become

$$\int d\xi f_L \psi_\alpha(\xi) [\phi(\epsilon^*, \xi) - 1] = 0 ,$$

$$\psi_\alpha(\xi, \theta) \leftrightarrow (1, \xi_\gamma, \xi^2) .$$
(15)

These conditions are verified by direct integration in Appendix A. Consequently, Eqs. (12), or equivalently (14), provide an exact solution to the nonlinear BGK equation. As mentioned above, for $\epsilon = 0$ we have $f \rightarrow f_L$, and therefore the dimensionless parameter ϵ^* provides a measure of how far a given state is from equilibrium. The derivation places no restrictions on ϵ^* , so highly nonequilibrium states can be described. The qualitative features of the velocity distribution function are illustrated in Fig. 1 for $\epsilon^* = 0.1$, 0.5, and 1.0. To restrict the number of variables, the quantity illustrated is the reduced distribution for velocities along the x axis,

$$\overline{\phi}(\epsilon^*, \xi_x) \equiv \int d\xi_y d\xi_z f / \int d\xi_y d\xi_z f_L . \tag{16}$$

As the local equilibrium distribution gives no heat flux and since the heat flux is directed opposite the temperature gradient, there must be an excess population for large negative velocities relative to the local equilibrium

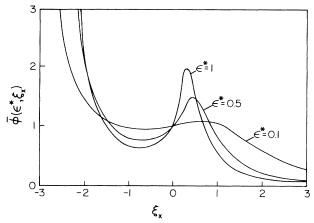


FIG. 1. Reduced velocity distribution [Eq. (16)] for several values of the dimensionless temperature gradient ϵ^* .

distribution. This excess grows rapidly for large negative ξ_x . In addition, there is a maximum for $\xi_x > 0$ that increases with ϵ^* .

$$R^{(N)}(\epsilon^*,\xi) = (\operatorname{sgn}\xi_x)(N+1)!(\xi_x\epsilon^*)^N \int_0^\infty dt \ \Theta((1-t)\operatorname{sgn}\xi_x)t^{-(7/2+N)} \exp\{(t-1)[(\epsilon^*\xi_x)^{-1} + \xi^2t^{-1}]\} L_{N+1}^{3/2}(\xi^2/t) \ . \tag{19}$$

The convergence of the Chapman-Enskog series has been the subject of much speculation, with few specific results. On the basis of general arguments by Grad^8 , it is expected that the series should be at least asymptotic for small ϵ^* even if it does not converge. For the specific case considered here we can be more precise.

- (1) The Chapman-Enskog series diverges pointwise for all finite ξ .
 - (2) The series is asymptotic as $\epsilon^* \rightarrow 0$.

To prove (1) it is sufficient to show that $C_n(\xi)$ does not vanish as $n \to \infty$. This follows from the dependence of C_n on Laguerre polynomials given by (18), which have the asymptotic behavior for large n, ⁷

III. CHAPMAN-ENSKOG EXPANSION

The Chapman-Enskog method leads to an expansion of the distribution function in gradients of the thermodynamic variables. Here the only spatial variation is due to the temperature, so the Chapman-Enskog solution is identified as the expansion of $\phi(\epsilon^*, \xi)$ in powers of ϵ^* . Integrating by parts N+1 times in Eq. (14) gives

$$\phi(\epsilon^*, \xi) = \phi_{CE}^{(N)}(\epsilon^*, \xi) + R^{(N)}(\epsilon^*, \xi) . \tag{17}$$

Here $\phi_{\mathrm{CE}}^{(N)}(\epsilon^*,\xi)$ is the Chapman-Enskog expansion to order N.

$$\phi_{CE}^{(N)}(\epsilon^*, \xi) = \sum_{n=0}^{N} C_n(\xi) \epsilon^{*n} ,$$

$$C_n(\xi) \equiv n! \xi_x^n L_x^{3/2}(\xi^2) ,$$
(18)

where $L_n^{3/2}(\xi^2)$ are Laguerre polynomials.⁷ The remainder $R^{(N)}$ in Eq. (17) is

$$L_n^{3/2}(\xi^2) = -\frac{1}{\sqrt{\pi}} e^{\xi^2/2} \xi^{-2} n^{1/2} \cos[2(n\xi^2)^{1/2}] + O(n^0) .$$

Therefore the Chapman-Enskog series diverges. To prove that the series is asymptotic requires (for fixed N)

$$\lim_{\epsilon^* \to 0} (\epsilon^*)^{-N} R^{(N)}(\epsilon^*, \xi) = 0.$$
 (21)

For positive values of the argument the Laguerre polynomials have the bound⁹

$$|L_N^{3/2}(x)| < \frac{\Gamma(N + \frac{5}{2})}{N!\Gamma(\frac{5}{2})} e^{x/2}$$
 (22)

Using (22) and the fact that $e^{-\xi^2/2t}t^{-(7/2+N)}$ has its maximum at $\xi^2/(2N+7)$, we obtain the bound

$$|(\epsilon^*)^{-N}R^{(N)}(\epsilon^*,\xi)| < \epsilon^* \frac{|\xi_x|^{N+1}\Gamma(N+\frac{7}{2})}{\Gamma(\frac{5}{2})} \exp[\xi^2 - (\frac{7}{2} + N)] \left[\frac{\xi^2}{7+2N} \right]^{-(N+\frac{7}{2})} [1 - \Theta(\operatorname{sgn}\xi_x)e^{-1/\epsilon^*\xi_x}]. \tag{23}$$

Therefore the limit in (21) is verified and the Chapman-Enskog solution is asymptotic.

To illustrate the useful domain for the Chapman-Enskog expansion, Fig. 2 compares $\overline{\phi}(\epsilon^*, \xi_x)$ and $\overline{\phi}_{CE}^{(N)}(\epsilon^*, \xi_x)$ at $\epsilon^*=0.1$ for several values of N. Several features may be noted. For large positive velocities the Chapman-Enskog expansion is always a poor approximation, often leading to a negative distribution. The discrepancies at large negative velocities are less dramatic but quantitatively significant. The asymptotic nature of the expansion is apparent; agreement improves with increasing N up to 3, but is somewhat worse for N=4. Fig-

ure 3 shows the same comparison at $\epsilon^* = 0.5$. Here, the leading approximation is only qualitative and higher approximations are worse.

IV. MOMENT HIERARCHY

In many cases the most important properties of the distribution function are the low-order velocity moments, such as those of Eq. (2). Then it is reasonable to study the equations for the moments themselves instead of looking for the full solution to the kinetic equation. For example, the velocity moments are defined by

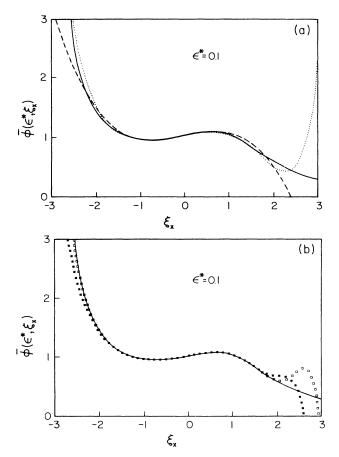


FIG. 2. (a) Comparison of the velocity distribution function at $\epsilon^* = 0.1$ with the Chapman-Enskog expansion [Eq. (18)] for N = 1 (--) and N = 2 ($\cdot \cdot \cdot \cdot$). (b) Same as (a) for N = 3 (\square) and N = 4 (\blacksquare).

$$M_{k,l}(\sigma) \equiv \int d\mathbf{v} \, v^{2k} v_x^l f(\sigma, \mathbf{v}) . \tag{24}$$

Then it follows from (1) and (3) that the moments obey a hierarchy of equations,

$$\frac{\partial}{\partial \sigma} M_{k,l+1}(\sigma) + M_{k,l}(\sigma) = M_{k,l}^{(0)}(\sigma) , \qquad (25)$$

where $M_{k,l}^{(0)}(\sigma)$ are the moments associated with the local equilibrium distribution. Various methods for determining the moments based on truncation of the hierarchy have been suggested. It may be instructive to see how the physically motivated assumptions (7) leads to an exact solution for this hierarchy as well. First, define the dimensionless moments,

$$M_{k,l}^* = \int d\xi \, \xi^{2k} \xi_x^l f^*(\epsilon^*, \xi) ,$$
 (26)

where f^* is the dimensionless distribution function

$$f^*(\epsilon^*, \xi) \equiv p^{-1}2^{3/2}T^{5/2}f(\mathbf{v}) = \pi^{-3/2}e^{-\xi^2}\phi(\epsilon^*, \xi)$$
. (27)

Since $M_{k,l}^*$ depends on σ only through $\epsilon^*(\sigma)$, the hierarchy equations become

$$\frac{\epsilon^*}{2} \left[[2(k-1)+l+1] M_{k,l+1}^* - \epsilon^* \frac{\partial}{\partial \epsilon^*} M_{k,l+1}^* \right] + M_{k,l}^*$$

$$= \begin{cases} \frac{(2k+l+1)!!}{(l+1)2^{k+l/2}}, & l = \text{even} \\ 0, & l = \text{odd} \end{cases}$$
(28)

The form on the left-hand side of this equation suggests a solution where $M_{k,l}^*$ is a polynomial of degree 2(k-1)+l. In fact, this is correct with the precise form given by

$$M_{00}^{*} = 1, \quad M_{01}^{*} = 1, \quad M_{10}^{*} = \frac{3}{2},$$

$$M_{k,l}^{*} = (-1)^{l} 2^{-(2k+l)} \sum_{r=0}^{2(k-1)+l} \frac{(2k+l+r+1)!}{[k-1+(l-r)/2]![k+(l+r)/2](l+r+1)} (\epsilon^{*}/2)^{r},$$
(29)

as may be verified by direct substitution into (28). The last of Eqs. (29) applies for l+2(k-1)>0. This result was first obtained in Ref. 1 using formal properties of the BGK kinetic equation.

Since the macroscopic variables n, T, and U here are the same as in Sec. II, it is expected that the two solutions are closely related. It is proved in Appendix B that all of the moments calculated directly from the distribution function (14) are the same as those given by (29). The inverse problem, construction of the distribution function from the moments, is more difficult. To explore this possibility a new set of moments is defined,

$$N_n(\sigma) = \int d\mathbf{v} \psi_n(\mathbf{v}) f(\sigma, \mathbf{v}) . \tag{30}$$

The functions $\psi_n(\mathbf{v})$ are polynomials of order n, so the N_n are linear combinations of moments considered above. To construct the distribution function, the ψ_n are chosen

to be a complete orthonormal set in the Hilbert space with scalar product,

$$(a,b) = \int d\mathbf{v} \ W(\mathbf{v}) a^*(\mathbf{v}) b(\mathbf{v}) \ . \tag{31}$$

A positive weight factor $W(\mathbf{v})$ is required for the polynomials to have finite norm, but is otherwise arbitrary. Then, assuming f/W is also in this space, an expansion of f in terms of the moments results,

$$f(\sigma, \mathbf{v}) = W(\mathbf{v}) \sum_{n} N_{n}(\sigma) \psi_{n}(\mathbf{v}) . \tag{32}$$

To proceed it is necessary to choose a set of polynomials, or equivalently, $W(\mathbf{v})$. Commonly used examples are Sonine polynomials and Hermite polynomials. In the former case the $\psi_n(\mathbf{v})$ are given by 10

$$\psi_{klm}(\xi) = C_{klm} Y_{lm}(\theta, \phi) \xi^{l} L_{(k-l)/2}^{l+1/2}(\xi^{2}) , \qquad (33)$$

where C_{klm} are normalization constants, k and l are positive integers with $0 \le l \le k$, $k+l = \mathrm{even}$, m is an integer with $-l \le m \le l$, and $Y_{lm}(\theta,\phi)$ are the spherical harmonics. This choice corresponds to a Gaussian weight factor, $W(\mathbf{v}) = f_L(v)$. The hierarchy of equations for the new moments $N_{klm}(\sigma)$ is easily obtained from the kinetic equation and the first several moments have been calculated explicitly. Convergence is assured if the norm of $\phi = f/f_L$ is finite,

$$\|\phi\| = \sum_{k,l,m} |N_{klm}|^2 < \infty$$
 (34)

Figure 4 shows the contribution to this norm from partial sums up through k=6. The results strongly suggest that the series does not converge. Since the moments N_{klm} obtained from the hierarchy equations are the same as those calculated directly from Eq. (14), this implies that the solution ϕ of Sec. II does not exist in the chosen Hilbert space. A closer inspection of ϕ shows for $\xi_x < 0$ and large ξ an asymptotic behavior,

$$\phi(\epsilon^*, \xi) \sim \pi^{1/2} (\epsilon^* |\xi_x|)^{-3/2} \xi^{-2} \exp\left[\xi^2 - 2\left[\frac{\xi^2}{\epsilon^* |\xi_x|}\right]^{1/2}\right].$$
(35)

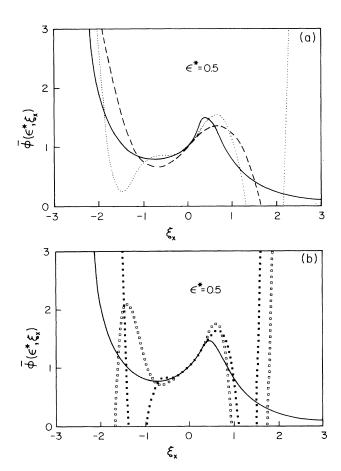


FIG. 3. (a) Same as Fig. 2(a) at ϵ^* = 0.5. (b) Same as Fig. 2(b) at ϵ^* = 0.5.

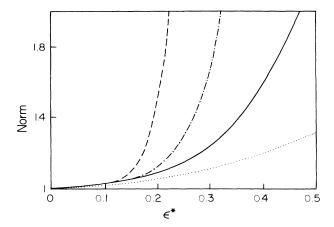


FIG. 4. Norm of ϕ calculated from (34) using partial sums with k=3 (...), k=4 (...), k=5 (...), and k=6 (...)

Thus $(1,\phi)$ is finite, as required for normalization, but (ϕ,ϕ) is infinite.

This analysis indicates that there is no simple and direct representation of the distribution function in terms of its moments. The failure of ϕ to exist in the Hilbert space is of no physical importance beyond the above comment. In fact, the Hilbert space L_2 admits the full solution f. A basis set in this space would provide a systematic expansion, but the coefficients would generally obey a more complex hierarchy than the simple velocity moments and would have a more remote physical significance.

V. DISCUSSION

In Secs. II-IV we have obtained and analyzed a nonequilibrium distribution function that is an exact solution of the BGK kinetic equation. This solution has been used to study the range of validity of some approximation methods commonly used in kinetic theory. To put these results in context and clarify some points the following comments are relevant.

(1) The validity of a kinetic theory is usually tested indirectly by its hydrodynamic fields and transport coefficients. The distribution function provides a more stringent test since it includes all implications of the kinetic equation itself. Unfortunately, under typical laboratory conditions the deviation from local equilibrium is small and experimental measurement of the nonequilibrium distribution function is very difficult.11 Large temperature gradients may occur under more extreme conditions, such as in solar flares or laser-compressed matter, leading to highly distorted electron velocity distributions. Also, there have been attempts recently to apply nonequilibrium molecular dynamics simulation methods for determination of the distribution function in low-density gases. 12 We hope the distribution function obtained here will provide motivation for additional simulations.

(2) The divergence of the Chapman-Enskog expansion does not have any serious physical consequences for the macroscopic transport, since the heat flux is exactly

linear in the temperature gradient. This is in contrast to other conditions we have studied for the BGK equation (combined Couette flow and heat transport) using the moment equations. ^{13,14} In this latter case the divergence of the Chapman-Enskog expansion is associated with a non-analytic dependence of the fluxes on the velocity gradient.

(3) The dimensionless parameter ϵ^* characterizes the deviation of the distribution function from local equilibrium. According to Eqs. (3) and (13) it is related to the actual value of the local temperature gradient through

$$\epsilon^* = l(x) \frac{\partial \ln T(x)}{\partial x} , \qquad (36)$$

where $l(x) = [2T(x)]^{1/2}/v(x)$ is the local mean free path. Therefore, ϵ^* is the ratio of the mean free path to the relevant hydrodynamic length (the distance over which the temperature has a given relative change).

- (4) It might be expected from the simplicity of the temperature field and the heat flux that the distribution function itself would have a simple form for strong symmetry. If this were the case, variational methods, such as maximizing the information entropy, could be used to construct an approximate distribution function from limited macroscopic data (e.g., low-order moments). However, the exact distribution function appears to be considerably more complex both with respect to its ϵ^* dependence and its behavior for large velocities. Further investigation of this point is in progress.
- (5) The relevance of the BGK equation as a model for the Boltzmann equation in this case is supported by the results of Asmolov *et al.* ¹⁵ They show that the moment

equations from the nonlinear Boltzmann equation for Maxwell molecules have an exact solution for the same state as considered here [Eqs. (5)–(7)]. As in Sec. IV, they find the velocity moments are polynomials in the temperature gradient and the heat flux is given exactly by Fourier's law. This suggests that the corresponding distribution function should be qualitatively similar to that given here.

(6) The simplicity of the macroscopic state is due to the absence of any boundary layer for the idealized infinite system considered. More realistic boundary conditions applied to a finite domain lead to deviations from the linear temperature profile near the walls. It is generally expected that a Hilbert-class or "normal" solution, such as that given here, should apply far from the walls. This question is addressed in the following paper, where the relationship of this idealized solution to that for physically more realistic boundary conditions is given.

ACKNOWLEDGMENTS

This research was supported by the U.S.-Spain Joint Committee for Scientific and Technological Cooperation through Grant No. CCB-8402062. C.S.K. and J.W.D. also acknowledge support from National Science Foundation Grant No. CHE-8411932, and A.S. and J.J.B. from Dirección General de Investigación Cientifica y Técnica (Spain) Grant No. PB86-0205.

APPENDIX A: CONSISTENCY CONDITIONS

In this appendix a proof of the consistency conditions (15) is given. Let us start from Eqs. (17)–(19) with N=0:

$$\phi(\epsilon^*, \xi) = 1 + (\operatorname{sgn}\xi_x) \int_0^\infty dt \ \Theta((1-t)\operatorname{sgn}\xi_x) t^{-7/2} e^{(t-1)/\epsilon^*\xi_x} e^{-\xi^2(1-t)/t} L_1^{3/2}(\xi^2/t) \ . \tag{A1}$$

The first integral that must vanish is

$$\int d\xi \, e^{-\xi^2} (\phi - 1) = 2\pi \int_{-1}^1 du (\operatorname{sgn} u) \int_0^\infty dt \, \Theta((1 - t) \operatorname{sgn} u) t^{-2} F_{2,0} \left[\frac{1 - t}{\sqrt{t} \, \epsilon^* u} \right] , \tag{A2}$$

where $u \equiv \xi_x / \xi$ and we have introduced the auxiliary function

$$F_{n,N}(\alpha) \equiv \int_0^\infty dy \, y^n e^{-\alpha/y} e^{-y^2} L_{N+1}^{3/2}(y^2) , \qquad (A3)$$

which has the properties

$$F_{n,N}(\alpha) = -\frac{\partial}{\partial \alpha} F_{n+1,N}(\alpha), \quad F_{4,N}(0) = 0 = F_{n,N}(\infty)$$
 (A4)

Now, if we make the changes $u \rightarrow -u$, $t \rightarrow 1/t$ for u < 0, Eq. (A2) becomes

$$\int d\xi \, e^{-\xi^{2}} (\phi - 1) = 2\pi \int_{0}^{1} du \, \int_{0}^{1} dt (t^{-2} - 1) F_{2,0} \left[\frac{1 - t}{\sqrt{t} \, \epsilon^{*} u} \right]$$

$$= 4\pi \epsilon^{*2} \int_{0}^{1} du \, u^{2} \int_{0}^{\infty} d\alpha \, \alpha F_{2,0}(\alpha)$$

$$= -\frac{4\pi}{3} \epsilon^{*2} \int_{0}^{\infty} d\alpha \frac{\partial}{\partial \alpha} [F_{4,0}(\alpha) + \alpha F_{3,0}(\alpha)]$$

$$= 0,$$
(A5)

where in the last steps use has been made of (A4). The second consistency condition is

$$\int d\xi \, e^{-\xi^2} \xi_x(\phi - 1) = 2\pi \int_{-1}^1 du |u| \int_0^\infty dt \, \Theta((1 - t) \operatorname{sgn} u) t^{-3/2} F_{3,0} \left[\frac{1 - t}{\sqrt{t} \, \epsilon^* u} \right]$$

$$= 2\pi \int_0^1 du \, u \, \int_0^1 dt (t^{-3/2} + t^{-1/2}) F_{3,0} \left[\frac{1 - t}{\sqrt{t} \, \epsilon^* u} \right]$$

$$= 4\pi \epsilon^* \int_0^1 du \, u^2 \int_0^\infty d\alpha \, F_{3,0}(\alpha)$$

$$= -\frac{4\pi}{3} \epsilon^* \int_0^\infty d\alpha \, \frac{\partial}{\partial \alpha} F_{4,0}(\alpha)$$

$$= 0. \tag{A6}$$

Finally, the conservation of energy is preserved:

$$\int d\xi \, e^{-\xi^2} \xi^2 (\phi - 1) = 2\pi \int_{-1}^1 du \, (\operatorname{sgn} u) \int_0^\infty dt \, \Theta((1 - t) \operatorname{sgn} u) t^{-1} F_{4,0} \left[\frac{1 - t}{\sqrt{t} \, \epsilon^* u} \right]$$

$$= 2\pi \int_0^1 du \, \int_0^1 dt \, (t^{-1} - t^{-1}) F_{4,0} \left[\frac{1 - t}{\sqrt{t} \, \epsilon^* u} \right]$$

$$= 0. \tag{A7}$$

APPENDIX B: VELOCITY MOMENTS

In this appendix the velocity moments of the distribution function considered in the main text are evaluated. According to the decomposition (17)-(19), one can write

$$M_{kl}^{*}(\epsilon^{*}) \equiv \pi^{-3/2} \int d\xi \, e^{-\xi^{2}} \xi^{2k} \xi_{x}^{l} \phi(\epsilon^{*}, \xi) = M_{kl}^{*(N)} + \Delta_{kl}^{(N)}, \qquad (B1)$$

where

$$M_{kl}^{*(N)} = \pi^{-3/2} \int d\xi \, e^{-\xi^2} \xi^{2k} \xi_k^l \phi_{CE}^{(N)} , \qquad (B2)$$

$$\Delta_{kl}^{(N)} = \pi^{-3/2} \int d\xi \, e^{-\xi^2} \xi^{2k} \xi_x^l R^{(N)} \,. \tag{B3}$$

Let us compute the term $\Delta_{kl}^{(N)}$ first. By making the same steps as in Appendix A, one easily gets

$$\Delta_{kl}^{(N)} = \frac{2}{\sqrt{\pi}} (N+1)! \epsilon^{*N} \int_{-1}^{1} du (\operatorname{sgn} u) u^{l+N} \int_{0}^{\infty} dt \, \Theta((1-t) \operatorname{sgn} u) t^{k-2+(l-N)/2} F_{N+l+2(k+1),N} \left[\frac{1-t}{\sqrt{t} \, \epsilon^{*} u} \right] \\
= \frac{2}{\sqrt{\pi}} (N+1)! \epsilon^{*N} \int_{0}^{1} du \, u^{l+N} \int_{0}^{1} dt \left[t^{k-2+(l-N)/2} - (-1)^{l+N} t^{-k-(l-N)/2} \right] F_{N+l+2(k+1),N} \left[\frac{1-t}{\sqrt{t} \, \epsilon^{*} u} \right] . \tag{B4}$$

Now, if we choose N = 2(k-1) + l, we have $\Delta_{kl}^{(N)} = 0$. (This excludes the cases k = l = 0 and k = 0, l = 1, which have been considered separately in Appendix A.) Therefore

$$\begin{aligned}
&M_{kl}^{*}(\epsilon^{*}) = M_{kl}^{*(N)}(\epsilon^{*}) \\
&= \pi^{-3/2} \sum_{n=0}^{2(k-1)+l} \epsilon^{*n} n! \int d\xi \, e^{-\xi^{2}} \xi^{2k} \xi_{x}^{l+n} L_{n}^{3/2}(\xi^{2}) \\
&= \frac{2}{\sqrt{\pi}} \sum_{n=0}^{2(k-1)+l} \epsilon^{*n} \frac{n!}{l+n+1} \int_{0}^{\infty} dx \, e^{-x} x^{k+(l+n+1)/2} L_{n}^{3/2}(x) \\
&= (-1)^{l} \frac{2}{\sqrt{\pi}} \sum_{n=0}^{2(k-1)+l} \frac{\epsilon^{*n}}{l+n+1} \int_{0}^{\infty} dx \, x^{k+(l+n+1)/2} \left[\left[\frac{\partial}{\partial t} \right]^{n} \frac{e^{-x/t}}{t^{5/2}} \right]_{t=1} \\
&= (-1)^{l} \frac{2}{\sqrt{\pi}} \sum_{n=0}^{2(k-1)+l} \frac{[k+(l+n)/2-1]!}{[k+(l-n)/2-1]!} \frac{\Gamma(k+(l+n+3)/2)}{l+n+1} \epsilon^{*n} .
\end{aligned} \tag{B5}$$

- ¹A. Santos, J. J. Brey, and V. Garzo, Phys. Rev. A **34**, 5047 (1986).
- ²The only other example we can quote is for uniform shear flow, R. Zwanzig, J. Chem. Phys. **71**, 4416 (1979).
- ³See, for example, J. R. Dorfman and H. van Beijeren, in *Statistical Mechanics, Part B: Time Dependent Processes*, edited by B. J. Berne (Plenum, New York, 1977).
- ⁴H. Grad, in *Principles of the Kinetic Theory of gases*, Vol. 12 of *Handbüch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1958).
- ⁵C. Truesdell and R. G. Muncaster, Fundamentals of Maxwell's Kinetic Theory of a Simple Monatomic Gas (Academic, New York, 1980).
- ⁶C. Cercignani, in *Nonequilibrium Phenomena I. The Boltzmann Equation*, edited by J. L. Lebowitz and E. W. Montroll (North-Holland, Amsterdam, 1983).
- ⁷I. S. Gradshteyn and I. M. Ryzhik, Table of Integrals, Series

- and Products (Academic, New York, 1980), p. 1039.
- ⁸H. Grad, Phys. Fluids 6, 147 (1963).
- ⁹M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1965).
- ¹⁰J. A. McLennan, Introduction to Nonequilibrium Statistical Mechanics (Prentice-Hall, Englewood Cliffs, NJ, 1989).
- ¹¹B. S. Douma, H. F. P. Knapp, and J. J. M. Beenakker, Chem. Phys. Lett. **74**, 421 (1980).
- ¹²W. Loove and S. Hess, Phys. Rev. Lett. **58**, 2243 (1987).
- ¹³A. Santos, J. J. Brey, and J. W. Dufty, Phys. Rev. Lett. 56, 1571 (1986).
- ¹⁴J. J. Brey, A. Santos, and J. W. Dufty, Phys. Rev. A 36, 2842 (1987)
- ¹⁵E. S. Asmolov, N. K. Makarhev, and V. I. Nosik, Dokl. Akad. Nauk SSSR **249**, 577 (1979) [Sov. Phys.—Dokl. **24**, 892 (1979)].