## Hilbert-class or "normal" solutions for stationary heat flow

C. S. Kim and J. W. Dufty

Department of Physics, University of Florida, Gainesville, Florida 32611

### A. Santos and J. J. Brey

Departamento de Fisica Teorica, Universidad de Sevilla, Apartados Correos 1065, Sector Sur, E-41080 Sevilla, Spain (Received 27 April 1988)

The concept of a Hilbert-class or "normal" solution in kinetic theory refers to one whose space and time dependence is determined entirely through the hydrodynamic variables. Such solutions are expected to apply sufficiently far from the boundaries. We investigate this concept quantitatively for the nonlinear Bhatnagar-Gross-Krook equation to describe a gas between two infinite parallel planes at different uniform temperatures. For sufficiently small average Knudsen numbers, spatial domains are identified for which a normal solution applies. It is shown that these conditions include states far from equilibrium, in the sense that deviations of the normal solution from the first Chapman-Enskog approximation can be large. The special exact solution of the preceding paper is found to be the normal solution in the limit of constant temperature gradient.

#### I. INTRODUCTION

The equilibrium state of a physical system is specified by the appropriate conserved quantities or their conjugate variables. In contrast, a general characterization of the nonequilibrium states is quite difficult because the appropriate properties to be specified can differ from state to state and may depend on the space and time scales of the nonequilibrium process considered. For spatially inhomogeneous states a minimal description should include the space and time dependence of the local conserved densities (e.g., mass, energy, and momentum densities). These variables obey local conservation laws relating their time dependence to gradients of the associated macroscopic fluxes. Under favorable conditions, it is often possible to express the space and time dependence of the fluxes entirely as a general function of the conserved variables. The conservation laws then become a closed set of equations for the macroscopic state of the system. An important example is the hydrodynamic description of a simple fluid, which applies for a wide range of nonequilibrium states and types of fluids. The conditions under which the fluxes can be specified in terms of the hydrodynamic variables characterize what is known as a Hilbert-class or "normal" state. Often a more detailed description of a nonequilibrium state is desired. For normal states the additional properties of interest also should have generic forms specified as functionals of the hydrodynamic variables. Normal states are therefore a class of nonequilibrium states that share some of the generic features of equilibrium states in the sense that they can be specified in terms of a relatively few number of variables.

The objective here is to investigate quantitatively this concept of a normal state for a specific class of nonequilibrium states. The system considered is a simple dilute gas between parallel walls held at different temperatures. In this case all macroscopic variables can be determined from the single-particle phase-space distribution function. At low density the distribution function is determined from the Boltzmann equation, whose solutions define the nonequilibrium states of the gas. We address two coupled questions: what are the conditions required for a normal state, and what is the form of the normal distribution function?

Although the concept of normal states is not limited to gases, the most complete discussion has been provided by Grad<sup>1</sup> in the context of solutions to the Boltzmann equation. Grad identified three boundary layers outside of which a normal solution might exist. The boundary layers are (1) short times after specified initial conditions, (2) positions close to spatial boundaries on which conditions have been imposed, and (3) regions separated by discontinuities of the hydrodynamic variables (e.g., shock fronts). Outside these boundary layers it is expected that the gas has a sufficiently regular behavior for a normal solution to exist. The justification for this expectation is closely related to the success of the first Chapman-Enskog approximation for the solution to the Boltzmann equation.<sup>2</sup> The Chapman-Enskog method generates a normal solution by expanding the distribution function in powers of a uniformity parameter. Although the first approximation seems to be in excellent agreement with experiment, through indirect prediction of transport coefficients, there is significant evidence that the method is not convergent.<sup>1,3-5</sup> This leaves open the question of the existence of normal states that are not asymptotically close to the equilibrium state. The results presented here suggest that the failure of the Chapman-Enskog method does not imply a breakdown of the normal state but only a limitation of the method.

Attention is restricted to stationary states, so only the spatial boundary layer is relevant. Two independent parameters are used to generate the class of nonequilibrium stationary states studied. The first is the Knudsen number  $\lambda$ , which is a measure of the average mean free path relative to the system size. The second is the uniformity

39

parameter  $\epsilon^*$ , which is a measure of the relative temperature change over a mean free path. The size of the boundary layer decreases with decreasing Knudsen number, so for small Knudsen numbers there is a domain away from the walls in which a normal solution is expected to apply. At larger Knudsen numbers the boundary layer encompasses the entire system, and a normal state is not possible. To study normal states far from equilibrium (outside the domain of the first Chapman-Enskog approximation) it is necessary to have conditions of relatively large uniformity parameter while maintaining small Knudsen number. States far from equilibrium also require consideration of the nonlinear Boltzmann equation, instead of its simpler linearization. To allow for detailed quantitative analysis we consider instead the Bhatnagar-Gross-Krook (BGK) model for the nonlinear Boltzmann equation.<sup>6</sup> The model equation is actually more highly nonlinear, but it can be solved as a functional of the hydrodynamic variables for a wide class of boundary conditions. The hydrodynamic variables are then determined from a closed set of nonlinear integral equations that can be solved numerically. In this way problems associated with the validity of the Chapman-Enskog method or boundary conditions for the associated differential equations are circumvented. Only diffuse boundary conditions are considered, corresponding to complete accommodation of the particle by the wall. The conclusions drawn here concerning normal states should be representative of other boundary conditions as well.

A normal solution is defined to be a local solution to the kinetic equation whose space and time dependence occurs entirely through the hydrodynamic variables. It need not have a local differential dependence on these variables, as in the Chapman-Enskog method, but more generally it may be a functional of these variables. Its form should be generic rather than specific to a given problem, and the solution does not have to satisfy the specified boundary conditions since it is applicable only outside the boundary layers. Actually, this is a characterization rather than a definition and it may not be sufficient to uniquely determine the normal solution. Nevertheless, on physical grounds it is expected that there should be only one such solution. The success of the first Chapman-Enskog solution suggests that it is an asymptotic representation of the normal solution for small uniformity parameters. For the special case of the BGK equation, a general form for the normal solution suggests itself. The solution to this equation can be written as the sum of a particular solution to the BGK equation plus a second function describing all of the given boundary conditions. The particular solution satisfies the above criteria for a normal function, i.e., it depends on space only through the hydrodynamic variables and is generic. Furthermore, the boundary condition function decays exponentially for points far from the boundary. Consequently, for conditions such that the boundary function is small, the particular solution behaves as a normal solution. (Actually, somewhat stronger conditions are required as indicated in Sec. III.) In Sec. IV we explore in some detail these conditions. For favorable conditions we determine the relative accuracy of a normalstate description of the hydrodynamic variables, the heat flux, and the distribution function.

The questions addressed are old and largely unsolved. There are two main reasons for their reconsideration now. First, there have been several attempts to study nonequilibrium states directly by novel computer-simulation methods. These methods typically have to compromise between a faithful simulation of physical boundary conditions and practical limitations of computer time and system size. In many cases the simulation artificially modifies the boundary layers so that "bulk" properties (e.g., transport coefficients) can be studied directly. These methods presume the validity of a normal state even far from equilibrium. Other methods use more realistic boundary conditions but for very small systems. In these cases it is not clear how well boundary effects can be separated from bulk properties.

A second motivation is to understand and interpret the only two known exact solutions to the nonlinear Boltzmann equation for inhomogeneous states: uniform shear flow<sup>9</sup> and stationary heat flow.<sup>10</sup> They are both obtained as solutions to the infinite hierarchy of equations for moments of the distribution function. However, the boundary conditions are not explicitly stated or imposed. The associated hydrodynamic variables have no boundary layers, so the solutions apparently represent idealized normal states. There is evidence that the boundary conditions are actually nonlocal<sup>11</sup> or unrealistic,<sup>3</sup> so the relationship of these special solutions to those for more physical boundary conditions is not a priori clear.

The corresponding exact solutions also have been obtained for the BGK equation. 12,13 For the case of steady heat flow, the distribution function is obtained in the preceding paper<sup>3</sup> as a function of the temperature gradient. This solution is a special case of the boundaryvalue problem posed here in the limit of an infinitely large system with constant temperature gradient. In this limit, it represents a normal solution that is exact in a finite domain sufficiently far from the hot boundary. Alternatively, it can be viewed as an approximate local solution for the finite boundary-value problem in a domain where the temperature gradient is nearly constant. We show that under such conditions this special solution is indeed a good approximation. However, for the finite boundary case the special solution is not a normal solution in the sense defined above since it is not generic. Instead it is a special solution that is applicable only when the temperature gradient is sufficiently linear in some domains.

The concept of a normal solution is complex and even subjective in some respects. The objective here is to provide some insight for a specific example amenable to quantitative study. Some preliminary conclusions and generalizations are discussed in Sec. V.

## II. SOLUTION TO THE BGK EQUATION

The numerical solution to the BGK equation for heat transport between parallel plates has been discussed elsewhere, <sup>14</sup> primarily for calculation of the dependence of the heat flux on Knudsen number. For completeness and

to define notation, a brief description of the equation and its solution is repeated in this section. For stationary states and the chosen geometry the BGK equation is

$$v_x \frac{\partial}{\partial x} f(x, \mathbf{v}) = -v(x) [f(x, \mathbf{v}) - f_L(x, \mathbf{v})] . \tag{2.1}$$

Here  $f(x, \mathbf{v})$  is the distribution of velocities at position -L < x < L, and  $f_L(x, \mathbf{v})$  is the local equilibrium distribution function,

$$f_L(x,\mathbf{v}) = \Theta(L^2 - x^2) n(x) [2\pi k_B T(x)/m]^{-3/2}$$

$$\times \exp\{-m[\mathbf{v} - \mathbf{U}(x)]^2 / 2k_B T(x)\}.$$
 (2.2)

The Heaviside step function  $\Theta$  restricts the domain to be between the surfaces, and the temperature, T(x), density, n(x), and flow velocity, U(x), are determined self-consistently from  $f(x, \mathbf{v})$  by

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

$$3n(x)k_B T(x)/2 = \int d\mathbf{v} \frac{1}{2} m(\mathbf{v} - \mathbf{U})^2 f(x, \mathbf{v}) ,$$

$$n(x)\mathbf{U}(x) = \int d\mathbf{v} \mathbf{v} f(x, \mathbf{v}) .$$
(2.3)

Also, v(x) is the collision frequency whose dependence on x occurs entirely through T(x) and n(x). The specific functional form of v(x) is determined by the interatomic potential. It is clear that Eqs. (2.1)-(2.3) constitute a highly nonlinear set of equations for  $f(x, \mathbf{v})$ . A unique solution is obtained once boundary conditions are specified at x = -L and x = L. A wide class of local boundary conditions is given by  $^{15}$ 

$$\begin{split} \Theta(\mp v_x) f(x = \pm L, \mathbf{v}) = & \Theta(\mp v_x) \int d\mathbf{v}' K(\mathbf{v}, \mathbf{v}', \pm L) \\ & \times \Theta(\pm v_x') \\ & \times f(x = \pm L, \mathbf{v}') \; . \end{split}$$

The kernels  $K(\mathbf{v}, \mathbf{v}', \pm L)$  describe the distribution of velocities coming off each surface in terms of the distribution of velocities incident on the surfaces. They are restricted by requirements of normalization and the existence of an equilibrium solution, but are otherwise arbitrary. Here we limit attention to diffuse boundary conditions, for which  $K(\mathbf{v}, \mathbf{v}', \pm L)$  is given by

$$K(\mathbf{v}, \mathbf{v}', \pm L) = \frac{1}{2\pi} \left[ \frac{m}{k_B T_{\pm}} \right]^2 |v_x'| e^{-m(\mathbf{v} - \mathbf{U}_{\pm})^2 / 2k_B T_{\pm}}.$$
(2.5)

The constants  $T_{\pm}$  and  $\mathbf{U}_{\pm}$  are specified parameters characterizing the temperature and velocity of the surface at  $x=\pm L$ . Diffuse boundary conditions correspond to complete accommodation of the particle on interaction with the surface. It is possible to consider more realistic boundary conditions, but it is not expected to be important for the qualitative questions of interest here. Equations (2.1)–(2.5) completely specify the problem to be solved.

To simplify these expressions it is useful to introduce a

dimensionless velocity  $\mathbf{v}^*$  and position s by

$$\mathbf{v}^* = \mathbf{v}/v_0, \quad s = (\lambda/v_0) \int_{-L}^{x} dx' v(x') ,$$
 (2.6)

where  $v_0 = (2k_B T_0/m)^{1/2}$  is the thermal velocity at some reference temperature  $T_0$ , and  $\lambda$  is the ratio of an average mean free path to the distance between the surfaces,

$$\lambda = v_0 \left[ \int_{-L}^{L} dx \ v(x) \right]^{-1} . \tag{2.7}$$

Equivalently,  $\lambda$  is an effective Knudsen number. Finally, the dimensionless distribution functions are given by

$$f^*(s, \mathbf{v}^*) = v_0^3 n_0^{-1} f(x, \mathbf{v})$$
, (2.8)

$$f_I^*(s, \mathbf{v}^*) = \Theta(s - s^2) n^*(s) [\pi T^*(s)]^{-3/2}$$

$$\times \exp\{-[\mathbf{v}^* - \mathbf{U}^*(s)]^2 / T^*(s)\},$$
 (2.9)

where  $n_0$  is some reference density,  $n^* = n/n_0$ ,  $T^* = T/T_0$ , and  $U^* = U/v_0$ , and the step function enforces the domain 0 < s < 1. In the following it is understood that only the dimensionless quantities occur, unless otherwise specified, and the asterisks will be deleted. In dimensionless form Eq. (2.1) becomes

$$\left[1 + \lambda v_x \frac{\partial}{\partial s}\right] f(s, \mathbf{v}) = f_L(s, \mathbf{v}) . \tag{2.10}$$

A general, but implicit, solution to this equation is easily obtained by direct integration,

$$f(s,\mathbf{v}) = f_p(s,\mathbf{v}) + f_b(s,\mathbf{v}) . \tag{2.11}$$

The first term on the right-hand side is a particular solution to Eq. (2.10),

$$f_p(s, \mathbf{v}) = \int_0^\infty dt \ e^{-t} f_L(s - \lambda v_x t, \mathbf{v}) \ , \tag{2.12}$$

as may be verified by direct substitution. Since  $f_L$  depends on s only through the hydrodynamic variables,  $f_p(s, \mathbf{v})$  has the characteristics of a normal solution.

The second term on the right-hand side of (2.11) is given by

$$f_b(s, \mathbf{v}) = A(\mathbf{v})e^{-s/\lambda v_x} . \tag{2.13}$$

It can be verified that  $f_p(s, \mathbf{v})$  vanishes at s = 0 for  $v_x > 0$  and at s = 1 for  $v_x < 0$ , so the boundary conditions are entirely contained in  $f_b(s, \mathbf{v})$ . The function  $A(\mathbf{v})$  is determined by (2.4) and (2.5) to be

$$A(\mathbf{v}) = \Theta(v_x) n_- (\pi T_-)^{-3/2} e^{-(\mathbf{v} - \mathbf{U}_-)^2 / T_-}$$

$$+ \Theta(-v_x) e^{1/\lambda v_x} n_+ (\pi T_+)^{-3/2} e^{-(\mathbf{v} - \mathbf{U}_+)^2 / T_+}.$$
(2.14)

The constants  $n_+$  and  $n_-$  are twice the density of particles coming off the surfaces at s=1 and 0, respectively. Their values must be determined self-consistently from the distribution function. The parameters  $T_\pm$  and  $U_+$  can be specified arbitrarily.

Equations (2.11)-(2.14) provide only an implicit solution since there is still a dependence on the unknown variables n(s), T(s), and the constants  $n_+$  and  $n_-$ . These must be determined self-consistently from Eqs.

(2.3). We now specialize to the case of pure heat flow by setting  $U_+=U_-=0$ . Then the velocity field inside the system vanishes everywhere. Substituting (2.11)–(2.14) into Eqs. (2.3) gives

$$n(s) = n_{+}J_{0} \left[ \frac{1-s}{\lambda} \right] + J_{0} \left[ \frac{s}{\lambda\sqrt{T_{-}}} \right] + \frac{1}{\lambda} \int_{0}^{1} dt \frac{n(t)}{\sqrt{T(t)}} J_{-1} \left[ \frac{|s-t|}{\lambda\sqrt{T(t)}} \right],$$

$$\frac{3}{2}p(s) = n_{+} \left[ J_{0} \left[ \frac{1-s}{\lambda} \right] + J_{2} \left[ \frac{1-s}{\lambda} \right] \right] + T_{-} \left[ J_{0} \left[ \frac{s}{\lambda\sqrt{T_{-}}} \right] + J_{2} \left[ \frac{s}{\lambda\sqrt{T_{-}}} \right] \right]$$

$$+ \frac{1}{\lambda} \int_{0}^{1} dt \frac{p(t)}{\sqrt{T(t)}} \left[ J_{-1} \left[ \frac{|s-t|}{\lambda\sqrt{T(t)}} \right] + J_{1} \left[ \frac{|s-t|}{\lambda\sqrt{T(t)}} \right] \right], \qquad (2.15)$$

$$n(s)U_{x}(s) = 0 = -n_{+}J_{1} \left[ \frac{1-s}{\lambda} \right] + \sqrt{T_{-}}J_{1} \left[ \frac{s}{\lambda\sqrt{T_{-}}} \right] + \frac{1}{\lambda} \int_{0}^{1} dt \operatorname{sgn}(s-t)n(t)J_{0} \left[ \frac{|s-t|}{\lambda\sqrt{T(t)}} \right].$$

Here p(s) = n(s)T(s) and the normalization of temperature and density has been taken relative to  $T_+$  and  $n_-$ , respectively. The functions  $J_l(t)$  are defined in Appendix A. The above provide a closed set of equations for the temperature, density, and  $n_+$ . Once their solutions have been given these parameters can be substituted into Eq. (2.11) to obtain the distribution function as well. This is one of the simplifying features of the BGK equation: for a wide class of boundary conditions a closed set of equations for the hydrodynamic variables applies, independent of the distribution function.

Equations (2.15) are a set of nonlinear, singular integral equations. There are no general methods available to discuss the existence or qualitative features of the solutions,

and numerical methods fail at very small Knudsen numbers. Nevertheless, it is possible to obtain the solution over an interesting domain  $0.1 \le \lambda \le \infty$ , for a wide range of temperature ratios,  $T_{-}$ . The details of the calculation are given in Appendix A.

In addition to the hydrodynamic variables, the fluxes of energy and momentum can be calculated. For example, the heat flux in the direction of the temperature gradient is

$$q(s) = \int d\mathbf{v} \, v_x v^2 f(s, \mathbf{v}) \ . \tag{2.16}$$

Using the general solution (2.12) and (2.13) this can be expressed in terms of the hydrodynamic variables,

$$q(s) = T_{-}^{3/2} \left[ J_{1} \left[ \frac{s}{\lambda \sqrt{T_{-}}} \right] + J_{3} \left[ \frac{s}{\lambda \sqrt{T_{-}}} \right] \right] - n_{+} \left[ J_{1} \left[ \frac{1-s}{\lambda} \right] + J_{3} \left[ \frac{1-s}{\lambda} \right] \right] + \frac{1}{\lambda} \int_{0}^{1} dt \operatorname{sgn}(s-t) p(t) \left[ J_{0} \left[ \frac{|s-t|}{\lambda \sqrt{T(t)}} \right] + J_{2} \left[ \frac{|s-t|}{\lambda \sqrt{T(t)}} \right] \right].$$

$$(2.17)$$

Therefore, once the hydrodynamic variables have been calculated, it is straightforward to obtain the heat flux. In spite of the apparent dependence on s the heat flux is actually constant, as follows from energy conservation. This constancy is used as a check on the numerical accuracy of the solution to the nonlinear integral equations.

## III. NORMAL SOLUTIONS

Both Eq. (2.11) for the distribution function and Eqs. (2.15) for the hydrodynamic variables have an explicit dependence on the boundary contribution  $f_b$ . This is responsible for a boundary layer near each wall in which the form and parameters of the boundary conditions are very important. However, far from the walls  $f_b$  can be small and the effects of the boundary conditions occur only implicitly through the values of hydrodynamic variables. For example, the particular solution  $f_p$  of Eq.

(2.12) becomes a normal solution in this case since its space dependence appears entirely as a functional of the hydrodynamic variables. Also, the special solution given in Ref. 3 is normal for the case of a constant temperature gradient. Three possible choices for a normal solution are described in the following, for comparison with the exact solution of Sec. II. It is convenient to describe the various distribution functions relative to the local equilibrium distribution,

$$\phi(s,\xi) = f(s,\mathbf{v})/f_I(s,\mathbf{v}) , \qquad (3.1)$$

where now  $\xi = \mathbf{v}/\sqrt{T(s)}$  is the velocity relative to the local thermal velocity at the point s.

#### A. Chapman-Enskog solution

In the Chapman-Enskog method, a uniformity parameter  $\epsilon^*$  is introduced to measure the mean free path rela-

tive to a characteristic distance over which the hydrodynamic variables vary. For the problem here this is the mean free path times the relative temperature gradient,

$$\epsilon^*(s) = l(x) \frac{\partial}{\partial x} \ln T(s) = \lambda \sqrt{T(s)} \frac{\partial}{\partial s} \ln T(s)$$
 (3.2)

Here,  $l(x)=v_0\sqrt{T(x)}/v(x)$  is the local mean free path. This uniformity parameter is the same as that of Ref. 3. The Chapman-Enskog method leads to an expansion in powers of  $\epsilon^*(s)$ . Therefore the result is assumed to be valid near equilibrium in a spatial domain far from the walls. To first order in  $\epsilon^*$  the Chapman-Enskog solution for steady heat flow is

$$\phi_{\text{CE}}(s,\xi) = 1 - \epsilon^* \xi_x (\xi^2 - \frac{5}{2})$$
 (3.3)

It is easily verified that Eqs. (2.3) are satisfied by Eq. (3.3). The heat flux in the first Chapman-Enskog approximation can be calculated from (3.3) to get

$$q_{\rm CE}(s) = -\frac{5}{4} \epsilon^*(s) p(s) \sqrt{T(s)} . \tag{3.4}$$

Equation (3.4) is Fourier's law, expressing the heat flux proportional to the temperature gradient or, equivalently,  $\epsilon^*$ . Corrections to Fourier's law involving a nonlinear dependence on  $\epsilon^*$  are expected from higher-order approximations in the Chapman-Enskog expansion. Since this expansion is probably only asymptotic, it is not useful to calculate these higher-order terms.

## B. The particular solution

The function  $f_p$  is an exact solution to the BGK equation (2.1) for given hydrodynamic fields. Thus, whenever a normal solution exists, it must agree with  $f_p$ . This particular solution is a good approximation in a region of the system for which the boundary function  $f_b$  in Eq. (2.11) is negligible. An estimate of the conditions for this can be obtained from the requirement  $\phi_b \ll 1$ . Equation (2.14) shows that  $\phi_b$  decreases exponentially with the distance from the boundary for

$$s \gg \lambda(s)\xi_x[1+\xi_x\xi^2\epsilon^2(s)T(s)/T_-]^{-1}, \quad \xi_x > 0$$
 (3.5)

$$1-s \gg \lambda(s)|\xi_x|[1-|\xi_x|\xi^2\epsilon^*(s)T(s)]^{-1}, \quad \xi_x < 0$$

where  $\lambda(s) = \lambda \sqrt{T(s)}$  is a local Knudsen number. The region for which conditions (3.5) do not hold (near the boundaries) will be referred to as the boundary layers. These conditions simplify for velocities near the thermal velocity ( $\xi_x \sim 1$ ) and for small  $\epsilon^*(s)$  to approximately  $\lambda(s)|\xi_x| \ll s \ll 1 - \lambda(s)|\xi_x|$ . Consequently, when both Knudsen number and velocity are small there is a large region away from the boundaries in which  $f_p$  should be a good normal solution. For large velocities with positive  $\xi_x$  and large  $\epsilon^*$  this domain actually increases, as seen from the first of conditions (3.5). However, under the same conditions for negative  $\xi_x$  the boundary layer is large and substantial differences between  $f_p$  and f are expected. The exponential separation of the particular solution from the boundary layer defines a more general

normal solution than that obtained from the Chapman-Enskog expansion, which is limited to states near equilibrium. It can be verified that the Chapman-Enskog result follows from the particular solution by a formal expansion of  $f_L(s-\lambda v_x,\mathbf{v})$  about  $f_L(s,\mathbf{v})$  for small values of the uniformity parameter.

The hydrodynamic variables depend on integration over the velocity and their effective boundary layers are determined from the functions  $J_l(s/\lambda \sqrt{T_-})$  and  $J_I[(1-s)/\lambda]$  in Eqs. (2.15). The functions are small for  $\lambda \sqrt{T_{-}} \ll s \ll 1 - \lambda$  but they are not exponentially small like  $f_h$ . In this case it is only the average Knudsen number that determines the relative size of the boundary layer. Consequently, for a given Knudsen number, the particular solution may be a good normal solution for a range of small velocities but the hydrodynamic parameters may still require including boundary effects in Eqs. (2.15). The two requirements that a solution must satisfy away from the boundaries are the BGK equation (2.1) and the consistency conditions (2.3). Therefore all properties derive from  $f_p(x, \mathbf{v})$  will be normal (functionals of the hydrodynamic variables only) whenever  $f_p$  satisfies both of these requirements.

#### C. A special solution

In Ref. 3, an exact solution to the BGK equation was obtained for an infinite system with temperature equal to zero at the cold wall and infinite at the remote hot wall. The temperature for this case is exactly linear in s with constant pressure. The space dependence of this solution is characterized simply by the temperature gradient, and therefore it is normal. This special solution is easily regained from Eqs. (2.11)–(2.14) in the limit of  $T_- \to 0$  at constant  $e^*$  and  $s \to 0$ . (The limit on s corresponds to a finite distance s from the cold wall.) It is therefore a special case of the diffuse boundary-value problem considered here.

It is also possible to interpret this special solution with constant temperature gradient as applying to a finite system, but with contrived boundary conditions that elimi-

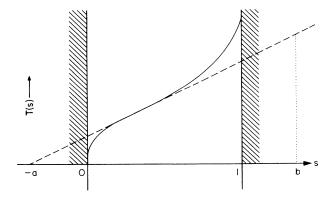


FIG. 1. Illustration of the extended domain  $-a \le s \le b$ , with temperature profile for diffuse boundary conditions ( —— ) and for conditions (B8) ( — — ).

nate the boundary layer. The constant temperature gradient of this special solution can be adjusted to fit locally the temperature field for the diffuse boundary conditions used here. This is illustrated schematically in Fig. 1. Since the solution is also local (i.e., a function rather than a functional of the hydrodynamic variables) it must agree with the diffuse boundary solution whenever the hydrodynamic fields are the same. It will appear in Sec. IV that the temperature gradient for diffuse boundary conditions is not strictly linear, even in the normal state. How-

ever, there are intervals over which the temperature is approximately linear and the special solution should provide a good description. It cannot be considered a normal solution for these boundary conditions in the strict sense, because the gradient must be adjusted differently for each such interval. Further comment on this point is given in Sec. IV. In essence, the finite domain is simply considered as part of the above infinite region. The details are given in Appendix B, and the distribution function is

$$\phi_s(\epsilon^*, \xi) = (1/\epsilon^* | \xi_x|) \int_0^\infty dt \,\Theta((1-t) \operatorname{sgn} \xi_x) t^{-5/2} \exp\{(t-1)[(\epsilon^* \xi_x)^{-1} + \xi^2 t^{-1}]\} . \tag{3.6}$$

The three normal solutions described above each have different conditions under which they are expected to apply. Since the normal solution should be unique, they should agree when their conditions for validity overlap. It is worth commenting that the identification of a normal solution does not provide a recipe for calculating the required hydrodynamic variables in the normal domain. This is a separate problem that must be addressed for application of the normal solution. For practical purposes it is necessary to have a method to connect the specified conditions at the boundaries to the hydrodynamic variables across the boundary layers. This problem lies outside the domain in the normal state and requires further knowledge of the details in the boundary layer. We do not address this connection problem here, but instead use the numerical solutions to the full Eqs. (2.15) for the hydrodynamic variables when required.

# IV. RESULTS

To discuss the possible relevance of normal solutions it is first necessary to determine the hydrodynamic variables. These are calculated numerically from Eqs. (2.15). The method and accuracy of the solution are discussed in Appendix A. Two cases are considered, temperature ratios  $T_{-}=0.2$  and 0.01, for Knudsen numbers  $0.1 \le \lambda \le 1.0$ . The qualitative features of the density, temperature, and pressure are the same at all Knudsen numbers. The temperature gradient and the pressure are always approximately constant with respect to s, while the density is simply defined by n=p/T. Figure 2 shows the variation of the temperature with Knudsen number at

 $T_{-}$ =0.2. The main feature is a temperature slip at each boundary that increases with Knudsen number. In addition, there is a point in each case for which the temperature is approximately independent of Knudsen number, although this invariance fails at larger Knudsen numbers. We have not yet understood this property of the solutions.

The heat flux was calculated from these hydrodynamic variables using Eq. (2.17), and is shown in Fig. 3 as a function of the Knudsen number. Also shown is the heat flux from Fourier's law, Eq. (3.4), calculated at s=0.4 for  $T_-=0.2$ . Similar results are found for  $T_-=0.01$ . There is agreement with Fourier's law up to  $\lambda=0.2$  for both temperature ratios, but significant deviations occur at larger values. There are two possible sources for this deviation, higher-order terms in the Chapman-Enskog solution and boundary effects. To estimate the latter, the contribution of  $f_b$  in Eq. (2.11) to the density is shown in Fig. 4. The boundary effects are seen to be significant at about the same Knudsen numbers for which Fourier's law fails. We conclude that the heat flux is normal for  $\lambda \lesssim 0.2$ .

The fact that Fourier's law is applicable only at small Knudsen numbers does not necessarily imply limitation to states near equilibrium (i.e., first Chapman-Enskog approximation). The converse is of course true, but it is possible that Fourier's law could hold under more general conditions. In fact, it is a surprising property of the special solution<sup>3</sup> that Fourier's law is *exact* for arbitrary magnitude of the temperature gradient. To explore this possibility in the present case and investigate the possibil-

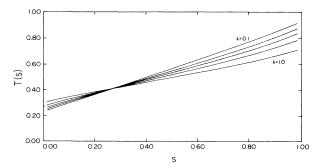


FIG. 2. Temperature profiles for  $\lambda = 0.1$ , 0.2, 0.3, 0.5, and 1.0 at  $T_{-} = 0.2$ .

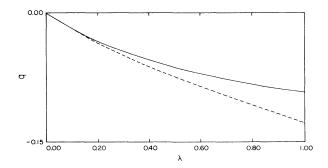


FIG. 3. Heat flux as a function of Knudsen number at  $T_{-}=0.2$ ; numerical ( —— ), Fourier's law ( — — ).

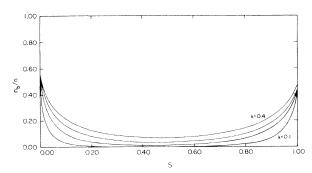


FIG. 4. Relative contributions to the density from the boundary term  $f_b$  for  $\lambda = 0.1, 0.2, 0.3,$  and 0.4 at  $T_- = 0.2$ .

ity of more general normal solutions it is necessary to study the distribution functions directly.

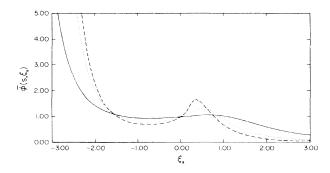
Consider the reduced distribution function  $\bar{\phi}$  obtained by integrating out the velocities in the y and z directions,

$$\overline{\phi}(s,\xi_x) = \int dv_y dv_z f(s,\mathbf{v}) / \int dv_y dv_z f_L(s,\mathbf{v}) . \tag{4.1}$$

Figure 5 illustrates the results for several combinations of Knudsen number and temperature ratio. There is an excess of particles with large velocities directed opposite the temperature gradient. The small peak at positive velocities is required to compensate for this excess, so that the total particle flux vanishes. As expected, the deviation from local equilibrium increases for larger Knudsen number or smaller temperature ratio.

For comparison with the various forms for a normal solution given in Sec. III, it is necessary to identify the range of s values for which the boundary terms are small. In Fig. 4 for  $T_-=0.2$  the relative boundary contribution to the density is about  $10^{-3}$  at s=0.4 and  $\lambda=0.1$ . Similarly, for  $T_-=0.01$  it is  $2\times10^{-3}$  at s=0.2 and  $\lambda=0.2$ . These are clearly conditions for which both a normal solution is expected to apply and Fourier's law is well verified. For  $T_-=0.2$  the uniformity parameter is  $\epsilon^*=0.1$  at s=0.4, while for  $T_-=0.01$  it is  $\epsilon^*=0.39$  at s=0.2. In the following, we refer to the conditions for  $\epsilon^*=0.1$  and  $\epsilon^*=0.39$  as cases 1 and 2, respectively.

Three candidates for a normal solution were identified in Sec. III: the Chapman-Enskog solution, the particular solution of Eq. (2.12), and the special solution of Ref. 3.



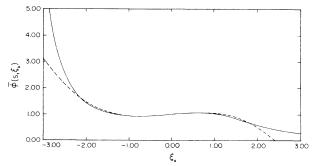


FIG. 6. Comparison of the reduced distribution function ( — ) with the first Chapman-Enskog approximation ( ---), for  $\lambda=0.1$ , and  $T_-=0.2$  at s=0.4.

The Chapman-Enskog solution is obtained from a power-series expansion in the uniformity parameter  $\epsilon^*$  and therefore applies only close to local equilibrium. Other conditions also are required for its validity. Since the series in  $\epsilon^*$  involves polynomials in the velocity, the latter must not be too large either. For case 1 these conditions are well satisfied for  $-2 \le \xi_x \le 2$ , as shown in Fig. 6. Although significant errors occur outside the range they are attenuated by the local equilibrium weight factor so that the consistency conditions (2.3) hold as well. As expected, Fig. 7 shows that the first Chapman-Enskog solution fails for case 2 since the uniformity parameter is no longer small. Nevertheless, Fourier's law is still found to be a good approximation so the differences indicated in Fig. 7 evidently do not contribute to the heat flux.

Only the first Chapman-Enskog approximation has been studied here since there is strong evidence that the expansion is only asymptotic. 1,3-5 A natural question, therefore, is whether the notion of a normal solution is similarly limited to states asymptotically close to equilibrium. To test this, an alternative to the Chapman-Enskog solution must be constructed that does not require small  $\epsilon^*$ . The particular solution  $f_p$  is a reasonable choice since it is a normal solution whenever the boundary contribution  $f_b$  is negligibly small. This condition places restrictions on the velocity and average Knudsen number, but not necessarily on the uniformity parameter  $\epsilon^*$ . For case 1, Fig. 8 shows that the particular solution is actually a better approximation than the first Chapman-Enskog solution. At the larger uniformity parameter, case 2, the particular solution is still a very good approximation as shown by Fig. 9. This is a primary re-

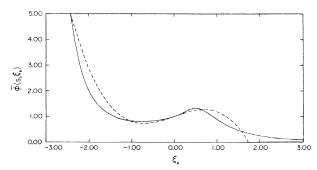


FIG. 7. Same as Fig. 6, for  $\lambda = 0.2$  and  $T_{-} = 0.01$  at s = 0.2.

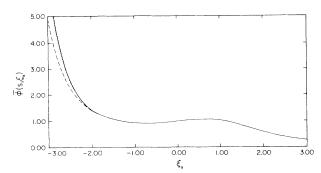


FIG. 8. Comparison of the reduced distribution function ( — ) with the particular solution ( — — ) and the special solution (  $\cdot \cdot \cdot \cdot$  ), for  $\lambda = 0.1$  and  $T_{-} = 0.2$  at s = 0.4.

sult of our analysis. It shows that the concept of a normal state extends beyond the limitations of the Chapman-Enskog method. Although we have not performed the calculations at still larger values of the uniformity parameter, we believe the present results suggests that the particular solution would still apply as long as  $\lambda \lesssim 0.2$ . Of course, there are discrepancies at large velocities, but for the reasons mentioned above conditions (2.3) are satisfied for both cases 1 and 2.

It is interesting to note that the particular solution can be a good approximation even for larger Knudsen numbers, for which a normal state is not expected to apply. This is shown in Fig. 10. Although the differences are now larger than in Fig. 9, the agreement is surprisingly good. However, the consistency conditions (2.3) no longer hold, since there are boundary contributions to the density of the order of several percent.

Finally, we consider the special solution of Ref. 3 as a possible approximation to f. As discussed above this solution is different in character from the Chapman-Enskog and particular solutions. The latter are generic solutions in the sense that their form is the same for a class of boundary-value problems, not just for the simple heat-flow case considered here. In contrast, the special solution applies only for states that show locally a linear temperature profile, constant pressure, and zero flow velocity. However, when these conditions hold locally, the special solution might apply over a wider range of Knudsen numbers than the particular solution. The reason is that conditions (2.3) are then automatically satisfied for the special solution even if  $f_b$  is not negligible. Figure 2 shows that the exact temperature gradient is approxi-

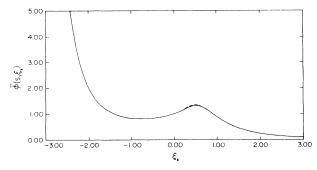


FIG. 9. Same as Fig. 8, for  $\lambda = 0.2$  and  $T_{-} = 0.01$  at s = 0.2.

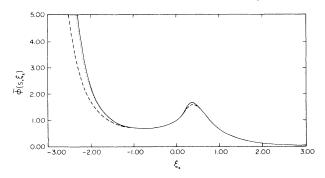


FIG. 10. Same as Fig. 8, for  $\lambda = 0.5$  and  $T_{-} = 0.01$  at s = 0.3.

mately constant over small intervals containing the points chosen for cases 1 and 2. And it is seen that the pressure is also constant over the entire range for both cases. Using the calculated temperature gradient in the special solution it can be compared with the exact distribution. Figures 8 and 9 show that the special solution is as good an approximation as  $f_p$  at small Knudsen numbers. Figures 10 and 11 show the same comparison at  $\lambda$ =0.5 and 1.0. The corresponding uniformity parameters are  $\epsilon^*$ =0.7 and 1.05. The special solution is now clearly a better approximation than  $f_p$ , although these conditions clearly do not admit a normal-state description.

The relationship of the heat flux to the distribution function is interesting and somewhat paradoxical. It turns out that most of the contribution to the heat flux comes from velocities in the range  $1 < |\xi_x| < 3$ . The reason for this is a near cancellation of the contributions from positive and negative velocities with magnitude  $|\xi_x|$  < 1, plus the slow decay of the distribution function for larger negative velocities. This is somewhat surprising since the first Chapman-Enskog solution differs substantially in this region (for large  $\epsilon^*$ ) and yet they predict the same heat flux. Evidently, these large differences exactly cancel. Conversely, the special solution and the exact solution appear to agree closely in Fig. 10 but their respective heat fluxes are significantly different. The explanation again lies in the significance of the contribution from relatively large negative velocities. A calculation of the ratio of the exact  $\bar{\phi}$  relative to that for the special solution shows there are large differences for large negative velocities that apparently have different contributions to the heat flux in this case.

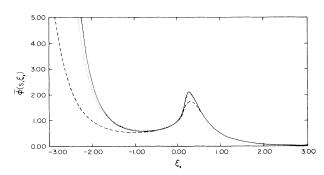


FIG. 11. Same as Fig. 8, for  $\lambda = 1.0$  and  $T_{-} = 0.01$  at s = 0.5.

#### V. DISCUSSION

The analysis of a simple gas in steady heat flow from the BGK equation has been given many years ago. Previous work has concentrated on the Knudsen number dependence of fluxes and the description of boundary layers. Here, we have considered the complementary problem of describing properties outside the boundary layers. Specifically, we have calculated properties for fixed, small Knudsen numbers as a function of the uniformity parameter at points far from the boundaries. The objective was to explore the possibility of a normal state for which the space dependence of the properties could be described as generic functionals of the hydrodynamic variables. Sufficient conditions for a normal state here are the existence of a normal solution to Eq. (2.1) with the consistency conditions (2.3). The following points summarize and highlight some of the results of the calculations given here.

- (1) The first Chapman-Enskog solution is a good approximation for the distribution function only at very small values for the uniformity parameter.
- (2) The heat flux is accurately described by Fourier's law for small values of the Knudsen number. However, this domain includes large values for the uniformity parameter. It appears that Fourier's law extends outside the domain of accuracy of the first Chapman-Enskog solution.
- (3) At small Knudsen numbers the particular solution, Eq. (2.12), behaves as a generic normal solution outside the boundary layers, even for large values of the uniformity parameter.
- (4) The special solution of Ref. 3 is a limiting case of the particular solution when the system size is taken large at fixed average temperature gradient. Therefore this is the limit in which the normal solution becomes exact.
- (5) The special solution can also approximate the distribution function for finite boundaries wherever the temperature gradient and pressure are approximately constant. This is true regardless of whether or not there are boundary effects at the points considered.

The analysis presented here can be extended to other boundary conditions. In particular, we have studied the case of combined heat and planar Couette flow. The results will be described elsewhere.

#### **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: SOLUTION OF EQS. (2.15)**

In this appendix, the numerical analysis used in solving the coupled singular nonlinear equations (2.15) is described. The transcendental functions  $J_m(x)$  in these expressions are defined by

$$J_m(x) \equiv \frac{1}{\sqrt{\pi}} \int_0^\infty dt \ t^m e^{-t^2} e^{-x/t} \ , \tag{A1}$$

with the properties

$$J_{m}(0) = \begin{cases} \Gamma[(1+m)/2]/2\sqrt{\pi}, & m \ge 0\\ \infty, & m \le -1 \end{cases}$$

$$J_{m}(x \to \infty) = 0,$$

$$\frac{d}{dx}J_{m}(x) = -J_{m-1}(x),$$

$$2J_{m}(x) = (m-1)J_{m-2}(x) + xJ_{m-3}(x),$$

$$x\frac{d^{3}}{dx^{3}}J_{m}(x) - (m-1)\frac{d^{2}}{dx^{2}}J_{m}(x) + 2J_{m}(x) = 0.$$
(A2)

Although Eqs. (2.15) are nonlinear, it is useful to write them in the quasilinear form

$$\psi_{\alpha}(s) = \phi_{\alpha}(s) + \int_{0}^{\infty} dt \ K_{\alpha\beta}(s,t) \psi_{\beta}(t) , \qquad (A3)$$

where  $\psi_{\alpha}(s)$  denotes the hydrodynamic variables,  $\phi_{\alpha}(s)$  the boundary contribution associated with  $f_b$ , and the kernels K(s,t) are defined in terms of the functions  $J_m$ . These kernels have an x dependence that arises through the temperature T(x), which is the source of nonlinearity. Also, they are singular in the limit of small |s-t|. To further simplify the notation (A3) is written in the abstract form

$$\psi = \phi + \hat{K}\psi . \tag{A4}$$

Three methods of solution were considered. The simplest is that of direct iteration of (A4), leading to the approximation

$$\psi^{(N)} \sim \sum_{n=0}^{N} (\hat{K}^{(n)})^n \phi$$
, (A5)

where  $\hat{K}^{(n)}$  is the kernel  $\hat{K}$  evaluated using the temperature obtained from the N=n-1 approximation. As indicated by previous studies, this method is quite effective for Knudsen numbers greater than 1, but has very poor convergence at smaller Knudsen numbers. The second method is a modification of Nystrom's method. A suitable quadrature rule is introduced to write (A3) approximately as

$$\psi_{\alpha}(s_i) = \phi_{\alpha}(s_i) + \sum_{j=1}^{M} w_j K_{\alpha\beta}(s_i, s_j) \psi_{\beta}(s_j)$$
, (A6)

where M is the number of quadrature points and  $w_i$  are the weight factors according to the quadrature rule. Equation (A6) is now a nonlinear matrix equation of the form

$$A_{ij}\psi_j = \phi_i , \qquad (A7)$$

where the index i now denotes both the hydrodynamic variable and the quadrature point. The matrix A depends on the temperature, so the solution to (A7) is still obtained by iteration, but now at each iteration (A7) is solved exactly by matrix inversion. This leads to an approximation

$$\psi_i^{(n)} \sim [A^{(n)}]_{ii}^{-1} \phi_i , \qquad (A8)$$

where  $A^{(n)}$  is the matrix A evaluated with the temperature obtained in the n-1 approximation. This method requires that the number of mesh points M be large enough to approximate well both the hydrodynamic variables and the kernel K(s,t). The former are smooth functions and cause no difficulty, but the singular domain of the kernels requires that M be very large. Consequently, the time and errors involved in the matrix inversion with large M limit this method severely.

In order to treat the singular domain properly, the integral in (A3) is first divided into M intervals as follows:

$$\psi_{\alpha}(s_i) = \phi_{\alpha}(s_i) + \sum_{j=1}^{M} \int_{t_j}^{t_{j+1}} dt \ K_{\alpha\beta}(s_i, t) \psi_{\beta}(t) \ .$$
 (A9)

Now, the number of points M is chosen to be large enough only to represent the smooth functions  $\psi_{\alpha}(t)$ . The latter are then approximately constant over each interval so (A9) becomes

$$\psi_{\alpha}(s_i) = \phi_{\alpha}(s_i) + \sum_{j=1}^{M} \int_{t_j}^{t_{j+1}} dt \ K_{\alpha\beta}(s_i, t) \psi_{\beta}(s_j) \ ,$$
 (A10)

where  $s_i \equiv (t_i + t_{i+1})/2$ . The remaining integrations can be performed using the third property of (A2), so the singularity of  $K_{\alpha\beta}(s,t)$  is now treated exactly. The resulting equations have the form of (A7) and are solved in the same way. The difference now is that M can be chosen small; in practice M=40 was used. The relative difference between input and output after 20 iterations was always less than  $10^{-4}$ . Internal consistency of the equations themselves was monitored by verifying that  $U_x(s) \sim 0$  and  $q(s) \sim \text{const.}$  For all data reported here the heat flux is constant to less than 1% and  $U_x(s)/v_0 < 10^{-2}$ . However, the method eventually fails (for constant M) at sufficiently small Knudsen number. For example, at  $\lambda = 0.01$  we were unable to obtain a heat flux with variation less than about 20%. The reason is that  $K_{\alpha\beta}(s,t)$  approaches a  $\delta$  function in s-t as  $\lambda \rightarrow 0$ , and almost any trial function is an approximate solution in this limit. Very small Knudsen numbers would require an increase in M. This method of solution, Eq. (A10), is an adaptation of one proposed by Cercignani<sup>16</sup> for the linearized equations.

The precise forms for Eq. (A10) are

$$n(s_{i}) = n_{+}J_{0}\left[\frac{1-s_{i}}{\lambda}\right] + J_{0}\left[\frac{s_{i}}{\lambda\sqrt{T_{-}}}\right] + \sum_{j=1}^{M}\left[\frac{1}{\lambda\sqrt{T(s_{j})}}\int_{t_{j}}^{t_{j+1}}dt J_{-1}\left[\frac{|s_{i}-t|}{\lambda\sqrt{T(s_{j})}}\right]\right]n(s_{j}),$$

$$\frac{3}{2}p(s_{i}) = n_{+}\left[J_{0}\left[\frac{1-s_{i}}{\lambda}\right] + J_{2}\left[\frac{1-s_{i}}{\lambda}\right]\right] + T_{-}\left[J_{0}\left[\frac{s_{i}}{\lambda\sqrt{T_{-}}}\right] + J_{2}\left[\frac{s_{i}}{\lambda\sqrt{T_{-}}}\right]\right]$$

$$+ \sum_{j=1}^{M}\left[\frac{1}{\lambda\sqrt{T(s_{j})}}\int_{t_{j}}^{t_{j+1}}dt \left[J_{-1}\left[\frac{|s_{i}-t|}{\lambda\sqrt{T(s_{j})}}\right] + J_{1}\left[\frac{|s_{i}-t|}{\lambda\sqrt{T(s_{j})}}\right]\right]\right]p(s_{j}), \tag{A11}$$

$$n(s_{i})U_{x}(s_{i}) = \sqrt{T_{-}}J_{1}\left[\frac{s_{i}}{\lambda\sqrt{T_{-}}}\right] - n_{+}J_{1}\left[\frac{1-s_{i}}{\lambda}\right] + \sum_{j=1}^{M}\left[\frac{1}{\lambda}\int_{t_{j}}^{t_{j+1}}dt \operatorname{sgn}(s_{i}-t)J_{0}\left[\frac{|s_{i}-t|}{\lambda\sqrt{T(s_{j})}}\right]\right]n(s_{j}).$$

As noted above the integrals in Eqs. (A11) can be performed exactly using the third of Eqs. (A2). To start the iteration, trial temperature and density profiles are put into the last of Eqs. (A11) to determine the unknown parameter  $n_+$ . Then the density and the pressure are calculated from the first and second of Eqs. (A11). These steps are repeated until the relative difference between each step is less than  $10^{-8}$  for all variables.

The heat flux is calculated from these hydrodynamic variables, using a discretized form of Eq. (2.17).

## APPENDIX B: SPECIAL SOLUTION

The special exact solution to the BGK equation obtained in Ref. 3 can be obtained as the limit of diffuse boundary conditions applied to an unbounded system. In this appendix that solution is rederived for a finite system, but with different boundary conditions, for comparison with the results of Sec. II.

The general solution to the boundary-value problem has the form of Eq. (2.11),

$$f(s,\mathbf{v}) = f_b(s,\mathbf{v}) + f_p(s,\mathbf{v}) , \qquad (B1)$$

where  $f_b(s, \mathbf{v})$  and  $f_p(s, \mathbf{v})$  are given by Eqs. (2.12) and (2.13). If the positive and negative velocity distributions are distinguished by a superscript + or -, respectively, then the boundary and particular distributions are explicitly

$$f_{b}(s,\mathbf{v}) = f^{+}(s=0,\mathbf{v}) \exp(-s/\lambda v_{x})$$

$$+ f^{-}(s=1,\mathbf{v}) \exp[(1-s)/\lambda v_{x}], \qquad (B2)$$

$$f_{p}(s,\mathbf{v}) = (\lambda v_{x})^{-1} \left[ \int_{0}^{s} dx \, f_{L}^{+}(x,\mathbf{v}) \exp[(x-s)/\lambda v_{x}] \right]$$

$$- \int_{s}^{1} dx \, f_{L}^{-}(x,\mathbf{v}) \exp[(x-s)/\lambda v_{x}] . \qquad (B3)$$

To isolate the solution of Ref. 3, the limits of the integration in the expression for  $f_p$  are extended to the range  $-a \le s \le b$  with a and b positive, and  $b \ge 1$ . The compensation for this additional contribution is grouped with the boundary term to rewrite Eq. (B1) as

$$f(s,\mathbf{v}) = f_b'(s,\mathbf{v}) + f_s(s,\mathbf{v}), \qquad (B4)$$

where  $f'_{h}$  and  $f_{s}$  are given by

$$f_b'(s, \mathbf{v}) = \left[ \left[ f^+(s = 0, \mathbf{v}) - (\lambda v_x)^{-1} \int_{-a}^0 dx \, f_L^+(x, \mathbf{v}) \exp(x / \lambda v_x) \right] + \left[ f^-(s = 1, \mathbf{v}) \exp(1 / \lambda v_x) + (\lambda v_x)^{-1} \int_1^b dx \, f_L^-(x, \mathbf{v}) \exp(x / \lambda v_x) \right] \exp(-s / \lambda v_x) ,$$
(B5)

$$f_{s}(s,\mathbf{v}) = (\lambda v_{x})^{-1} \left[ \int_{-a}^{s} dx \, f_{L}^{+}(x,\mathbf{v}) \exp[(x-s)/\lambda v_{x}] - \int_{s}^{b} dx \, f_{L}^{-}(x,\mathbf{v}) \exp[(x-s)/\lambda v_{x}] \right]. \tag{B6}$$

Comparison of (B6) and (B3) shows that  $f_s(s, \mathbf{v})$  is the particular solution for the extended domain, as illustrated in Fig. 1. Also indicated in the figure is a hypothetical linear temperature profile that vanishes at s = -a,

$$T_0(s) = T(s_0)(s+a)/(s_0+a)$$
, (B7)

where  $s_0$  is an arbitrary reference point.

The special solution of Ref. 3 refers to an infinite system, so  $b = \infty$  is chosen in the above expressions. Next, to justify  $T_0(s)$  as the true temperature profile, i.e., that given by (2.3), the contribution from  $f_b$  must vanish. This requires imposing the boundary conditions

$$f^{+}(s=0, \mathbf{v}) = (\lambda v_{x})^{-1} \int_{-a}^{0} dx \, f_{L}^{+}(x, \mathbf{v}) \exp(x / \lambda v_{x}) ,$$

$$f^{-}(s=1, \mathbf{v}) = -(\lambda v_{x})^{-1} \int_{1}^{\infty} dx \, f_{L}^{-}(x, \mathbf{v})$$

$$\times \exp[(x-1) / \lambda v_{x}] .$$
(B8)

These are not physical boundary conditions, but they have a simple interpretation. The distribution of velocities off the wall at s=0 is that produced by the particular solution for the domain  $-a \le s \le 0$ . Similarly, the distribution off the wall at s=1 is that produced by the particular solution for the domain  $1 \le s$ . These two particular solutions act as perfect reservoirs to produce an exactly linear temperature gradient in the physical domain  $0 \le s \le 1$ .

The form (3.6) for the special solution is obtained by expressing the parameters a and  $\lambda$  in terms of  $\epsilon^*$ , using Eqs. (B8) and (3.2), and introducing the scaled velocity  $\xi = \mathbf{v}/\sqrt{T(s)}$ . Although this result is the solution to a different boundary-value problem than that given in the text, it is clear from Fig. 1 that the point  $s_0$  in Eq. (B7) can be chosen to make the temperature and its gradient agree for the two solutions. If a normal solution is appropriate at this point, the specific boundary conditions should not matter and the two solutions are expected to agree.

<sup>&</sup>lt;sup>1</sup>H. Grad, Phys. Fluids **6**, 147 (1963).

<sup>&</sup>lt;sup>2</sup>See, for example, J. R. Dorfman and H. van Beijeren, in *Statistical Mechanics, Part B: Time Dependent Processes*, edited by B. Berne (Plenum, New York, 1977).

<sup>&</sup>lt;sup>3</sup>A. Santos, J. J. Brey, C. S. Kim, and J. W. Dufty, preceding paper, Phys. Rev. A 39, 320 (1988).

<sup>&</sup>lt;sup>4</sup>A. Santos, J. J. Brey, and J. W. Dufty, Phys. Rev. Lett. **56**, 1571 (1986).

<sup>&</sup>lt;sup>5</sup>J. J. Brey, A. Santos, and J. W. Dufty, Phys. Rev. A **36**, 2842 (1987).

<sup>&</sup>lt;sup>6</sup>P. Bhatnagar, E. Gross, and M. Krook, Phys. Rev. **94**, 511 (1954).

<sup>&</sup>lt;sup>7</sup>A. Lees and S. Edwards, J. Phys. C 5, 128 (1972); for a review of recent applications and modifications see the articles by J. J. Erpenbeck, D. J. Evans, and W. G. Hoover, in *Nonlinear Fluid Behavior*, edited by H. Hanley (North-Holland, Amsterdam, 1983).

<sup>&</sup>lt;sup>8</sup>C. Trozzi and G. Ciccotti, Phys. Rev. A 29, 916 (1984); A. Tennenbaum, G. Ciccotti, and R. Gallico, *ibid.* 25, 2778 (1982);

M. Mareschal and E. Kestemont, ibid. 30, 1158 (1984).

<sup>&</sup>lt;sup>9</sup>C. Truesdell, J. Ration. Mech. Anal. 5, 55 (1956).

<sup>&</sup>lt;sup>10</sup>E. Asmolov, N. Makarev, and V. Nosik, Dokl. Akad. Nauk. SSSR **249**, 577 (1979) [Sov. Phys.—Dokl. **24**, 892 (1979)]; A. Santos, J. J. Brey, and J. W. Dufty (unpublished).

<sup>&</sup>lt;sup>11</sup>J. W. Dufty, A. Santos, J. J. Brey, and R. F. Rodriguez, Phys. Rev. A 33, 459 (1986).

<sup>&</sup>lt;sup>12</sup>R. Zwanzig, J. Chem. Phys. **71**, 4416 (1979).

<sup>&</sup>lt;sup>13</sup>A. Santos, J. J. Brey, and V. Garzo, Phys. Rev. A 34, 5047 (1986).

<sup>&</sup>lt;sup>14</sup>D. Willis, in *Rarefied Gas Dynamics*, edited by J. Laurman (Academic, New York, 1963), Vol. 1, p. 209; D. Anderson, J. Fluid Dyn. 25, 271 (1966); C. Cercignani and G. Tironi, in *Rarefied Gas Dynamics*, edited by C. Brundin (Academic, New York, 1967), Vol. 1, p. 441.

<sup>&</sup>lt;sup>15</sup>C. Cercignani, Theory and Application of the Boltzmann Equation (Elsevier, New York, 1975).

<sup>&</sup>lt;sup>16</sup>C. Cercignani and A. Daneri, J. Appl. Phys. 34, 3509 (1963).