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Numerical solutions of the Krook kinetic equation

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Because of the relative simplicity of the statistical model for molecular interactions, numerically exact solutions of the Krook kinetic equation can be obtained. Comparison of exact and approximate solutions of the model equation allows the evaluation of approximate procedures for solving the Boltzmann equation. Exact and approximate numerical solutions have been obtained for Couette flow with heat transfer and the structure of a plane shock wave. The present paper summarizes the work of the author in obtaining the numerically exact solutions.

1. Introduction

Krook (1955, 1959) has pointed out that the relative simplicity of the statistical model for molecular interactions allows numerically exact solutions of the Krook kinetic equation to be obtained. An opportunity is thereby provided for evaluating various approximate procedures for solving the Boltzmann equation by comparing exact and approximate solutions of the model equation. Exact and approximate numerical solutions have been obtained for two steady, one-dimensional problems: Couette flow with heat transfer and the structure of a plane shock wave. The present paper summarizes the work of the author (Anderson 1963) in obtaining the numerically exact solutions. Comparisons with the approximate results of Macomber are to be found in Anderson & Macomber (1965) and Macomber (1965).

In §2, we derive the equations defining the Couette-flow problem. In §3, we consider the numerical methods employed to solve these equations, and, in §4, we consider the general character of the solutions. In §§5–7, the shock structure problem is treated in parallel fashion.

2. Couette-flow equations

Consider a monatomic gas ɔh no internal degrees of freedom confined between two parallel plates $x_1 = 0$ and $x_1 = l$. The plate $x_1 = 0$ is at rest and is maintained at a constant temperature T_0; the plate $x_1 = l$ is translating in its plane with constant velocity $W\hat{x}_2$ and is maintained at a constant temperature T_1. The problem is steady and one-dimensional in the sense that the velocity distribution function $f(\mathbf{v}; x_1)$ describing the state of the system depends only on x_1.

In order to specify the interaction of molecules with the boundaries, we assume that molecules which strike a plate are subsequently emitted with a Maxwellian

velocity distribution characterized by the plate temperature and velocity. Since the boundary conditions involve only the emitted particles, it is convenient to define half-range distribution functions by

$$\left.\begin{aligned} f_+(\mathbf{v};\, x_1) &= f(\mathbf{v};\, x_1) \quad \text{for} \quad v_1 > 0, \\ \text{and} \qquad f_-(\mathbf{v};\, x_1) &= f(\mathbf{v};\, x_1) \quad \text{for} \quad v_1 < 0. \end{aligned}\right\} \tag{1}$$

The boundary conditions can then be written

$$\left.\begin{aligned} f_+(\mathbf{v};\, 0) &= n_0\,\Phi(\mathbf{v};\, T_0), \\ \text{and} \qquad f_-(\mathbf{v};\, l) &= n_1\,\Phi(\mathbf{v} - W\hat{x}_2;\, T_1), \end{aligned}\right\} \tag{2}$$

where

$$\Phi(\mathbf{v};\, T) = (m/2\pi kT)^{\frac{3}{2}} \exp\left(-m\mathbf{v}^2/2kT\right). \tag{3}$$

m is the molecular mass and k is Boltzmann's constant. The parameters n_0 and n_1 are not known *a priori*; they are determined by some characteristic number density of the gas and the condition that there be no net mass flux normal to the plates.

The Krook kinetic equation describing the system reduces to

$$v_1\,\partial f/\partial x_1 = \nu[-f + n\Phi(\mathbf{v} - q\hat{x}_2, T)]; \tag{4}$$

n, q, and T are the local number density, flow velocity, and kinetic temperature, respectively. The collision frequency $\nu(x_1)$ is a function of the law of force between molecules but can be removed from the equation by a co-ordinate transformation. In this sense, the solutions obtained are universal. Define a characteristic velocity u_0 and a global Knudsen number λ by

$$u_0 = \sqrt{(kT_0/m)} \tag{5}$$

and

$$\lambda^{-1} = u_0^{-1} \int_0^l \nu(t)\, dt. \tag{6}$$

A universal co-ordinate τ is then defined as

$$\tau = \frac{\lambda}{u_0} \int_0^x \nu(t)\, dt. \tag{7}$$

We complete the definition of dimensionless variables as follows:

$$\left.\begin{aligned} &\mathbf{u} = \mathbf{v}/u_0, \quad \gamma = q/u_0, \quad \Gamma = W/u_0; \\ &\alpha = n/n_0, \quad \omega = n_1/n_0; \\ &\beta^2 = T/T_0, \quad \beta_1^2 = T_1/T_0; \\ \text{and} \qquad &F(\mathbf{u};\, \tau) = (u_0^3/n_0) f(\mathbf{v};\, x_1), \\ &\phi(\mathbf{u};\, \beta^2) = (2\pi\beta^2)^{-\frac{3}{2}} \exp\left(-\mathbf{u}^2/2\beta^2\right). \end{aligned}\right\} \tag{8}$$

The usual definitions of the low-order moments become

$$\alpha = \int F\, d\mathbf{u}, \quad \alpha\gamma = \int u_2 F\, d\mathbf{u} \quad \text{and} \quad 3\alpha\beta^2 = \int (\mathbf{u} - \gamma\hat{x}_2)^2 F\, d\mathbf{u}. \tag{9}$$

The kinetic equation becomes

$$\lambda u_1\, \partial F/\partial\tau + F = \alpha\phi(\mathbf{u} - \gamma\hat{x}_2;\, \beta^2), \tag{10}$$

with boundary conditions

$$\left.\begin{aligned} F_+(\mathbf{u};0) &= \phi(\mathbf{u};\,1) \\ \text{and} \qquad F_-(\mathbf{u};\,1) &= \omega\phi(\mathbf{u}-\Gamma\hat{x}_2;\,\beta_1^2). \end{aligned}\right\} \tag{11}$$

Formally integrating (10) and applying (11), we obtain

$$\left.\begin{aligned} F_+(\mathbf{u};\,\tau) &= \phi(\mathbf{u};\,1)\exp\left[-\tau/\lambda u_1\right]+\frac{1}{\lambda u_1}\int_0^\tau dt\,\alpha\phi\exp\left[-(\tau-t)/\lambda u_1\right] \\ \text{and} \quad F_-(\mathbf{u};\,\tau) &= \omega\phi(\mathbf{u}-\Gamma\hat{x}_2;\,\beta_1^2)\exp\left[-(1-\tau)/\lambda|u_1|\right] \\ &\quad +\frac{1}{\lambda|u_1|}\int_\tau^1 dt\,\alpha\phi\exp\left[-(t-\tau)/\lambda|u_1|\right]. \end{aligned}\right\} \tag{12}$$

With the statistical model, the distribution function is characterized completely by its low-order moments. When α, β^2, γ, and ω are known, higher moments, such as the stress tensor and heat-flux vector, can be evaluated by quadrature.

Define

$$G_n(q) = \frac{1}{\sqrt{(2\pi)}}\int_0^\infty dt\,t^{n-2}\exp\left[-\tfrac{1}{2}t^2-q/t\right]. \tag{13}$$

Substituting (12) in (9) yields the following set of singular, non-linear integral equations:

$$\alpha(\tau) = G_2\left(\frac{\tau}{\lambda}\right)+\omega G_2\left(\frac{1-\tau}{\lambda\beta_1}\right)+\frac{1}{\lambda}\int_0^1 dt\,\frac{\alpha}{\beta}G_1\left(\frac{|\tau-t|}{\lambda\beta}\right), \tag{14}$$

$$\alpha\gamma = \omega\Gamma G_2\left(\frac{1-\tau}{\lambda\beta_1}\right)+\frac{1}{\lambda}\int_0^1 dt\,\frac{\alpha\gamma}{\beta}G_1\left(\frac{|\tau-t|}{\lambda\beta}\right), \tag{15}$$

$$\begin{aligned} \text{and} \quad 3\alpha\beta^2+\alpha\gamma^2 &= 3G_2\left(\frac{\tau}{\lambda}\right)+\left(\frac{\tau}{\lambda}\right)G_1\left(\frac{\tau}{\lambda}\right)+3\omega\beta_1^2G_2\left(\frac{1-\tau}{\lambda\beta_1}\right)+\omega\Gamma^2G_2\left(\frac{1-\tau}{\lambda\beta_1}\right) \\ &\quad +\omega\beta_1^2\left(\frac{1-\tau}{\lambda\beta_1}\right)G_1\left(\frac{1-\tau}{\lambda\beta_1}\right)+\frac{1}{\lambda}\int_0^1 dt\,\alpha\beta\left[G_3\left(\frac{|\tau-t|}{\lambda\beta}\right)\right. \\ &\quad \left.+2G_1\left(\frac{|\tau-t|}{\lambda\beta}\right)\right]+\frac{1}{\lambda}\int_0^1 dt\,\frac{\alpha\gamma^2}{\beta}G_1\left(\frac{|\tau-t|}{\lambda\beta}\right). \end{aligned} \tag{16}$$

These equations define α, β^2, and γ; simultaneously, the parameter ω is determined by the condition that the conserved mass flux normal to the plates be zero. This condition yields

$$0 = G_3\left(\frac{\tau}{\lambda}\right)-\omega\beta_1G_3\left(\frac{1-\tau}{\lambda\beta_1}\right)+\frac{1}{\lambda}\int_0^1 dt\,\mathrm{sgn}\,(\tau-t)\,\alpha G_2\left(\frac{|\tau-t|}{\lambda\beta}\right), \tag{17}$$

where $\mathrm{sgn}\,(x) = x/|x|$. The kernel function $G_n(q)$ is the subject of a separate publication (Anderson & Macomber 1964).

The problem so formulated is characterized by three dimensionless parameters: the Knudsen number λ, the temperature ratio β_1^2, and the velocity ratio Γ. Since we propose to compare exact and approximate solutions in order to assess the efficacy of the latter, this self-contained, universal formulation is very convenient. If it is desired *a posteriori* to obtain results in physical co-ordinates, it is necessary to re-dimensionalize. This presents no difficulty for β^2 and γ, since

T_0 and W are well defined. However, n_0 must be determined in such a way as to be consistent with the given values of λ and l. The collision frequency ν can be related to the transport properties of the gas by applying the Chapman–Enskog procedure to the Krook kinetic equation. Usually, ν is chosen as a function of α and β^2 so as to model the viscosity of a given gas. Conversion from τ to x_1 then reduces to a simple quadrature. Finally, n_0 can be chosen so as to be consistent with the model for ν and the given values of λ and l.

3. Numerical solution of the Couette-flow equations

The analytic problem formulated in §2 involves the solution of three coupled, singular, non-linear integral equations for α, β^2, and γ; and the simultaneous determination of ω from a fourth such equation. To approach the problem numerically, we first replace the analytic equations by discrete analogues. This yields a finite set of non-linear transcendental equations which are then solved iteratively.

We replace the integral operators by Gaussian quadrature formulae. The kernel function $G_n(q)$ behaves logarithmically near $q = 0$. This is an important feature of the analytic problem and was retained in the discrete analogue by developing special Gaussian quadrature formulae adapted to the logarithmic singularity (Anderson 1965*a*). The necessity of orienting the quadrature sample points relative to the singularity, and hence making them τ-dependent, dictates a continuous rather than a discrete representation of the dependent variables. $\alpha\beta^2$, β^2 and γ were therefore represented as finite expansions in Chebyshev polynomials (Lanczos 1952). To determine the expansion coefficients, the discretized equations were enforced at a set of interpolation sample points. When these sample points are chosen as the roots or extrema of a Chebyshev polynomial of appropriate degree, there is a duality between the values of the function at the sample points and the expansion coefficients, through the well-known discrete orthogonality conditions. Furthermore, the distribution of these interpolation sample points—clustered somewhat near the boundaries—is appropriate for a problem in which we anticipate Knudsen layers. For reasons of computational efficiency, it is necessary to optimize the discretization by minimizing the required number of quadrature and interpolation sample points. The discretization described above is 'near-optimum'.

The solutions of the discrete problem are sets of expansion coefficients or, dually, sets of sample values. Rather than reformulating the equations explicitly in terms of one of these sets of unknowns, it is convenient to retain the equations as they arise naturally from the discretization of the analytic problem and to retain the dual sets of unknowns. The discrete equations are then solved iteratively. The straightforward successive substitution iteration suggested by the form of the equations proves to be adequate for large λ. However, the successive substitution iteration becomes ill-conditioned and slowly convergent for $\lambda \lesssim 1$ —as observed by Willis (1962, 1963) in the linearized problem. This behaviour is due to the fact that the equations tend to become identities as $\lambda \to 0$; that is, the kernel functions become almost reproducing. For very small λ, it is necessary to remove this 'identity' by a preliminary integration by parts, at the expense,

however, of introducing additional dependent variables. For the range of transition Knudsen numbers considered here ($\lambda = 10$ to $\frac{1}{10}$), such a reformulation of the problem did not prove to be necessary. After considerable experimentation, suitable iterative procedures, which are reported elsewhere (Anderson 1965*b*), were developed.

Experiments suggest that the solutions obtained have four significant figures. As usual, most of these experiments are of the nature of internal self-consistency checks on the numerical procedure. However, an additional check on the results is available. *A posteriori*, the stress tensor and heat-flux vector components were calculated. Among these components are three conserved quantities which are not used explicitly in the calculation. The degree to which these conserved quantities, as well as the conserved normal mass flux defining ω, are constant may attest to the validity of the results.

4. Solutions of the Couette-flow equations

Solutions have been obtained for the following values of the characteristic parameters:

$$\lambda = 10, 4, 2, 1, \tfrac{1}{2}, \tfrac{1}{4}, \tfrac{1}{6}, \tfrac{1}{8}, \tfrac{1}{10};$$

$$\beta_1^2 = 1, \tfrac{7}{10}, \tfrac{4}{10}, \tfrac{1}{10}$$

and

$$\Gamma = 0, \tfrac{4}{10}, 1, 5.$$

A selected set of solutions is presented graphically in the Appendix.

The general character of the solutions is much as one would expect, though somewhat smoother than anticipated. By and large, the graphs will be allowed to speak for themselves. My remarks will be confined to a few observations on the graphs and a few comments on some subsidiary calculations.

One interesting observation is the linear dependence of the γ profiles on Γ: In figure 1 (see the Appendix) the curves for $\Gamma = \frac{4}{10}$ and 1 are seen to be identical to graphical accuracy. This is somewhat surprising since the pressure and temperature, and hence density, show pronounced frictional effects, proportional to Γ^2, which might be expected to affect the velocity. The linear dependence of γ on Γ is probably due to the use of the reduced co-ordinate τ; in physical co-ordinates, this linear dependence would be destroyed by the dependence of ν on α and β^2.

Two limiting effects are evident in the graphs: For large λ (near-free-molecular flow), the velocity profiles for varying β_1^2 are of essentially the same shape, differing only in the slip at the plates. In this limit of strong global coupling, the solutions are essentially superpositions of the wall conditions, and the dependence of ω on β_1^2 (and weakly on Γ) accounts for the change in the slip. As λ decreases, the coupling becomes more and more local and differential effects of local rather than global Knudsen number become apparent. Note, for example, the convergence of the profiles near $\tau = 0$ where the local mean free path, and hence the slip, is determined by λ, while it varies as $\lambda\beta_1$ near $\tau = 1$. The frictional effects also become more pronounced and non-uniform for small λ.

Non-linear, kinetic-theory phenomena are most evident in the pressure $\alpha\beta^2$, which in continuum theory is constant. While the reduced variable used

in plotting the pressure curves does exaggerate the effect somewhat, a global pressure gradient and local Knudsen layers appear whenever there are temperature and/or density gradients.

For selected cases, the non-zero components of the stress tensor and heat-flux vector were evaluated by quadrature. Attempts were made to correlate the results for different cases by defining viscosity, heat conductivity, and slip coefficients. These coefficients were found to be as variable as the original data, and no useful correlations were found. It seems reasonable to assume that such continuum concepts as transport and slip coefficients are simply inappropriate in the range of transition Knudsen numbers.

Further evidence of non-continuum effects is seen in the fact that the diagonal components of the stress tensor are far from equal in some cases. Furthermore, there is a significant heat-flux vector component parallel to the plates whose value—and even sign—is a strong function of λ, β_1^2, Γ and τ.

One criterion for 'non-linearity' in this problem is that the macroscopic variables change significantly on the scale of the mean free path. From continuum theory, one anticipates smooth, slowly varying interior solutions which are accommodated to the boundary conditions by rapidly varying Knudsen layers. The solutions obtained are in fact smooth and slowly varying everywhere, with simply slip at the boundaries. The problem seems not really to be of 'boundary layer' character. This may or may not be the case for more general collision models and boundary conditions. The 'non-linearity' of a given problem is a rather complicated function of the full set of characteristic parameters. The sets of parameters selected *a priori*, and shown above, may err in being too 'linear', but the computational procedure will handle a wider range of the β_1^2 and Γ parameters. It would be easy to extend the results to larger Knudsen numbers (from the transition to the free-molecular flow régime), but much smaller values of λ (tending toward the continuum régime) would require a new approach to the problem, for the reasons outlined above.

In and of themselves, the exact solutions of the Couette flow with heat transfer problem with the Krook equation are not particularly interesting. Their usefulness lies primarily in their role as standards for comparing and assessing various approximate procedures applied to the model problem. A set of solutions for some 72 cases is presented in condensed form in an appendix to Anderson (1965*c*).

5. Shock-wave equations

Consider a plane shock wave in a reference frame moving with the shock, choosing the x-axis normal to the shock. We take cylindrical co-ordinates in velocity space: u_n is the component of velocity normal to the shock; the transverse velocity u_t and the angle ζ form polar co-ordinates in the plane of the shock. We anticipate that the only non-zero component of the flow velocity is $q_n \equiv q$ and that the distribution function $f(u_n, u_t; x)$ is independent of ζ.

For this steady, one-dimensional problem, the Krook kinetic equation reads

$$u_n \partial f/\partial x = \nu[-f + n\Phi(\mathbf{u} - q\hat{\mathbf{x}}; T)]. \tag{18}$$

Far upstream ($x \to -\infty$) and downstream ($x \to +\infty$), the gas relaxes to thermodynamic equilibrium states (n_1, q_1, T_1) and (n_2, q_2, T_2) respectively, with the corresponding Maxwellian distribution functions. We define a reduced independent variable τ (to remove the collision frequency ν from the equation), dimensionless dependent variables α, β^2, and γ, and corresponding distribution functions by

$$u_2 = \sqrt{(kT_2/m)}, \tag{19}$$

$$\left.\begin{aligned} \tau &= u_2^{-1}\int_0^x \nu(t)\,dt, \\ \alpha &= n/n_2, \quad \beta^2 = T/T_2, \quad \gamma = q/u_2, \\ F(v,w;\tau) &= (u_2^3/n_2) f(u_n, u_t; x), \\ \text{and} \quad \phi(v,w;\gamma,\beta^2) &= (2\pi\beta^2)^{-\frac{3}{2}} \exp\{-[(v-\gamma)^2+w^2]/2\beta^2\}, \\ \text{where} \quad v &= u_n/u_2 \quad \text{and} \quad w = u_t/u_2. \end{aligned}\right\} \tag{20}$$

There is no characteristic origin or scale of co-ordinates in this problem; thus, we cannot define a global Knudsen number. We simply anticipate that the interesting structure occurs 'near' $\tau = 0$.

The kinetic equation and boundary conditions now read

$$v\,\partial F/\partial\tau + F = \alpha\phi, \tag{21}$$

$$\left.\begin{aligned} F(v,w;\,-\infty) &= \alpha_1\phi(v,w;\,\gamma_1,\beta_1^2), \\ \text{and} \quad F(v,w;\,+\infty) &= \alpha_2\phi(v,w;\,\gamma_2,\beta_2^2). \end{aligned}\right\} \tag{22}$$

Defining half-range distribution functions by

$$\left.\begin{aligned} F_+ &= F \quad \text{for} \quad v > 0 \\ \text{and} \quad F_- &= F \quad \text{for} \quad v < 0, \end{aligned}\right\} \tag{23}$$

we formally integrate (21) to obtain

$$\left.\begin{aligned} F_+ &= \int_{-\infty}^{\tau} dt \frac{\alpha}{v}\phi e^{-(\tau-t)/v} \\ \text{and} \quad F_- &= \int_{\tau}^{\infty} dt \frac{\alpha}{|v|}\phi e^{-(t-\tau)/|v|}. \end{aligned}\right\} \tag{24}$$

The boundary conditions are implicit in these equations in the sense that the integrals reduce to the correct Maxwellian form when α, β^2, and γ take on constant values.

Since the full-range distribution function is known at the boundaries, certain conserved quantities can be evaluated explicitly; this yields the usual Rankine–Hugoniot relations between the upstream and downstream equilibrium states. In terms of a shock Mach number M, these relations yield

$$\alpha_1 = (M^2+3)/4M^2, \quad \beta_1^2 = 16M^2/(M^2+3)(5M^2-1), \tag{25}$$

$$\text{and} \quad \gamma_1 = \sqrt{\tfrac{5}{3}}\,\beta_1 M.$$

By definition, we have $\alpha_2 = \beta_2 = 1$. γ_2 can be obtained from the fact that $\alpha\gamma$ is a conserved quantity. Indeed, it is convenient to eliminate α in favour of γ through the conservation law

$$\alpha\gamma = \alpha_1\gamma_1. \tag{26}$$

There seems little point in retaining three dependent variables. The mode of convergence of any iterative process for solving the problem will depend on the number of unknowns, but the same solutions will result if the process is self-consistent.

We obtain singular, non-linear integral equations for β^2 and γ by substituting the formal integrals (24) in the definitions of the low-order moments:

$$\left.\begin{aligned} \alpha &= \int_{-\infty}^{\infty} dt \frac{\alpha}{\beta} H_1\left(\operatorname{sgn}(\tau-t)\frac{\gamma}{\beta}, \frac{|\tau-t|}{\beta}\right) \\ 3\alpha\beta^2+\alpha\gamma^2 &= \int_{-\infty}^{\infty} dt\, \alpha\beta\left[H_3\left(\operatorname{sgn}(\tau-t)\frac{\gamma}{\beta}, \frac{|\tau-t|}{\beta}\right)\right. \\ &\qquad \left. +2H_1\left(\operatorname{sgn}(\tau-t)\frac{\gamma}{\beta}, \frac{|\tau-t|}{\beta}\right)\right]. \end{aligned}\right\} \tag{27}$$

The kernel function

$$H_n(p,q) \equiv \frac{1}{\sqrt{(2\pi)}}\int_0^{\infty} du\, u^{n-2}\exp\{-\tfrac{1}{2}(u-p)^2-q/u\} \tag{28}$$

is the subject of a separate publication (Anderson & Macomber 1964).

The problem so formulated is characterized by a single dimensionless parameter—the Mach number M. Again, in the terms of reference of the present research, the self-contained, universal τ formulation is the most convenient. Results in physical co-ordinates can be obtained *a posteriori* by quadrature, once a model for the collision frequency is specified.

6. Numerical solution of the shock-wave equations

The numerical procedures employed in the shock-structure problem parallel those described above for the Couette-flow problem; thus, the discussion here can be abbreviated somewhat. In many ways the shock-wave problem is the easier of the two; there are only two functions to be determined and only a single characteristic dimensionless parameter, the Mach number. However, for reasons inherent in the problem, it is more difficult to obtain a satisfactory numerical solution.

The analytic problem is first replaced by a discrete analogue and then the resulting discrete problem is solved iteratively. The integral operators are replaced by Gaussian quadrature formulae oriented with respect to the singularity at $t = \tau$; again, the logarithmic singularity is retained by means of special quadrature formulae. The considerably more complicated structure of the kernel functions and the infinite interval of integration make a satisfactory, and yet efficient, discretization of the integral operators more difficult than in the Couette-flow problem. As a consequence of the increased number of quadrature sample points required and the fact that it is considerably more time consuming to evaluate H_n than G_n, one iteration in the shock problem requires ten to twenty times the computation time required for one iteration in the Couette-flow problem—of the order of half a minute on an IBM 7094. While there are fewer problems to run, since there is but a single free parameter, the program development was somewhat curtailed by economics.

To retain the 'near-optimum' Chebyshev interpolation, the interval

$$-\infty < \tau < \infty$$

was mapped into the interval $-1 < z < 1$ by the transformation pair

$$z = \tanh(\tau/\Delta) \quad \text{and} \quad \tau = \tfrac{1}{2}\Delta \ln[(1+z)/(1-z)]. \tag{29}$$

The Chebyshev collocation points in the z domain are mapped into a set of points clustered about the origin in the τ domain. This particular transformation was suggested by the classical weak shock solution of Taylor (Hayes 1960). The interpolation sample points at which the equations are enforced are chosen as the extrema of an appropriate Chebyshev polynomial, including the points $z = \pm 1$, so as to impose the known boundary conditions on all potential iterates. The dual sets of unknowns are retained, as before. The parameter Δ is chosen so that roughly 98 % of the variation of the profiles occurs in the interval $-3\Delta < \tau < 3\Delta$.

Because of the nature of the discretization, it is convenient to choose initial iterates as appropriately normalized hyperbolic tangent profiles. The iterative procedures described in Anderson (1965*b*) proceed satisfactorily at first but after 10–15 iterations—the equivalent of 30–50 successive substitution iterations —the process becomes stationary. That is, the iterates oscillate among a class of final states and convergence ceases. As a result, one can be confident of only two to three significant figures in the solutions. The obvious explanation of round-off error accumulation is easily ruled out; we shall discuss briefly one possible explanation of this behaviour.

The equations (27) are invariant under translation of the origin of co-ordinates and there are, therefore, a set of solutions which are isomorphic under translation. To obtain a well-set problem with a unique solution, one must divide the potential iterates (monotonic profiles taking on the correct boundary values) into equivalence classes based, for example, on the value of γ at the origin. The unique solution is defined to be a member of the canonical equivalence class characterized by γ taking on its median value at the origin.

At each stage, when a new iterate is determined from a set of collocation points oriented with respect to the *nominal origin* $\tau = 0$, one can determine an *effective origin* $\tau = \tau_0$ with respect to which the new iterate falls into the canonical equivalence class. If the iteration were carried out analytically, it is reasonable to assume that, if each iterate is mapped into the canonical equivalence class at each stage, a convergent iterative process can be obtained (cf. Altman 1955). In the analytic iteration, τ_0 would converge to zero, but in general this is not the case with the numerical iteration. While the analytic problem is translationally invariant, the numerical problem is not in the large, since only a finite number of collocation points are used. A *natural solution* of the discrete problem (with, in general, $\tau_0 \neq 0$) is induced by this lack of invariance of the discretization. It is possible—indeed probable—that this natural solution exists only in a 'least squares' sense. That is, the non-linear equations constituting the discrete problem may not have a real solution but only some profile which satisfies

the equations best in some sense. In non-linear numerical problems, this question of existence of a solution of the discrete equations is usually ignored as unanswerable. One depends on the analogy with the well-posed analytic problem to define a 'solution' satisfying the equations to a satisfactory degree. A rather unpleasant side-effect is the fact that the natural solution depends on the discretization. We must accept the τ_0 appropriate to the given discretization and seek the corresponding natural solution iteratively, without mapping the iterates into the canonical equivalence class at each stage.

Any consistent discrete analogue of the translationally invariant analytic problem is translationally invariant in the small, and there is a whole set of profiles, isomorphic under translation, which satisfy the equations equally well. In the neighbourhood of the natural solution, the iterates orbit in a class of profiles which the procedure is powerless to distinguish, and the iteration is asymptotically only neutrally stable.

Considerable experimentation with this and other simpler model problems has failed to yield a satisfactory resolution of this insidious kind of ill-conditioning. The degree of indeterminacy of the solution is extremely problem-dependent and, unfortunately, is relatively large ($\sim 5 \times 10^{-4}$) for the problems of interest. The results obtained are adequate for preliminary comparison with the corresponding approximation-procedure results; however, since some of these procedures seem to yield quite accurate results, the problem would bear further study if some new insight can be found.

The shock-structure problem with the Krook kinetic equation has also been studied by Liepmann, Narasimha, & Chahine (1962) and Chahine (1963*a*). They employed a rather more complicated numerical procedure in which the kernel function was evaluated by numerical quadrature and the universal τ co-ordinate was not used; a particular model for the collision frequency was chosen *a priori*. As a result, their computation time for one iteration was between one and two orders of magnitude longer than in my case. It is not surprising, therefore, that their original results were inaccurate, due to the all too common error of mistaking an ill-conditioned, slowly convergent, successive substitution iteration for a rapidly converging one. This is one of the most difficult problems in numerical work of this kind. In addition, their numerical treatment of the logarithmic singularity of the kernel was less than adequate. These defects have been remedied in the more recent work of Chahine & Narasimha (1965), by increased attention to the singular region and an increase of an order of magnitude in the number of iterations performed.

I have translated my results into physical co-ordinates using the collision-frequency–viscosity correlation employed by Chahine & Narasimha. To the limits of graphical comparison, no significant discrepancy between the results seems to remain. However, the temperature profiles seem to agree somewhat more satisfactorily than the density profiles. As pointed out in Chahine (1963*b*), the fact that the logarithmic singularity of the kernel is not retained has its predominant effect on the density profile, in particular on the downstream side of the shock.

No problem with the translational invariance of the equations is reported by

Chahine. As mentioned above, the effect of the invariance is very problem dependent. I feel that the fact that the τ variable was not used by Chahine means that the discrete problem so formulated is less invariant in the small, and the iterates—including the initial Navier–Stokes profile—are more tightly coupled. Consequently, the effect of the invariance is reduced, but not eliminated. The use of the τ variable, while it enhances the invariance problem, simplifies the numerical problem considerably and is the most suitable frame of reference for comparisons with the results of approximation procedures. In addition, I believe the role of the τ variable in distributing the discretization sample points optimally with respect to the natural local mean-free-path scaling of the problem to be quite significant.

Because of the invariance problem, one cannot say definitely which set of results is closer to the true solution. However, the satisfactory agreement of profiles obtained by quite different numerical procedures and the rather spectacular agreement of certain of the approximation-procedure curves with the present results indicate that the problem has been solved adequately for all practical purposes.

7. Solutions of the shock-wave equations

With the reservations noted above, results have been obtained for $M = 1{\cdot}2$, $1{\cdot}5$, $2{\cdot}0$, $3{\cdot}0$, $5{\cdot}0$, and $10{\cdot}0$. A selected set of these results is presented graphically in the Appendix; the profiles which have been suppressed are quite similar. For comparison, curves in the τ and the x domains are given.

The distortion involved in the translation from the universal τ-co-ordinate to the physical x-co-ordinate is much more significant in the shock-wave problem than in the Couette-flow problem. Through the shock, there are large gradients of the macroscopic dependent variables and hence a strong variation of the collision frequency ν. In the τ domain, the solutions are considerably smoother and more symmetrical than in the x domain. Other characteristic velocities than that defined in (19) could have been used to define τ. The results suggest that, in this particular τ-co-ordinate system, the profiles tend to limiting profiles as $M \to \infty$. The profiles for $M = 5{\cdot}0$ and $10{\cdot}0$ are essentially identical.

A more complete selection of shock profiles is presented in condensed form in an appendix to Anderson (1965*c*).

8. Conclusion

Numerically exact solutions of the Krook kinetic equation have been obtained for two steady, one-dimensional problems: Couette flow with heat transfer and the structure of a plane shock wave. These have served (Anderson & Macomber 1965, and Macomber 1965), and will serve, as standards for comparing and evaluating approximation procedures applied to these model problems. Such comparisons may supply some modicum of justification for the application of such approximation procedures in more complicated problems whose exact solution is not feasible.

The numerically exact solutions do not in themselves yield any particularly unexpected results. They may prove useful in attempting to assess the efficacy

of the statistical model as a physical rather than a mathematical tool. For example, it would be interesting to see if a self-consistent empirical specification of the collision frequency ν is possible. However, perhaps the most useful by-product of the research is the experience gained in solving such problems numerically.

The author would like to acknowledge the contributions of Professor Max Krook and Dr H. K. Macomber through many helpful discussions. This work was supported by the Smithsonian Astrophysical Observatory and the National Science Foundation.

Appendix

The Couette-flow problem is characterized by three dimensionless parameters: the Knudsen number λ, the plate temperature ratio β_1^2 and the plate velocity Γ. For this problem, we define the following reduced dependent variables:

$$\left.\begin{aligned} \bar{\alpha} &= (\alpha-1)/(\omega-1), \quad \bar{\beta}^2 = (1-\beta^2)/(1-\beta_1^2), \\ \alpha\beta^2 &= [\alpha\beta^2 - \tfrac{1}{2}(1+\beta_1)]/[1-\tfrac{1}{2}(1+\beta_1)], \\ \bar{\gamma} &= \gamma/\Gamma \\ \text{and} \qquad \bar{\omega} &= (\omega-\beta_1^{-1})/(\beta_1^{-2}-\beta_1^{-1}). \end{aligned}\right\} \tag{A 1}$$

A selected set of curves of these dependent variables plotted versus τ for various values of the characteristic parameters follows (figures 1–8). In each figure, there are a number of curves labelled a, b, ... In the figure legend, the set of characteristic parameters involved is specified by a triplet of numbers: $(\lambda, \beta_1^2, \Gamma)$.

The shock-wave problem is characterized by a single dimensionless parameter: the Mach number M. For this problem, we define the following reduced dependent variables:

$$\left.\begin{aligned} \bar{\alpha} &= (\alpha-\alpha_1)/(1-\alpha_1), \\ \bar{\beta}^2 &= (\beta^2-\beta_1^2)/(1-\beta_1^2), \\ \text{and} \qquad \bar{\gamma} &= (\gamma-\gamma_2)/(\gamma_1-\gamma_2). \end{aligned}\right\} \tag{A 2}$$

Two sets of shock profiles are given: first, profiles versus τ/Δ using the nominal origin and, second, profiles versus $\pi x/4\Lambda$ using the effective origin. We define a characteristic upstream mean free path Λ by

$$\Lambda = \sqrt{(\tfrac{1}{2})}\pi\mu_1/n_1\sqrt{(mkT_1)}. \tag{A 3}$$

The viscosity μ, related to the collision frequency ν by

$$\mu\nu = nkT, \tag{A 4}$$

is assumed to have a temperature dependence given by

$$\mu/\mu_1 = (T/T_1)^s. \tag{A 5}$$

This yields

$$x/\Lambda = \sqrt{\frac{2}{\pi}}\alpha_1\beta_1^{1-2s}\int_{\tau_0}^{\tau} d\tau\, \beta^{2s}/\alpha\beta^2. \tag{A 6}$$

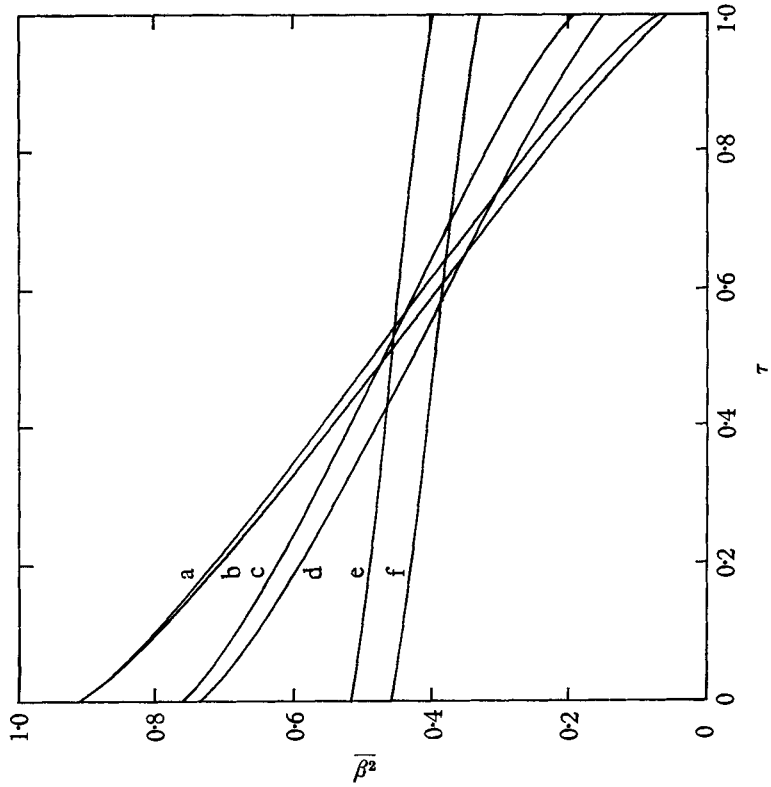

FIGURE 2. Temperature profiles for $\Gamma = 0{\cdot}0$: a (0·1, 0·4, 0·0); b (0·1, 0·7, 0·0); c (0·5, 0·4, 0·0); d (0·5, 0·7, 0·0); e (10·0, 0·4, 0·0); f (10·0, 0·7, 0·0).

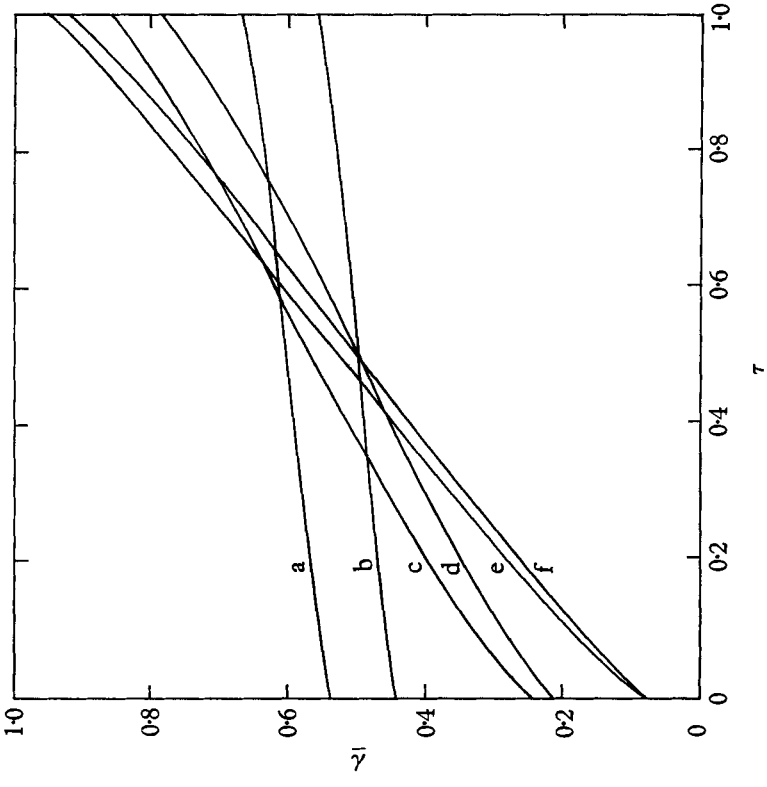

FIGURE 1. Velocity profiles for $\beta_1^2 = 1{\cdot}0$ and 0·4: a (10·0, 0·4, 0·4 *and* 10·0, 0·4, 1·0); b (10·0, 1·0, 0·4 *and* 10·0, 1·0, 1·0); c (0·5, 0·4, 0·4 *and* 0·5, 0·4, 1·0); d (0·5, 1·0, 0·4 *and* 0·5, 1·0, 1·0); e (0·1, 0·4, 0·4 *and* 0·1, 0·4, 1·0); f (0·1, 1·0, 0·4 *and* 0·1, 1·0, 1·0).

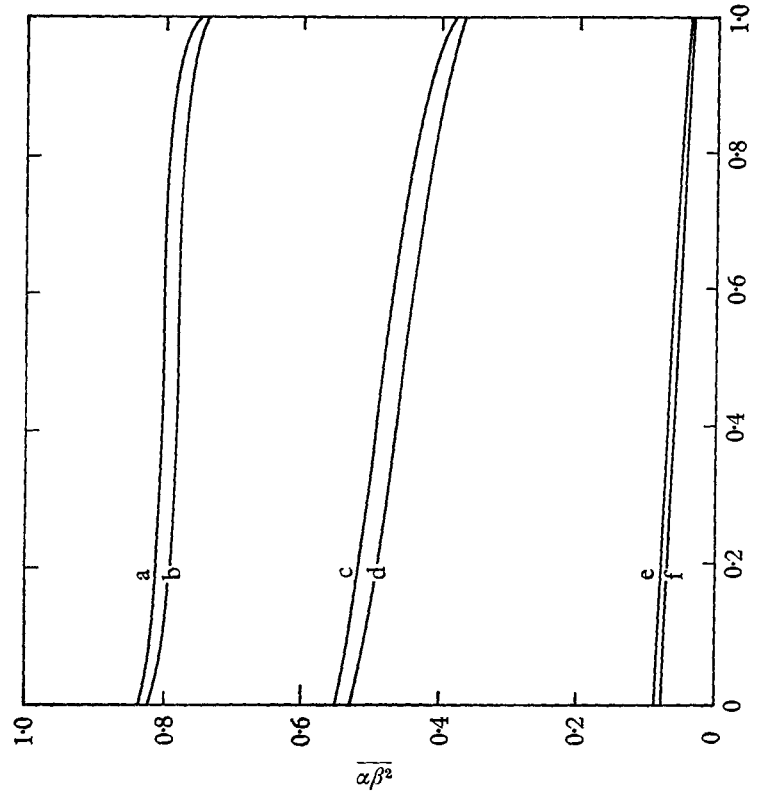

FIGURE 4. Pressure profiles for $\Gamma = 0{\cdot}0$: a (0·1, 0·4, 0·0); b (0·1, 0·7, 0·0); c (0·5, 0·4, 0·0); d (0·5, 0·7, 0·0); e (10·0, 0·4, 0·0); f (10·0, 0·7, 0·0).

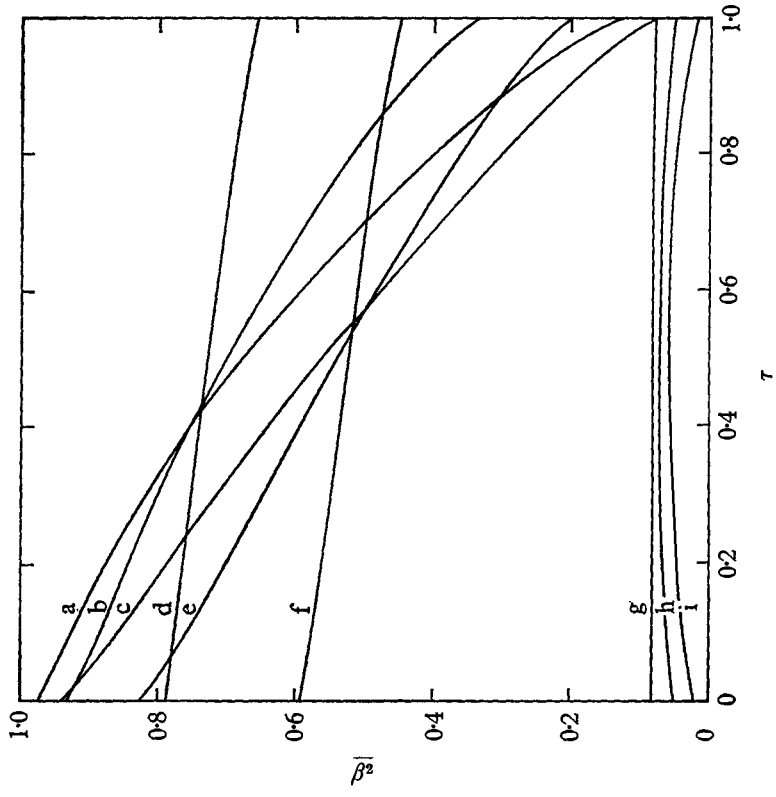

FIGURE 3. Temperature profiles for $\Gamma = 1{\cdot}0$: a (0·1, 0·7, 1·0); b (0·5, 0·7, 1·0); c (0·1, 0·4, 1·0); d (10·0, 0·7, 1·0); e (0·5, 0·4, 1·0); f (10·0, 0·4, 1·0); g (10·0, 1·0, 1·0); h (0·5, 1·0, 1·0); i (0·1, 1·0, 1·0).

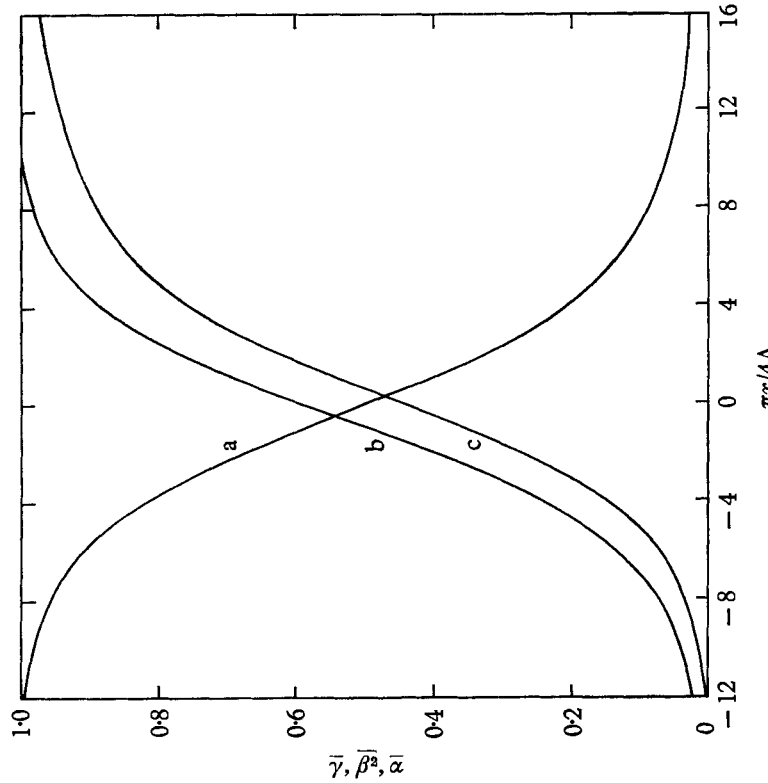

FIGURE 6. Shock profiles *vs.* $\pi x/4\Lambda$ for $M = 1{\cdot}2$ and $\mu \sim T^{0{\cdot}816}$:
a, velocity ; b, temperature; c, density.

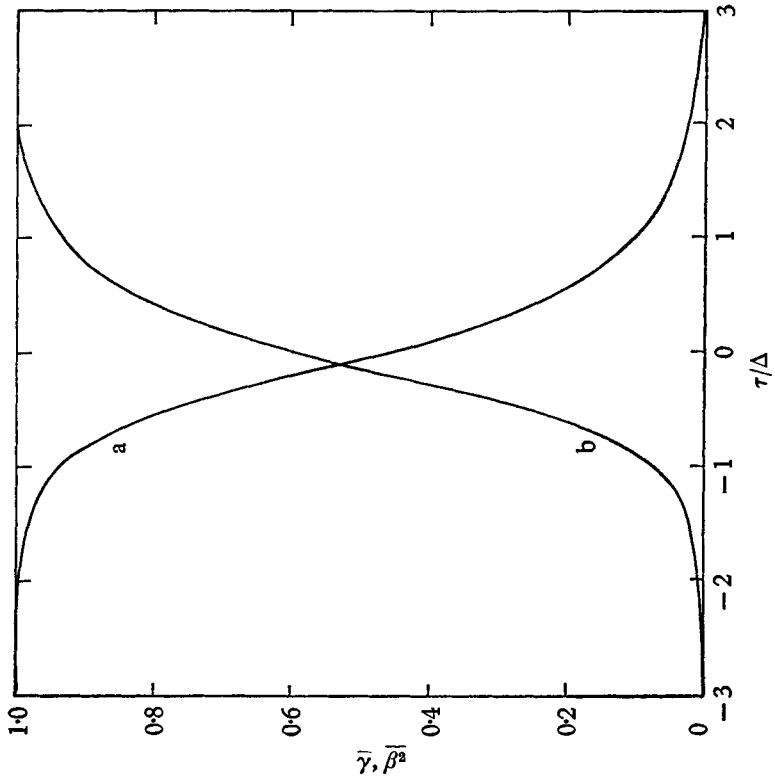

FIGURE 5. Shock profiles *vs.* τ/Δ for $M = 1{\cdot}2$ and $\Delta = 11{\cdot}0$:
a, velocity; b, temperature.

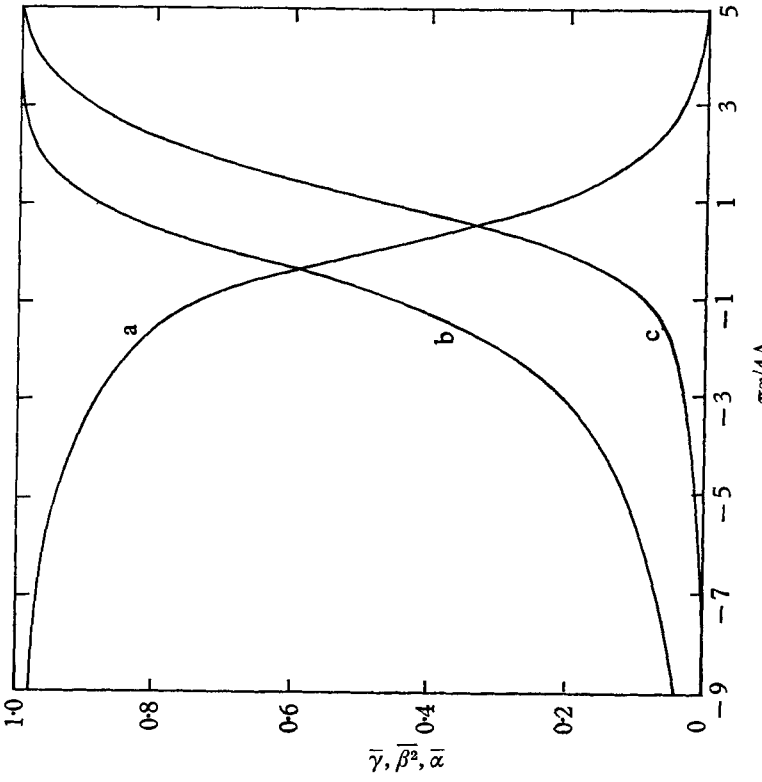

FIGURE 8. Shock profiles *vs.* $\pi x/4\Lambda$ for $M = 10{\cdot}0$ and $\mu \sim T^{0{\cdot}816}$: a, velocity ; b, temperature; c, density.

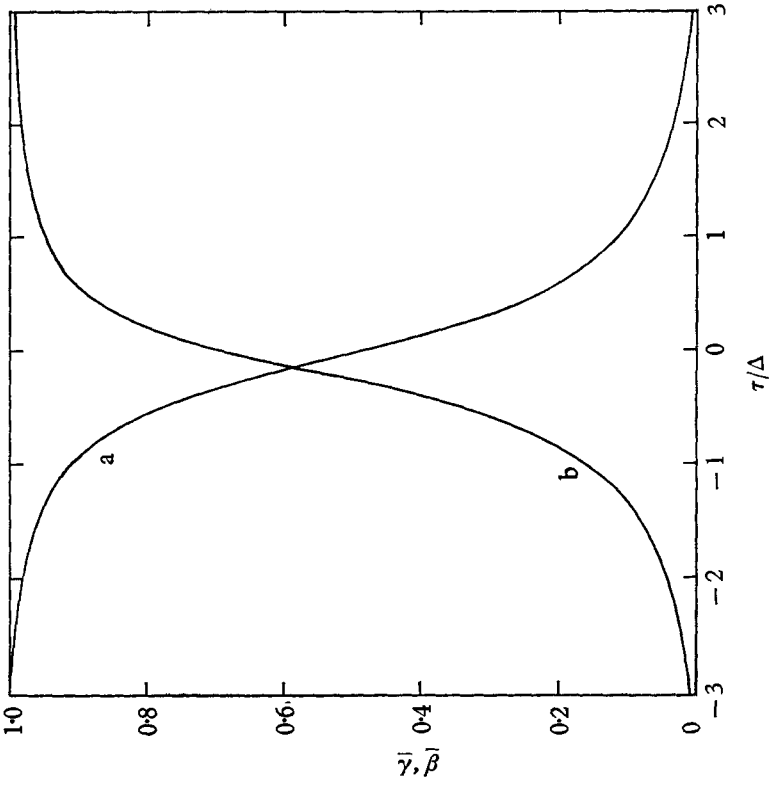

FIGURE 7. Shock profiles *vs.* τ/Δ for $M = 10{\cdot}0$ and $\Delta = 2{\cdot}0$: a, velocity; b, temperature.

With $s = 0{\cdot}816$, the pseudo-gas of the Krook kinetic equation models the viscosity of argon, under some conditions. Owing to the fact that this simplest of the hierarchy of statistical models contains but a single free parameter ν, the Prandtl number of the pseudo-gas is unity.

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