Journal of Statistical Physics, Vol. 1, No. 2, 1969

A Variational Principle for Boundary Value Problems in Kinetic Theory

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Received April 3, 1969

A variational principle which applies directly to the integrodifferential form of the linearized Boltzmann equation is introduced. Extremely general boundary conditions and collision terms are allowed. For a class of interesting problems, the value of the functional to be varied is shown to be closely related to quantities of great physical interest. The formalism is applied to the treatment of plane Couette flow for different forms of the collision term (BGK model, rigid spheres, Maxwell's molecules).

KEY WORDS: kinetic theory; boundary value problems; variational principles; Couette flow; transition regime; Boltzmann equation; rarefied gas dynamics.

1. INTRODUCTION

Variational methods have been recently used by different authors dealing with kinetic theory, and excellent results have been obtained for the Bhatnagar, Gross, and Krook (BGK) model(1–7) as well as for more-refined models.(8–10)

All these papers make use of the integral form of the linearized Boltzmann equation; accordingly, the trial function does not need to satisfy any boundary conditions, and this fact has been exploited to obtain extremely accurate results in the transition and nearly free regimes by such unreasonable trial functions as Chapman–Enskog solutions with gross variables satisfying the Navier–Stokes equations. A disadvantage of the methods employed so far is that they require a splitting of the collision operator into two parts in order to build up an integral equation; this fact has the consequence that the basic functional changes from problem to problem. Also, even simple trial functions produce rather complicated expressions for the basic quantities to be evaluated.

Research sponsored by the Air Force Office of Scientific Research under contract F 61(052)-68-C-0020, through the European Office of Aerospace Research, OAR, United States Air Force.

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In this paper, we consider a variational principle which applies directly to the integrodifferential form of the linearized Boltzmann equations. The formalism developed is then applied to the treatment of a simple standard problem, plane Couette flow, for different forms of the collision term (BGK model, rigid spheres, Maxwell's molecules).

Although new in the kinetic theory of gases, the variational principle presented in this paper is closely related to a variational method for the monoenergetic neutron transport equation, proposed independently by Pomraning and Clark(11'12) and by the present author.(13) A preliminary form of the principle is also sketched in a recent book of the author's.(14)

2. FORMALISM

The steady linearized Boltzmann equation can be written as follows:

$$\mathbf{c} \cdot \partial h/\partial \mathbf{x} = Lh + g_0 \qquad (1)$$

where h is the perturbation of a suitable Maxwellian f_0, $\mathbf{x}$ the position vector of a general molecule, $\mathbf{c}$ the molecular velocity vector, L the collision operator, and g_0 a source term, which is usually, but not always, zero.

The boundary conditions to be matched with Eq. (1) have the following form(14,15):

$$h(\mathbf{x}, \mathbf{c}) = h_0(\mathbf{x}, \mathbf{c}) + \int_{\mathbf{c}'\cdot\mathbf{n}<0} A(\mathbf{c}' \to \mathbf{c})\, h(\mathbf{x}, \mathbf{c}')\, d\mathbf{c}' \qquad (\mathbf{x} \in \partial\Omega) \qquad (2)$$

where $\partial\Omega$ is the boundary of the region Ω where the gas is contained, and $\mathbf{n}$ the normal at $\mathbf{x}$ pointing into Ω. Here $A(\mathbf{c}' \to \mathbf{c})$ is a suitable kernel describing the influence on h of the interaction with the solid walls bounding the gas, $h_0(\mathbf{x}, \mathbf{c})$ a given function of $\mathbf{x}$ and $\mathbf{c}$ ($\mathbf{x} \in \partial\Omega$) depending upon the local state of the wall. We shall write Eq. (2) in the following more-compact form

$$h^+ = h_0 + Ah^- \qquad (3)$$

The operator A transforms functions defined for $\mathbf{c} \cdot \mathbf{n} < 0$ into functions defined for $\mathbf{c} \cdot \mathbf{n} > 0$ and has some notable properties.

To begin with, we have(14,15)

$$(f, ARg)_B = (ARf, g)_B \qquad (4)$$

where f and g are any two functions defined for $\mathbf{c} \cdot \mathbf{n} > 0$ and belonging to a Hilbert space $\mathscr{B}$ where the scalar product is defined as follows:

$$(f, g)_B \equiv \int_{\mathbf{c}\cdot\mathbf{n}<0} fgf_0 \,|\, \mathbf{c} \cdot \mathbf{n} \,|\, d\mathbf{c} \qquad (5)$$

The reflection operator R is defined by

$$R[f(\mathbf{x}, \mathbf{c})] = f(\mathbf{x}, -\mathbf{c}) \qquad (6)$$

Accordingly, AR is an operator transforming functions defined for $\mathbf{c} \cdot \mathbf{n} > 0$ into functions of the same type. Equation (4) shows that AR is symmetrical with respect to the scalar product defined by Eq. (5). Further properties of the operator A are its positiveness and its boundedness (with unit norm). In other words, we have

$$(g, ARg)_B \geqslant 0 \tag{7}$$

$$(g, ARg)_B \leqslant \| g \|_n^2 \tag{8}$$

where g is defined for $\mathbf{c} \cdot \mathbf{n} > 0$ and, by definition,

$$\| f \|_B^2 = (f, f) \tag{9}$$

Actually, Eqs. (4), (7), and (8) were shown to hold[14,15] when R is replaced by R_n, the operator of specular reflection with respect to the normal; since, however, $R = R_n R_t$, where R_t, the reflection operator in the tangent plane, commutes with both R_n and A, Eqs. (4), (7), and (8) follow.

The equality sign in Eq. (8) holds if, and only if, g is a constant with respect to $\mathbf{c}$. In fact, AR leaves a constant unchanged (for a nonporous wall); as a consequence of this fact, using Eq. (4) gives

$$(1, ARg)_B = (1, g)_B \tag{10}$$

The latter equation, if we put $g = Rh^-$, expresses conservation of mass at the wall.

We observe that because of Eq. (4) and well-known properties of symmetrical operators, Eqs. (7) and (8) also give

$$\| ARg \|_B^2 \leqslant \| g \|_B^2 \tag{11}$$

The properties of the collision operator L are perhaps more widely known (see, e.g., Cercignani[14]):

$$(g, Lh) = (Lg, h) \tag{12}$$

$$(h, Lh) \leqslant 0 \tag{13}$$

where, for any two functions $g(\mathbf{c})$ and $h(\mathbf{c})$,

$$(g, h) = \int g h f_0 \, d\mathbf{c} \tag{14}$$

This equation defines a scalar product in a Hilbert space $\mathscr{H}$, to which h and g are supposed to belong.

The equality sign in Eq. (13) holds if, and only if, h is a linear combination of the five collision invariants 1, c_i $(i = 1, 2, 3)$, c^2, usually denoted by ψ_α $(\alpha = 0, 1, 2, 3, 4)$. The scalar product defined by Eq. (14) induces the following norm

$$\| h \|^2 = (h, h) \tag{15}$$

We have introduced two kinds of scalar products for functions defined in velocity space: Eq. (5), to be used at each $\mathbf{x} \in \partial\Omega$, and Eq. (14), to be used at each $\mathbf{x} \in \Omega$. In order to discuss the operator $D = \mathbf{c} \cdot (\partial/\partial\mathbf{x})$, it is necessary to introduce scalar products for functions defined in both velocity space and Ω (or $\partial\Omega$). Therefore, we consider the Hilbert spaces $\mathscr{H} \otimes \mathscr{R}$ and $\mathscr{B} \otimes \mathscr{S}$, where the scalar products are defined as follows:

$$((g, h))_B = \int_{\partial\Omega} (g, h)_B \, dS \tag{16}$$

$$((g, h)) = \int_{\Omega} (g, h) \, d\mathbf{x} \tag{17}$$

where $d\mathbf{x}$ and dS are the volume and surface elements, respectively. Together with these scalar products, we introduce the corresponding norms:

$$|||\, h \,|||_B^2 = ((h, h))_B = \int_{\partial\Omega} \|\, h \,\|_B^2 \, dS \tag{18}$$

$$|||\, h \,|||^2 = ((h, h)) = \int_{\Omega} \|\, h \,\|^2 \, d\mathbf{x} \tag{19}$$

We note that all the relations previously established for scalar products in $\mathscr{B}$ and $\mathscr{H}$ hold unchanged in $\mathscr{B} \otimes \mathscr{S}$ and $\mathscr{H} \otimes \mathscr{R}$ with the new scalar products replacing the previous ones.

If we consider now the operator $D = \mathbf{c} \cdot (\partial/\partial\mathbf{x})$ with the homogeneous boundary conditions obtained by putting $h_0 = 0$ in Eq. (2) or (3), we immediately realize that D is not symmetrical with respect to the scalar product introduced with Eq. (17). We have, however, the following result:

$$\begin{aligned} ((g, RDh)) &= ((RDg, h)) + \int \mathbf{c} \cdot \mathbf{n} g R h \, dS \, d\mathbf{c} \\ &= ((RDg, h)) + ((Ag^-, Rh^-))_B - ((Rg^-, Ah^-))_B \end{aligned} \tag{20}$$

Equation (4) with the replacements $f \to Rg^-$ and $g \to Rh^-$ (note that $R^2 = I$, the identity operator) shows that the last two terms cancel. Therefore,

$$((g, RDh)) = ((RDg, h)) \tag{21}$$

i.e., the operator RD is symmetrical with respect to the scalar product in $\mathscr{H} \otimes \mathscr{R}$.

We finally observe that, for any central interaction, L commutes with R (as well as with any operator equivalent to an orthogonal transformation on $\mathbf{c}$). Accordingly,

$$(g, RLh) = (g, LRh) = (Lg, Rh) = (RLg, h) \tag{22}$$

where Eq. (12) has been used. Accordingly, RL is symmetrical in $\mathscr{H}$ and, as a consequence, in $\mathscr{H} \otimes \mathscr{R}$.

In other words, although the operator $D - L$ is not symmetrical in $\mathscr{H} \otimes \mathscr{R}$, $R(D - L)$ is symmetrical, or, if we prefer, $D - L$ is symmetrical in the pseudo-Hilbert space with a pseudonorm based on the "scalar product" $((f, g))_R \equiv ((f, Rg))$. This "scalar product" has all the usual properties except that $((f, f))_R$ is not a norm, because it is not necessarily positive. This circumstance, however, does not influence the well-known connection between symmetrical operators and variational principles. In fact, if we consider the functional

$$J(\tilde{h}) = ((\tilde{h}, R(D - L)\tilde{h} - 2Rg_0)) + ((\tilde{h}^+ - A\tilde{h}^- - 2h_0, Rh^-))_B \tag{23}$$

where $\tilde{h}$ is an arbitrary function, we have

$$\begin{aligned}\delta J = {} & ((\delta\tilde{h}, R(D - L)\,\tilde{h} - 2Rg_0)) + ((\tilde{h}, R(D - L)\,\delta\tilde{h})) \\ & + ((\delta\tilde{h}^+, R\tilde{h}^-))_B - ((A\,\delta\tilde{h}^-, R\tilde{h}^-))_B + ((\tilde{h}^+ - A\tilde{h}^- - 2h_0, R\,\delta\tilde{h}^-))_B\end{aligned} \tag{24}$$

The symmetry of $R(D - L)$ can now be exploited, taking into account, however, that $\tilde{h}$ will not satisfy, in general, the boundary conditions; accordingly,

$$((\tilde{h}, R(D - L)\,\delta\tilde{h})) = ((R(D - L)\,\tilde{h}, \delta\tilde{h})) + ((\tilde{h}^+, R\,\delta\tilde{h}^-))_B - ((R\tilde{h}^-, \delta\tilde{h}^+))_B \tag{25}$$

Also,

$$((A\,\delta\tilde{h}^-, R\tilde{h}^-))_B = ((R\,\delta\tilde{h}^-, A\tilde{h}^-)) = ((A\tilde{h}^-, R\,\delta\tilde{h}^-)) \tag{26}$$

because of Eq. (4) with $f = R\,\delta\tilde{h}^-$ and $g = R\tilde{h}^-$. Using Eqs. (25) and (26) in Eq. (24) gives

$$\delta J = 2((R(D - L)\,\tilde{h} - Rg, \delta\tilde{h})) + 2((\tilde{h}^+ - A\tilde{h}^- - h_0, R\,\delta\tilde{h}^-))_B \tag{27}$$

Accordingly, if $\tilde{h} = h$, where h is the solution of Eq. (1) with the boundary conditions given by Eq. (3), $\delta J = 0$. If, *vice versa*, $\delta J = 0$ for arbitrary $\delta\tilde{h}$ in Ω and on $\partial\Omega$, it follows that $\tilde{h} = h$.

3. SOME CONSEQUENCES

In the above section, we have shown that if $J(\tilde{h})$ is defined by Eq. (23), $\delta J = 0$ for any $\delta\tilde{h}$ is a necessary as well as sufficient condition for $\tilde{h}$ being equal to h, the solution of Eqs. (1) + (3). The variations given to $\tilde{h}$ are completely arbitrary both in Ω and on $\partial\Omega$. If, however, we restrict the class of admissible $\tilde{h}$ in such a way that all of them satisfy the boundary condition, then the expression for $J(\tilde{h})$ slightly simplifies as follows:

$$J(\tilde{h}) = ((\tilde{h}, R(D - L) - 2Rg_0)) - ((h_0, Rh^-))_B \tag{28}$$

It is interesting to examine the value attained by J when $\tilde{h} = h$; both Eq. (23) and (28) give

$$J(h) = -((Rg_0, h)) - ((h_0, Rh^-))_B \tag{29}$$

This result acquires its full meaning only when we examine the expressions for h_0 and g_0. The most typical case of $g_0 \neq 0$ is Poiseuille flow in a tube of arbitrary but constant section. In this case, $h_0 = 0$, and g_0 is equal to a constant times the component of **c** along the tube axis; accordingly, the value attained by J for $\tilde{h} = h$ is proportional to the flow rate.

In other interesting cases, $g_0 = 0$, and h_0 becomes the only source term in the problem. Now, h_0 is not a completely arbitrary function, because it arises(14,15) from linarization of the boundary conditions for the nonlinear Boltzmann equation. By means of the principle of detailed balance at the wall and using the general expression for h_0,(14,15) it is not difficult to show that h_0 has the following expression:

$$h_0 = \psi_0^+ - A\psi_0^- \tag{30}$$

where

$$\psi_0(\mathbf{x}, \mathbf{c}) = 2\mathbf{c} \cdot \mathbf{u}_0(\mathbf{x}) + (c^2 - 3/2)\,\tau_0(\mathbf{x}) \qquad (\mathbf{x} \in \partial R) \tag{31}$$

Here, $\mathbf{u}_0(\mathbf{x})$ and $\tau(\mathbf{x})$ are the deviations of the velocity and temperature of the boundary from those of the basic Maxwellian f_0; $\mathbf{c}$ and $\mathbf{u}$ are scaled with $(2kT_0/m)^{1/2}$ and τ with T_0, k being the universal Boltzmann constant, m the molecular mass, and T_0 the temperature in f_0.

Inserting $g_0 = 0$ and h_0 from Eq. (30) into Eq. (29), we find

$$\begin{aligned} J(h) &= -\,((\psi_0^+, Rh^-))_B + ((A\psi_0^-, Rh^-))_B \\ &= -((\psi_0^+, Rh^-))_B + ((R\psi_0^-, Ah^-))_B \\ &= -((R\psi_0^-, \psi_0^+, -\,A\psi_0^-)) + ((R\psi_0^-, h^+)) - ((\psi_0^+, Rh^-))_B \end{aligned} \tag{32}$$

The first term is a known function, while the second and the third terms can be written as follows:

$$\begin{aligned} ((R\psi_0^-, h^+)) - ((\psi_0^+, Rh^-))_B &= \int \mathbf{c} \cdot \mathbf{n}\ {}_0\psi_0(\mathbf{x}, -\,\mathbf{c})\, h(\mathbf{x}, \mathbf{c})\, d\mathbf{c}\, dS \\ &= -2 \int u_{0j}(\mathbf{x}) \Big[\int \mathbf{c} \cdot \mathbf{n} c_j f_0 h(\mathbf{x}, \mathbf{c})\, d\mathbf{c} \Big]\, dS \\ &\quad + \int \tau_0(\mathbf{x}) \Big[\int (c^2 - \tfrac{3}{2})\, \mathbf{c} \cdot \mathbf{n} f_0 h(\mathbf{x}, \mathbf{c})\, d\mathbf{c} \Big]\, dS \\ &= -2 \int \mathbf{u}_0 \cdot \mathbf{p}_n\, dS + 2 \int \tau_0 q_n\, dS \end{aligned} \tag{33}$$

Here, $\mathbf{p}_n$ is the normal stress vector (its components are $p_{ij}n_j$) or, rather, the pertubation part of the normal stress vector, and $q_n = \mathbf{q} \cdot \mathbf{n}$ is the normal component of heat flux. The mass conservation at the wall [Eq. (10) with $g = Rh^-$] has been taken into account.

We observe now that it is convenient, without loss of generality, to consider separately the two cases $\mathbf{u}_0 = 0$ and $\tau_0 = 0$, thanks to linearity. It is also frequent, albeit not necessary, that $\mathbf{u}_0$ and τ_0 can be taken to be constant ($\mathbf{u}_0$ equals the free-stream velocity in flows past a body, or the relative velocity of one wall with respect to the other in Couette flows, τ_0 the temperature difference). When the latter circumstance holds, the functional becomes proportional to a quantity of physical interest (e.g., a drag or heat transfer coefficient). We note that even if $\mathbf{u}_0$ is not constant, but describes a solid body rotation [$\mathbf{u}_0 = \boldsymbol{\omega}_0 \times (\mathbf{x} - \mathbf{x}_0)$, with $\boldsymbol{\omega}_0$ a constant], the functional acquires a simple meaning, being proportional to the torque upon the body.

These results were known previously(1–10) for the variational principles based on the integral version of the Boltzmann equation, but appeared as fortuitous coincidences arising from suitable manipulations to be repeated for each problem; in addition, the quoted papers$^{(1-10)}$ took into account particularly simple boundary conditions. Here, for the first time, as far as we know, a common root for all the different cases appears; also, the limits of applicability of the very useful connection between the functional and the physical quantities of basic interest are clearly shown.

4. APPLICATION TO PLANE COUETTE FLOW

As is well known, the practical advantages of the variational principle are of twofold nature: on the one hand, they give a standard recipe for writing down approximate equations for a "best fitting" of the parameters appearing in a suitably restricted class of trial functions; on the other hand, they allow the functional J to be evaluated with great accuracy, a particularly appealing circumstance when J can be related to quantities of great physical interest, as in the simple case to be treated here as an example, plane Couette flow.

Plane Couette flow is the flow of a gas between parallel plates located at $x = \pm\delta/2$ and moving with velocities $\mp U/2$ in the direction of the z axis.$^{(1,16,17)}$ If we assume as trial function

$$\tilde{h} = 2c_z(\alpha x + \beta c_x + \gamma \operatorname{sgn} c_x) \tag{34}$$

where α, β, and γ are adjustable constants, we shall certainly obtain results correct in both the free-molecular and continuum limits, at least for Maxwell molecules and the BGK model.

Inserting Eq. (34) into Eq. (23), we obtain

$$\begin{aligned} J(\tilde{h}) = &- [1/(2\sqrt{\pi})]\, \alpha^2\delta^2 + [(2/\sqrt{\pi}) - 4\delta I_3]\, \beta^2 \\ &+ [(2/\sqrt{\pi}) - 4\delta I_1]\, \gamma^2 + \delta\alpha\beta + (2/\sqrt{\pi})\, \delta\alpha\gamma \\ &+ (2 - 8\delta I_2)\, \beta\gamma + (U\delta/\sqrt{\pi})\, \alpha + U\beta + (2U/\sqrt{\pi})\, \gamma \end{aligned} \tag{35}$$

where velocities are scaled with $(2kT_0/m)$ as above, and diffuse reflection has been assumed at the walls; I_1, I_2, and I_3 are three quantities to be defined below. The condition $\delta J = 0$ gives

$$\begin{aligned} (\delta/\sqrt{\pi})\, \alpha - \beta - (2/\sqrt{\pi})\, \gamma &= U/\sqrt{\pi} \\ (\delta/2)\, \alpha + [(2/\sqrt{\pi}) - 4\delta I_3]\, \beta + (1 - 4\delta I_2)\, \gamma &= -U/2 \\ (\delta/\sqrt{\pi})\, \alpha + (1 - 4\delta I_2)\, \beta + [(2/\sqrt{\pi}) - 4\delta I_1]\, \gamma &= -U/\sqrt{\pi} \end{aligned} \tag{36}$$

Solving this system of three linear algebraic equations, we obtain

$$\begin{aligned} \alpha &= [8U\sqrt{\pi}(2\sqrt{\pi} I_2 - I_1 - 4I_3) + 16\pi\delta(I_1 I_3 - I_2^2)]/\Delta \\ \beta &= [4U\delta(\pi I_1 - 2\sqrt{\pi}\, I_2)]/\Delta \\ \gamma &= -[U(4 - \pi) - 4U\delta(\pi I_2 - 2\sqrt{\pi}\, I_3)]/\Delta \end{aligned} \tag{37}$$

where

$$\Delta = 16\pi(I_1 I_3 - I_2^2)\,\delta^2 + [16\pi I_2 - 2\sqrt{\pi}\,(4+\pi)\,I_1 - 16\sqrt{\pi}\,I_3]\,\delta + 2(4-\pi) \tag{38}$$

$$I_1 = \pi^{-3/2} \int c_z \operatorname{sgn} c_x\, L(c_z \operatorname{sgn} c_x) \exp[-c^2]\, d\mathbf{c} \tag{39}$$

$$I_2 = \pi^{-3/2} \int c_z \operatorname{sgn} c_x\, L(c_x c_z) \exp[-c^2]\, d\mathbf{c} \tag{40}$$

$$I_3 = \pi^{-3/2} \int c_x c_z L(c_x c_z) \exp[-c^2]\, d\mathbf{c} \tag{41}$$

An obvious advantage of the present variational principle with respect to the old one is that one obtain rational rather than transcendental expression in δ when using simple trial function; on the other hand, it must be expected that the previous method reflects better any effects of the kinetic boundary layers. If we evaluate the ratio of the shearing stress p_{xz} to its free-molecular value p^0_{xz}, we obtain

$$\begin{aligned} \frac{p_{xz}}{p^0_{xz}} &= -\frac{(\beta/2) + (\gamma/\sqrt{\pi})}{U/(2\sqrt{\pi})} \\ &= \frac{2[\sqrt{\pi}\,(8I_3 - 2\pi I_1)\,\delta + (4-\pi)]}{\Delta} \end{aligned} \tag{42}$$

The values of the integrals I_k ($k = 1, 2, 3$) are known for the BGK model, Maxwell molecules, and rigid spheres. In fact, the evaluation is trivial for the BGK model:

$$I_1 = -1/(2\theta), \qquad I_2 = -1/(2\sqrt{\pi}\,\theta), \qquad I_3 = -1/4\theta \tag{43}$$

For Maxwell molecules and rigid sphers, the three integrals are proportional to the homonymous integrals evaluated by Ziering$^{(18)}$ and Gross and Ziering.$^{(19)}$ The values for Maxwell molecules are

$$I_1 = -1.2392\alpha_1, \qquad I_2 = -0.3750\alpha_1, \qquad I_3 = -0.3323\alpha_1 \tag{44}$$

and, for rigid spheres,

$$I_1 = -1.0059\alpha_2, \qquad I_2 = -0.4343\alpha_2, \qquad I_3 = -0.4001\alpha_2 \tag{45}$$

where α_1 and α_2 are constants related to the constant of the force in the case of Maxwell molecules and the sphere diameter for the rigid-sphere model.
Equation (42) can be written as

$$p_{xz}/p^0_{xz} = (a + \sqrt{\pi}\,\delta)/(a + b\delta + c\delta^2) \tag{46}$$

where

$$a = \frac{4-\pi}{8I_3 - 2\pi I_1} \tag{47}$$

$$b = \frac{8\pi I_2 - \sqrt{\pi}\,(4+\pi)\,I_1 - 8\sqrt{\pi}\,I_3}{8I_3 - 2\pi I_1} \tag{48}$$

$$c = \frac{4\pi(I_1 I_3 - I_2^2)}{4I_3 - \pi I_1} \tag{49}$$

For large values of δ (continuum limit), Eq. (46) gives

$$p_{xz}/p_{xz}^0 \approx [\sqrt{\pi}/(c\delta)]\{1 - [(b/c) - (a/\sqrt{\pi})]/\delta\} + O(\delta^{-2}) \tag{50}$$

It is convenient to assume a length of the order of the mean free path as length scale; if we relate the mean free path to the viscosity coefficient μ, pressure p, and temperature T as follows:

$$l = (\mu/p)(\pi RT/2)^{1/2} \tag{51}$$

we assume $\lambda = (2l)/\sqrt{\pi}$ as length scale. In such a case, the asymptotic behavior of p_{xz}/p_{xz}^0 should be $(\sqrt{\pi}/\delta) + O(\delta^{-1})$;comparison with Eq. (50) gives

$$c = 1 \tag{52}$$

This relation is consistent for the BGK model and Maxwell molecules, since, in these cases, we have(20)

$$I_2/I_3 = 2/\sqrt{\pi}, \qquad I_3 = -\sqrt{\pi}/(8l) \tag{53}$$

Hence,

$$c = -4I_3 = \sqrt{\pi}/(2l) = 1/\lambda \tag{54}$$

If we assume λ as the scaling factor lengths, Eq. (52) is satisfied. For rigid spheres, the constant α_2 appearing in Eq. (45) is given by(19)

$$\alpha_2 = (2\pi)^{1/2}\, n\sigma^2 \tag{55}$$

where n is the number density ($n = \rho/m$) and σ the sphere diameter. Hence,

$$c = 1.7228(2\pi)^{1/2}\, n\sigma^2 \tag{56}$$

On the other hand, the viscosity coefficient for rigid spheres is(21)

$$\mu = 0.1792(kTm)^{1/2}/\sigma^2 \tag{57}$$

which gives

$$\lambda = (2l)/\sqrt{\pi} = \mu(2kT/m)^{1/2}/p = 0.1792\sqrt{2}\, kT/p\sigma^2 = 0.1792(\sqrt{2}/n\sigma^2) \tag{58}$$

Hence,

$$c = 1.0944/\lambda \tag{59}$$

which is not in agreement with Eq. (52) for $\lambda = 1$. The reason for this discrepancy is clearly related to the fact that the trial function cannot become the correct solution in the continuum limit, as was discussed elsewhere by the present author in another connection.(20) For the moment, we shall ignore this discrepancy and use Eq. (52) as normalization condition for the length scale, although not in agreement with

$\lambda = 1$ for rigid spheres. Then the constants appearing in Eq. (46) take on the following values:

$$a = (4 - \pi)/(\pi - 2), \qquad b = \pi \sqrt{\pi}/2(\pi - 2), \qquad c = 1 \tag{60}$$

$$a = 0.2225, \qquad b = 2.1400, \qquad c = 1 \tag{61}$$

$$a = 0.4741, \qquad b = 2.4014, \qquad c = 1 \tag{62}$$

The right hand side of Eq. (46) can be easily tabulated, and the results are given in Table I; as is seen, the results for the three models are very close to each other (but this could be artificial for rigid spheres, because of the chosen normalization).

In order to have an idea of the accuracy of the results, one can compare the results for the BGK model with the corresponding values obtained by Willis⁽¹⁶⁾ by means of an accurate numerical solution of the BGK equations. The moment method formula obtained by Lees⁽²²⁾

$$p_{xz}/p_{xz}^{0} = \sqrt{\pi}/(\delta + \sqrt{\pi}) \tag{63}$$

is also tabulated. It will be noticed that the maximum disagreement from Willis result is about 0.5% for Eq. (46) [with the BGK values for the constants given by Eq. (60)] and about 5% for the moment method. Both formulas give the exact continuum and free-molecular values, but a difference arises in the slip regime. In fact, Eqs. (50) and (63) give for the slip coefficient (in λ units)

$$\sigma = (\sqrt{\pi}/4) + (1/\sqrt{\pi}) = 1.0073, \quad \sigma = \sqrt{\pi}/2 = 0.8862 \tag{64}$$

the exact value being⁽²³⁾

$$\sigma = 1.0161 \tag{65}$$

Incidentally, the value given by Eq. (64) is the same given by the previous variational method with the simplest trial function.⁽¹⁾ A similar evaluation of the slip coefficient

Table I

			Variational method with trial function given by			
δ	Willis⁽¹⁶⁾ (BGK)	Lees' method [Eq. (63)]	Eq. (34), BGK model	Eq. (34), Maxwell molecules	Eq. (34), rigid spheres	Eq. (69), rigid spheres
0.1	0.9258	0.9466	0.9238	0.8953	0.8994	0.9147
1.0	0.6008	0.6393	0.6024	0.5933	0.5797	0.6051
2.0	0.4440	0.4698	0.4462	0.4430	0.4332	0.4496
3.0	0.3539	0.3714	0.3556	0.3542	0.3472	0.3583
4.0	0.2946	0.3070	0.2958	0.2951	0.2900	0.2980
5.0	0.2526	0.2617	0.2534	0.2529	0.2491	0.2550
7.0	0.1964	0.2020	0.1969	0.1967	0.1943	0.1980
10.0	0.1474	0.1506	0.1476	0.1476	0.1462	0.1483
20.0	0.0807	0.0814	0.0805	0.0805	0.0801	0.0807

can be made for Maxwell molecules. Using the values given by Eq. (61), we obtain

$$\sigma = (\sqrt{\pi}/4) + (1/\sqrt{\pi}) = 1.0073 \tag{66}$$

for Maxwell molecules, and

$$\sigma = 1.0669 \tag{67}$$

for rigid spheres. The value given by Eq. (66) is the same as the one in Eq. (64), thus confirming the fact(8,24) that the BGK model gives a value for σ very close to the value for Maxwell molecules. The value given by Eq. (67) is somewhat surprising, because all the available results(8,10) agree in giving a slip coefficient for rigid spheres somewhat lower than the corresponding value for Maxwell molecules (for a given viscosity, pressure, and temperature). However the disagreement between Eq. (67) and the expected result is of the same order as the discrepancy between the two normalizations $c = 1$ and $\lambda = 1$. If we adopt the latter rather than the former (as we know, the two are coincident for Maxwell molecules and the BGK model) we obtain

$$\sigma = 1.0669/1.0944 = 0.9749 \tag{68}$$

which is in a reasonably good agreement with the available results.(8–10) This means that the trial function given by Eq. (34), although not capable of giving correct values for the viscosity and the slip coefficients, gives a reasonably accurate estimate of their ratio. This conclusion has been reached *a posteriori* and does not avoid the circumstance that the trial function we have been using is not satisfactory for molecules other than Maxwell's (or models of Maxwell's molecules). This fact could have been easily foreseen on the basis of the discussion given by Cercignani(20) and can be avoided by the same kind of correction as the one proposed for the half-range expansions in the latter reference. A sketch of the modified computations is given in the next section.

5. A MORE-REFINED TRIAL FUNCTION

In this section, we assume as trial function for plane Couette flow:

$$\tilde{h} = 2c_z[\alpha x + \beta b(c)\, c_x + \gamma \operatorname{sgn} c_x] \tag{69}$$

where $b(c)$ is a function of the molecular speed satisfying

$$2c_x c_z = L[b(c)\, c_x x_z] \tag{70}$$

For Maxwell's molecules and the BGK model, $b(c)$ is a constant; accordingly, the new trial function reduces, in these cases, to the previous one. In general, however, inserting Eq. (69) into Eq. (23), we obtain

$$\begin{aligned} J(\tilde{h}) = &-[1/(2\sqrt{\pi})]\,\alpha^2\delta^2 + (4K - 8\delta J_1)\,\beta^2 + [(2/\sqrt{\pi}) - 4\delta I_1]\,\gamma^2 \\ &+ 4\delta J_1\alpha\beta + (2/\sqrt{\pi})\,\delta\alpha\gamma + [8J_1 - (8\delta/\sqrt{\pi})]\,\beta\gamma \\ &+ (U\delta/\sqrt{\pi})\,\alpha + 4UJ_1\beta + (2U/\sqrt{\pi})\,\gamma \end{aligned} \tag{71}$$

where I_1 is given by Eq. (39), and

$$J_1 = \pi^{-3/2} \int b(c)\, c_x^2 c_z^2 \exp[-c^2]\, d\mathbf{c} \tag{72}$$

$$K = \pi^{-3/2} \int [b(c)]^2 \mid c_x \mid^3 c_z^2 \exp[-c^2]\, d\mathbf{c} \tag{73}$$

The condition $\delta J = 0$ now gives

$$\begin{aligned} (\delta/\sqrt{\pi})\, \alpha - 4J_1\beta - (2/\sqrt{\pi})\, \gamma &= U/\sqrt{\pi} \\ (2J_1\delta)\, \alpha + (4K - 8\delta J_1)\, \beta + [4J_1 - (4\delta/\sqrt{\pi})]\, \gamma &= -2UJ_1 \\ (\delta/\sqrt{\pi})\, \alpha + [4J_1 - (4\delta/\sqrt{\pi})]\, \beta + [(2/\sqrt{\pi}) - 4\delta I_1]\, \gamma &= -U/\sqrt{\pi} \end{aligned} \tag{74}$$

i.e.,

$$\begin{aligned} \alpha &= -\, [4\delta(1 - 2\pi I_1 J_1) + 2\sqrt{\pi}\, I_1(2K\sqrt{\pi} - 4\pi J_1^2)]/\Delta' \\ \beta &= -2U\delta(1 - 2\pi I_1 J_1)/\Delta' \\ \gamma &= -U(2K\sqrt{\pi} - 4\pi J_1^2)/\Delta' \end{aligned} \tag{75}$$

where

$$\Delta' = [8\pi I_1 J_1 - 4]\, \delta^2 + (8J_1\sqrt{\pi} - 8\pi\sqrt{\pi}\, J_1^2 I_1 - 4\pi K I_1)\, \delta + (4K\sqrt{\pi} - 8\pi J_1^2) \tag{76}$$

The ratio of the shearing stress to its free-molecular value is

$$\frac{p_{xz}}{p^0_{xz}} = -\frac{(2J_1\beta + (\gamma/\sqrt{\pi})}{U/(2\sqrt{\pi})} \tag{77}$$

i.e., we find again an equation of the form shown in Eq. (46), with the following values for the constants

$$\begin{aligned} a &= \frac{2K\sqrt{\pi} - 4\pi J_1^2}{4J_1(1 - 2\pi I_1 J_1)} \\ b &= \frac{2J_1\sqrt{\pi} - 2\pi\sqrt{\pi}\, J_1^2 I_1 - \pi K I_1}{2J_1(1 - 2\pi I_1 J_1)} \\ c &= -1/(2J_1) \end{aligned} \tag{78}$$

J_1 is proportional to the homonymous integral given by Cercignani[(20)] and is therefore related to the mean free paths l and $\lambda = (2l)/\sqrt{\pi}$ as follows:

$$J_1 = -l/\sqrt{\pi} = -\lambda/2 \tag{79}$$

Accordingly, the agreement between the two normalizations ($\lambda = 1$ and $c = 1$) is automatically verified, as was to be expected. With this normalization, the slip coefficient becomes

$$\sigma = (\sqrt{\pi}/4) + (K/8J_1^2) \tag{80}$$

It is interesting to notice that the expression for σ turns out to be rather simple, and, for a simple molecular model with velocity-dependent collision frequency, Eq. (60) is in agreement with the formulas obtained from the older variational principle.(8–10)

The advantage, here, is that we used the true linearized Boltzmann equation, rather than special models approximating the latter. Also, one immediately sees that σ is the same for Maxwell molecules and the BGK model to this level of approximation; this was to be expected, because in these cases, the new trial function reduces to the one used in Section 4.

The fact that Eq. (80) is the same as the one obtained in previous paper has the further advantage that the ratio K/J_1^2 has already been evaluated with the $b(c)$ appropriate to rigid spheres.(8) Accordingly, we find from Eq. (80),

$$\sigma = 0.9790 \tag{81}$$

a value rather different from the one given in Eq. (67) [but close to the one given in Eq. (68)]. This fact shows the importance of choosing a sensibly correct dependence of the trial function upon the velocity variable.

By means of the numerical value for I_1, as given by Gross and Ziering,(19) and K, as deduced from the value for the slip coefficient given by Loyalka and Ferziger,(8) it is possible to evaluate the coefficients in Eq. (46) as given by Eq. (78), for the case of rigid spheres. Taking λ as length scale, the values of a, b, and c are

$$a = 0.3264, \qquad b = 2.1422, \qquad c = 1 \tag{82}$$

It is then possible to tabulate the stress *versus* the inverse Knudsen number δ (Table I). Even with the amended trial function, the influence of the molecular model on the stress is not very marked, the difference between rigid spheres and Maxwell's molecules reaching a maximum of about 2% in the nearly-free-molecular regime. It is also to be noted that in the latter regime, the results for the BGK model are closer to those for rigid spheres than those for Maxwell's molecules.

6. INFLUENCE OF THE BOUNDARY CONDITIONS

In the previous two sections, the boundary conditions of diffuse reflection were assumed at the wall. It is obvious that no problems arise in extending the previous calculations to any model of the boundary conditions one might wish to use. In particular, Maxwell's boundary conditions can be easily handled and do not produce any new integrals besides the already computed ones.

Equally easy is the use of finite-rank approximations to the operator A of the kind suggested previously;(14,15) new integrals arise for high-order approximations to A, but they are trivial to compute when the trial function of Section 4 is used (hence, the calculations are both simple and accurate for Maxwell's molecules). We note that within the limits of the accuracy of the computations presented in the previous sections a finite-rank operator with a kernel engendered by c_z, $c_x c_z$ should be a satisfactory approximation. A simpler boundary condition is based on a kernel engendered by c_z alone; in such a case, a single parameter enters which can be easily related to the accommodation coefficient for the tangential momentum.(25) There is no point in doing the calculations with the latter model for boundary conditions, since it can be shown$^{(25)}$ that the solution for a general value of the accommodation coefficient can be expressed in terms of the solution corresponding to diffuse reflection.

7. CONCLUDING REMARKS

A variational principle has been shown to hold for the linearized Boltzmann equation with fairly general boundary conditions; the functional having zero variation when the trial function becomes the true solution of the problem has been shown to be simply related to quantities of basic interest for a significant class of problems. It is to be noted that the principle is not a minimum or a maximum principle, since, in general, the points of zero variation will be saddle points; in spite of this, thanks to the connection between the physically interesting quantities and the basic functional, the principle lends itself to accurate evaluations of overall coefficients, such as drag, heat transfer, etc. The advantage with respect to the previously known methods$^{(1-10)}$ is that general molecular models can be used, including models with formally infinite collision frequency, and the resulting expression are rational in the Knudsen number. The latter circumstance can be particularly useful for making meaningful comparisons with correlations of experimental data.

The general method has been applied to a specific problem, plane Couette flow; the latter has been exhaustively studied by different authors and no new results could be expected, but just this fact makes the problem a significant one for a test of accuracy. The application of the method to less-simple problems, in cylindrical geometry, seems to constitute an interesting subject for future research.

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