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Shock-wave structure for some nonanalytical in-velocity closures

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The bimodal approach to the problem of shock structure is further investigated. The closing moments which are nonanalytical in molecular velocity, namely, $1/v_z$ and v_τ^2/v_z, are used. For rigid spheres, only the asymptotic ($M\rightarrow\infty$) values of the shock thickness were found. For pseudo-Maxwellian molecules, using Bobylev's method [A. V. Bobylev, Theor. Math. Phys. **60**, 820 (1984)] of the Fourier transformation of the Boltzmann equation, it was possible to reduce the problem to a one-dimensional integral and to obtain the full dependence of the thickness on the Mach number.

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I. INTRODUCTION

A lot of investigations have been dedicated during the last four decades or so to the problem of shock-wave structure on the basis of the Boltzmann equation. Mostly this research used the Mott-Smith bimodal ansatz [1] (see also the references in [2]). But the closing moments for the determination of the density profile in the shock wave were always analytical functions of the molecular velocity, usually power functions of its components.

In [2] we proposed using nonanalytical functions of velocity, namely $1/v_z$, which gives the equation for the density profile, and v_τ^2/v_z, which gives the equation for the profile of the transverse temperature. The aim in [2] was to obtain effective values of viscosity and thermal conductivity in the limit $M\rightarrow 1$ and compare them with the classical Chapman-Enskog values. The agreement turned out to be good for both the viscosity and thermal conductivity. The analysis in [2] was made for arbitrary inverse-power intermolecular potentials (including rigid spheres) but only for $M\rightarrow 1$. The results were in the form of one-dimensional integrals which were calculated numerically. Earlier, Yen and Ng [3] used the same moments in their Monte Carlo simulation. In [4] the transport coefficients were derived without any closure on the basis of the first correction to the bimodal distribution function for weak shock waves.

We would like to mention that recently a lot of important results, but pertaining mostly to the existence of longitudinal and transverse temperatures in weak and strong shock waves, have appeared in [5–8]. In the present paper we use the above closures to obtain the dependence of the shock wave thickness for arbitrary Mach numbers. However, for rigid spheres all we could do was to get the asymptotic values of the corresponding thicknesses for the infinite Mach number. But we were able to reduce the problem to one-dimensional integrals for the case of pseudo-Maxwellian molecules and calculate the thicknesses for any Mach number.

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II. ANALYSIS

Consider the one-dimensional stationary Boltzmann equation in the usual notation [9]:

$$v_z\partial f/\partial z=J(f,f)$$
$$=\int[f(\mathbf{v}')f(\mathbf{v}_1')-f(\mathbf{v})f(\mathbf{v}_1)]gb\,db\,d\varepsilon\,d^3v_1.$$

For the distribution function f we will use below the Mott-Smith bimodal ansatz [1]:

$$f=\nu(z)f_0(\mathbf{v})+[1-\nu(z)]f_1(\mathbf{v}),\tag{1}$$

where

$$f_i=n_i(2\pi kT_i/m)^{-3/2}\exp[-m(\mathbf{v}-\mathbf{u}_i)^2/2kT_i]$$

are the upstream ($i=0$) and downstream ($i=1$) Maxwellians. Though it is true that nowadays the Mott-Smith ansatz is not considered to be a good approximation for the distribution function, a judicious use of it can lead to good approximations to the shock thickness.

For the weighted density $\nu(z)$ we have $\nu(-\infty)=1$, $\nu(+\infty)=0$. Densities, velocities, and temperatures upstream and downstream are connected via the Rankine-Hugoniot relations which are obtained with the use of multiplication of the Boltzmann equation by collisional invariants when the moment of the collision integral is zero. The result is

$$u_1/u_0=n_0/n_1=(M^2+3)/4M^2,$$
$$T_1/T_0=(M^2+3)(5M^2-1)/16M^2,$$

where

$$M=u_0/(5RT_0/3)^{1/2}$$

is the upstream Mach number.

First we tried to apply the new closures $1/v_z$ and v_τ^2/v_z for a gas of rigid spheres. Deshpande and Narasimha [10] already calculated the collision integral for a combination of Maxwellians. Their result is in the form of a two-dimensional quadrature including confluent hypergeometric functions of a nonanalytical function of molecular velocity, $[\frac{1}{4}(c_0^2+c_1^2)^2-(\mathbf{c}_0\cdot\mathbf{c}_1)^2]^{1/2}$, where $\mathbf{c}_i=(2RT_i)^{-1/2}(\mathbf{v}-\mathbf{u}_i)$. Their expression turned out to be rather awkward and we found it impossible either to calculate analytically $\int\int dv_x\, dv_y\, J$ for arbitrary M or to reduce it to a one-dimensional quadrature. Hence all we could try to do was to treat their results for $M\to\infty$. They gave separate formulas for the region near the supersonic peak and for the rest of the velocity space. Combining these formulas, we obtained the following expression for the collision integral in the case of the bimodal distribution function (1):

$$J=8\nu(1-\nu)n_0^2\sigma^2/(2RT_1)\times[\pi^{-1/2}(|\mathbf{c}_1-\mathbf{c}_{10}|^{-1}-\tfrac{1}{2}|\mathbf{c}_1-\mathbf{c}_{10}|)\exp(-c_1^2)-\pi^{1/2}\delta(\mathbf{c}_1-\mathbf{c}_{10})\exp(-c_{10}^2)\,{}_1F_1(2,\tfrac{3}{2},c_{10}^2)],$$

where ${}_1F_1(2,\frac{3}{2},x)=\frac{1}{2}+\frac{1}{4}\sqrt{\pi}(x^{-1}+2x)\exp(x^2)\mathrm{erf}x$. Here $\mathbf{c}_{10}$ is directed along the z axis, $c_{10}=\sqrt{3/2}$, and σ is the diameter of a rigid sphere. After some algebra, we obtain

$$\int d^3v\; J/v_z=\sqrt{\pi}\nu(1-\nu)n_0^2\sigma^2\times\left\{4\exp(-\tfrac{3}{2})\int_{-\infty}^{+\infty}dz\,\exp(-\sqrt{6}z)\times[\tfrac{3}{2}\sqrt{\pi}\,\mathrm{erfc}|z|-|z|\exp(-z^2)]/(z+4/\sqrt{6})-\sqrt{6}[\exp(-\tfrac{3}{2})+2\sqrt{2/3\pi}\,\mathrm{erf}\sqrt{3/2}]\right\}.$$

The integral was taken numerically and the result turned out to be

$$\int d^3v\; J/v_z=-0.7354\sqrt{\pi}\nu(1-\nu)n_0^2\sigma^2.$$

But $\int d^3v\; J/v_z=(n_0-n_1)d\nu/dz=-3n_0 d\nu/dz>0$, so, unfortunately, this $1/v_z$ closure appears to describe the shock wave of infinite strength inadequately.

Hence we tried $v_\tau^2/v_z=(v_x^2+v_y^2)/v_z$ closure corresponding to the transport of transverse temperature in the shock wave. Similar calculations show that

$$\int d^3v\; Jv_\tau^2/v_z=2\sqrt{\pi}\exp(-\tfrac{3}{2})\nu(1-\nu)n_0^2\sigma^2RT_1B,$$

where

$$B=\int_{-\infty}^{+\infty}dz\,\exp(-\sqrt{6}z)[2|z|(1-z^2)+\sqrt{\pi}(1-6z^2)\mathrm{erfc}|z|]/(z+4/\sqrt{6})=0.021.$$

As $(d/dz)\int d^3v\; v_\tau^2 f=2R(n_0T_0-n_1T_1)d\nu/dz$ and $d\nu/dz=-(4/\delta)\nu(1-\nu)$, where $\delta=(n_1-n_0)/|dn/dz|_{\max}$ is the shock thickness, and introducing upstream mean free path $\lambda=(\sqrt{2}\pi n_0\sigma^2)^{-1}$, we see that in this case $\lambda/\delta=\exp(-\frac{3}{2})\sqrt{2/\pi}B/32=0.3553$.

In order to get, however, the full dependence of the shock thickness on the Mach number, we were forced to treat a model more artificial than the model of rigid spheres—pseudo-Maxwellian molecules. Segal and Ferziger [11] write about "quasi-Maxwell" molecules which scatter isotropically (like hard spheres) but with their diameters inversely proportional to the relative velocity. Kogan [12] says that if for Maxwellian molecules the Boltzmann equation is $df/dt=(16K/m)^{1/2}\int(f'f_1'-ff_1)\rho\, d\rho\, d\varepsilon\, d^3\xi_1$, where $\rho=b(mg^2/16K)^{1/4}$, then pseudo-Maxwellian molecules are such for which the Boltzmann equation can be written in the form

$$df/dt=(16K/m)^{1/2}\int f'f_1'\rho\, d\rho\, d\varepsilon\, d^3\xi_1-Af\int f_1\, d^3\xi_1.$$

For Maxwellian molecules $A=\infty$.

Segal [13] found a closed-form expression for J, and this result without derivation was cited in [11]. But there seem to be some errata in [11], because even the dimensionalities in the left- and right-hand sides of formula (29) of [11] are different. So we chose not to use this result, but to use instead the approach by Bobylev [14] of Fourier-transforming the Boltzmann equation. If

$$\varphi(\mathbf{k})=\int d^3v\; f(\mathbf{v})\exp(-i\mathbf{k}\cdot\mathbf{v}),$$

$$\Psi(\mathbf{k})=\int d^3v\; J(\mathbf{v})\exp(-i\mathbf{k}\cdot\mathbf{v}),$$

then, as Bobylev showed,

$$\Psi=\int d^2n\; g(\mathbf{k}\cdot\mathbf{n}/k)[\varphi(\mathbf{k}/2+k\mathbf{n}/2)\varphi(\mathbf{k}/2-k\mathbf{n}/2)-\varphi(\mathbf{k})\varphi(0)],$$

and here g is the product of the absolute value of the relative velocity and the collisional cross section (below we assume $g=\bar{g}/4\pi$, i.e., isotropic scattering), and the integration is over the surface of the unit sphere. Earlier one of us [15] obtained on the basis of Bobylev's results the expression for Ψ in the case of the bimodal distribution function (1):

$$\Psi=\nu(1-\nu)\bar{g}n_0n_1[2\varphi_0^{1/2}\varphi_1^{1/2}\sinh q/q-\varphi_0-\varphi_1].$$

Here

$$q=q(\mathbf{k})=\tfrac{1}{4}k(a_0^2-a_1^2)(k^2+2ik_z\kappa-\kappa^2)^{1/2},$$

$$\kappa=2(u_0-u_1)/(a_0^2-a_1^2),$$

$$\varphi_\mu=\exp(-\tfrac{1}{2}a_\mu^2k^2-ik_zu_\mu),\quad a_\mu^2=RT_\mu.$$

As

$$\int d^3v\; v_z^{-1}J(\mathbf{v})=(2\pi)^{-3}\int d^3k\; d^3v\; v_z^{-1}\Psi(\mathbf{k})\exp(i\mathbf{k}\cdot\mathbf{v})$$

and [16]

$$\int_{-\infty}^{+\infty} dv_{x,y} \exp(ik_{x,y}v_{x,y}) = 2\pi\delta(k_{x,y}),$$

$$\mathrm{P}\int_{-\infty}^{+\infty} dv_z\, v_z^{-1}\exp(ik_z v_z) = \pi i \operatorname{sgn}k_z,$$

(where P represents principal value) we have

$$\int d^3v\, v_z^{-1}J(\mathbf{v}) = \tfrac{1}{2}i\int_{-\infty}^{+\infty} dk_z\, \Psi(0,0,k_z)\operatorname{sgn}k_z$$
$$= \tfrac{1}{2}i\int_0^{+\infty} dk_z[\Psi(0,0,k_z) - \Psi(0,0,-k_z)]$$
$$= -\int_0^{+\infty} dk_z\, \mathrm{Im}\Psi(0,0,k_z).$$

If $\varphi_\mu(0,0,k_z) = \varphi_\mu^0$, $q(0,0,k_z) = q^0$ then

$$\int d^3v\, v_z^{-1}J(\mathbf{v}) = -\nu(1-\nu)\bar{g}n_0n_1\Bigg\{\int_0^{+\infty} dk_z\, \mathrm{Im}[(\varphi_1^0 - \varphi_0^0)/q^0]$$
$$- \sqrt{(1/2)\pi}a_0^{-1}\exp(-u_0^2/2a_0^2)\mathrm{erfi}(\sqrt{1/2}u_0/a_0) - \sqrt{(1/2)\pi}a_1^{-1}\exp(-u_1^2/2a_1^2)\mathrm{erfi}(\sqrt{1/2}u_1/a_1)\Bigg\}. \quad (2)$$

In order to make the shock-wave thickness λ/δ dimensionless, we used the upstream mean free path $\lambda = \mu_0/\rho_0(2RT_0/\pi)^{1/2}$ [11], where according to Chapman-Enskog theory [9], $\mu_0 = 5kT_0/8\Omega^{22} = 2kT_0/\bar{g}$.

The quadrature in Eq. (2) can be turned to a finite-domain one (it may be helpful for numerical procedures) using the fact that for arbitrary α and β the function $y(\lambda) = \int_0^{+\infty}dx(x+i\beta)^{-1}\exp(-\alpha x^2 - i\lambda x)$ is the solution of $dy/d\lambda = -\beta y - i\int_0^\infty dx \exp(-\alpha x^2 - i\lambda x)$. After that all we need is an appropriate textbook (e.g., [17]). As intermediate results, we had

$$\int_0^\infty dx\, x^{-1}[\exp(-\alpha_2x^2 - i\lambda_2x) - \exp(-\alpha_1x^2 - i\lambda_1x)] = -\tfrac{1}{2}\ln(\alpha_2/\alpha_1) + \tfrac{1}{2}\pi i[\mathrm{erf}(\tfrac{1}{2}\lambda_1/\alpha_1^{1/2}) - \mathrm{erf}(\tfrac{1}{2}\lambda_2/\alpha_2^{1/2})]$$
$$- \pi^{1/2}\int_{\lambda_1/2\alpha_1^{1/2}}^{\lambda_2/2\alpha_2^{1/2}} d\xi\, \exp(-\xi^2)\mathrm{erfi}\xi,$$

$$y(\lambda) = \tfrac{1}{2}\exp(\beta\lambda)\Bigg\{\Bigg[\exp(\alpha\beta^2)E_1(\alpha\beta^2) - 2\pi^{1/2}\int_0^{\lambda/2\alpha^{1/2}} d\xi\, \exp(-\xi^2 - 2\alpha^{1/2}\beta\xi)\mathrm{erfi}\xi\Bigg]$$
$$+ \pi i\, \exp(\alpha\beta^2)[2\,\mathrm{erf}(\alpha^{1/2}\beta) - \mathrm{erf}(\tfrac{1}{2}\lambda/\alpha^{1/2} + \alpha^{1/2}\beta) - 1]\Bigg\}.$$

After some simple manipulations we can obtain

$$\tfrac{1}{2}(u_0 - u_1)\mathrm{Im}\int_0^\infty dk_z\, \Psi(0,0,k_z) = -\pi^{1/2}\int_{x_1}^{x_0} d\xi\, \exp(-\xi^2)\mathrm{erfi}\xi + \tfrac{1}{2}\ln(T_1/T_0)$$
$$+ \tfrac{1}{2}(\tfrac{1}{2}\pi)^{1/2}[y_0\exp(-x_0^2)\mathrm{erfi}x_0 + y_1\exp(-x_1^2)\mathrm{erfi}x_1] + \tfrac{1}{2}\exp(2z_1)$$
$$\times\Bigg[\exp(t_1^2)E_1(t_1^2) - 2\pi^{1/2}\int_0^{x_1} d\xi\, \exp(-\xi^2 - 2^{3/2}t_1\xi)\mathrm{erfi}\xi\Bigg]$$
$$- \tfrac{1}{2}\exp(2z_0)\Bigg[\exp(t_0^2)E_1(t_0^2) - 2\pi^{1/2}\int_0^{x_0} d\xi\, \exp(-\xi^2 - 2^{3/2}t_0\xi)\mathrm{erfi}\xi\Bigg].$$

Here

$$x_\mu = \sqrt{1/2}u_\mu/a_\mu, \quad y_\mu = (u_\alpha - u_\beta)/a_\mu, \quad z_\mu = u_\mu(u_\alpha - u_\beta)/(a_\alpha^2 - a_\beta^2), \quad t_\mu = a_\mu(u_\alpha - u_\beta)/(a_\alpha^2 - a_\beta^2).$$

To proceed with v_τ^2/v_z closure, we differentiate our function Ψ twice and put $k_x = k_y = 0$:

$$G(k_z) = [(\partial^2/\partial k_x^2 + \partial^2/\partial k_y^2)\Psi](0,0,k_z)/\nu(1-\nu)\bar{g}n_0n_1$$
$$= 4(\varphi_0^0\varphi_1^0)^{1/2}\{-\tfrac{1}{2}(a_0^2 + a_1^2)\sinh q^0/q^0 + (\cosh q^0 - \sinh q^0/q^0)[1/k_z^2 + (a_0^2 - a_1^2)^2k_z^2/16q_0^2]\} - 2(a_0^2\varphi_0^0 + a_1^2\varphi_1^0)$$
$$= -2\{\tfrac{1}{2}(a_0^2 + a_1^2)(\varphi_1^0 - \varphi_0^0)/q^0 + [1/k_z^2 + (a_0^2 - a_1^2)^2k_z^2/16q_0^2][(\varphi_1^0 - \varphi_0^0)/q^0 - \varphi_0^0 - \varphi_1^0] - (a_0^2\varphi_0^0 + a_1^2\varphi_1^0)\}.$$

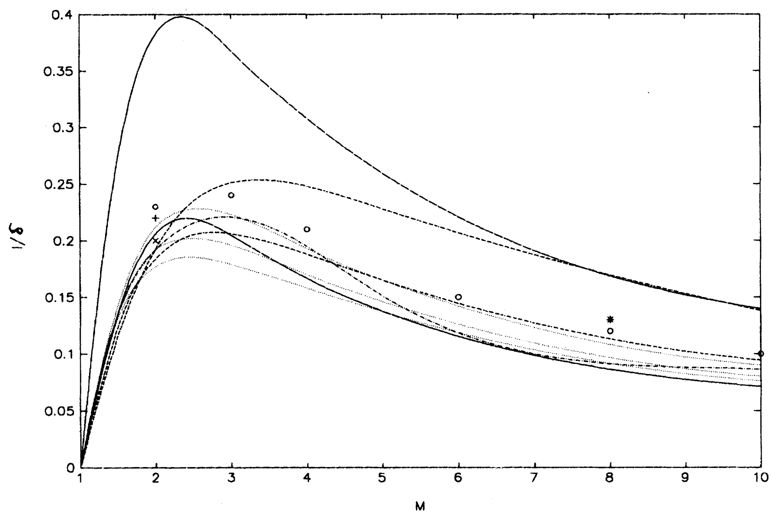

FIG. 1. Inverse shock thicknesses λ/δ_F (for $1/v_z$ closure; lower full line) and λ/δ_G (for v_τ^2/v_z closure; upper full line) versus the upstream Mach number for pseudo-Maxwellian molecules. Also the results of [19] (○), [20] (+), [8] (×), [19] (*), [1] (dashed lines, upper: v_z^3; lower: v_z^2), [21] (dotted lines, from bottom to top: v_z^2, v_z^3; $v_z^2, v_z v^2$; $v_z^3, v_z v^2$), and [22] (dash-dotted line) are shown.

If $F(k_z)=\Psi(0,0,k_z)/\nu(1-\nu)\bar{g}n_0n_1$ then for $1/v_z$ closure

$$\lambda/\delta_F=\tfrac{1}{4}(2\pi)^{1/2}(a_1/a_0)^{-1}(u_1/u_0-1)^{-1}\int_0^\infty dk_z\,\mathrm{Im}F(k_z),$$

and for v_τ^2/v_z closure

$$\lambda/\delta_G=\tfrac{1}{4}(2\pi)^{1/2}(a_1/a_0)^{-1}[(u_1/u_0)(a_1/a_0)^{-2}-1)]^{-1}\times\int_0^\infty dk_z\mathrm{Im}\,G(k_z).$$

In Fig. 1 we show the dependencies of λ/δ_F and λ/δ_G versus M. We made a comparison with Monte Carlo simulations [3,8,19,20] and previous approximate analytical solutions [1,21,22]. It is seen that the results obtained by Bird's DSMC method show a reasonable agreement with the curve corresponding to the moment $1/v_z$. We can see that these values tend to 0 for $M\to\infty$, as is the case for arbitrary closure. It is known that for molecules interacting via $\phi\propto r^{-p}$ the Mott-Smith collision integral decreases for $M\to\infty$ as $(T_0/T_1)^{1/2}$ [12,18]. Kogan [12] even explained this phenomenon qualitatively.

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